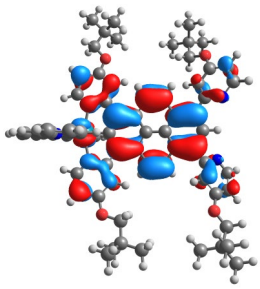
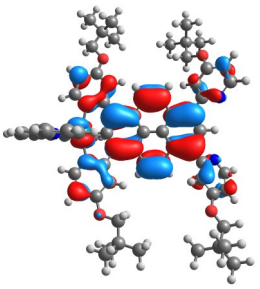
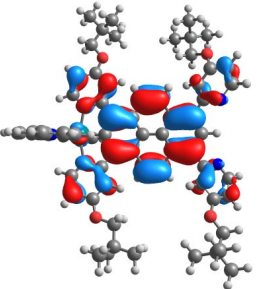
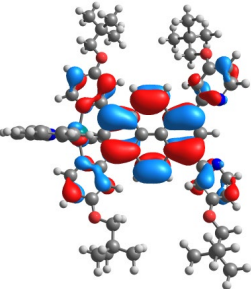
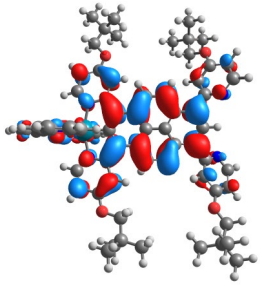
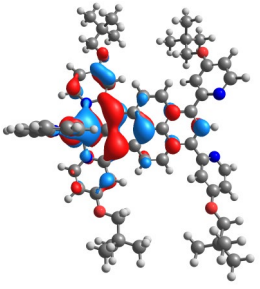
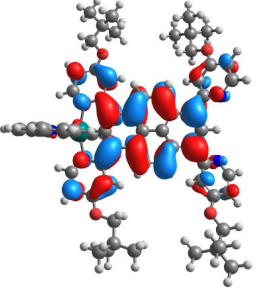
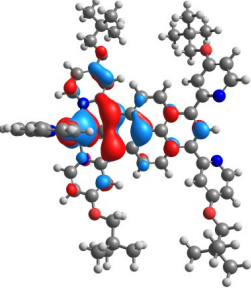
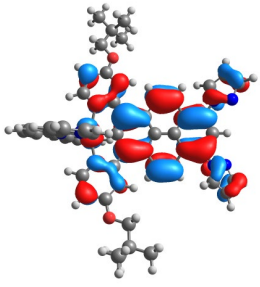
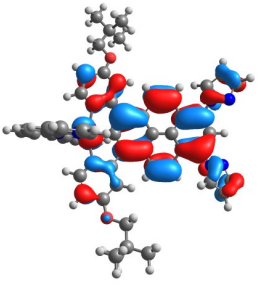
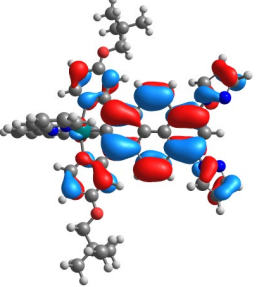
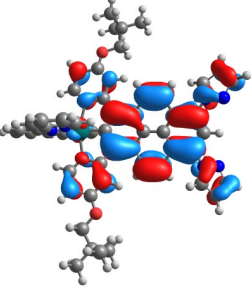
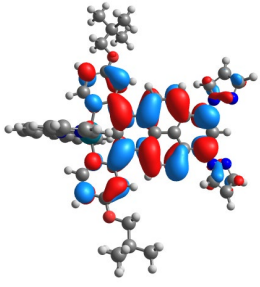
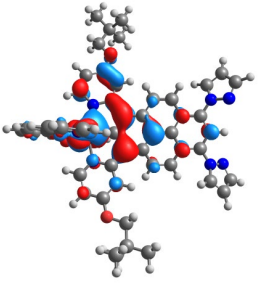
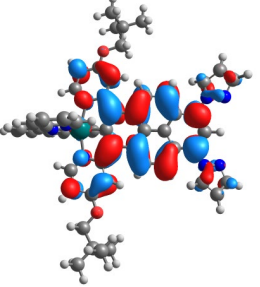
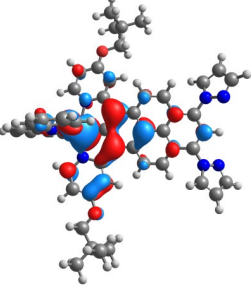
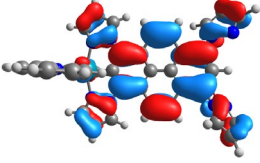
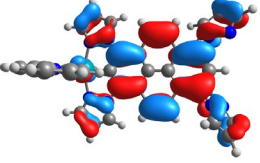
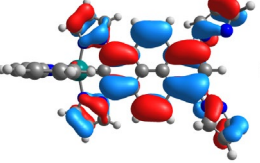
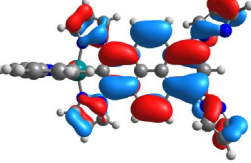
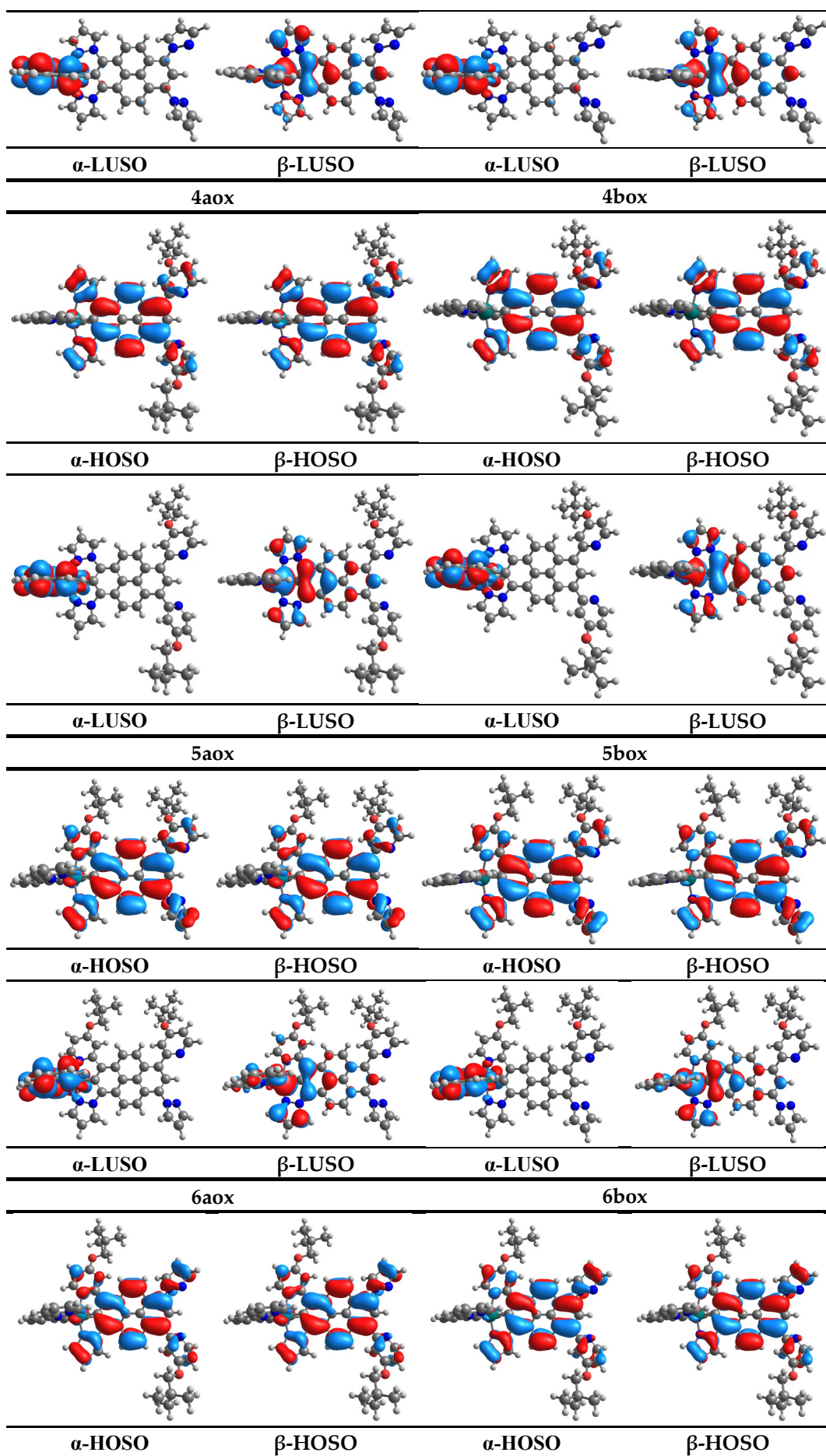
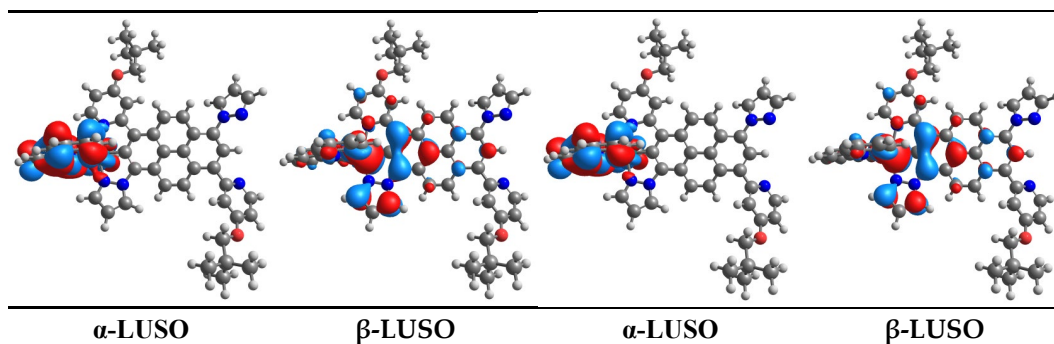


**Table S1.** The  $\alpha$ -HOSO,  $\beta$ -HOSO,  $\alpha$ -LUSO,  $\beta$ -LUSO contours for the complexes **1a**ox-**6a**ox and **1b**ox-**6b**ox.

1aox		1box	
			
$\alpha$ -HOSO	$\beta$ -HOSO	$\alpha$ -HOSO	$\beta$ -HOSO
			
$\alpha$ -LUSO	$\beta$ -LUSO	$\alpha$ -LUSO	$\beta$ -LUSO
2aox		2box	
			
$\alpha$ -HOSO	$\beta$ -HOSO	$\alpha$ -HOSO	$\beta$ -HOSO
			
$\alpha$ -LUSO	$\beta$ -LUSO	$\alpha$ -LUSO	$\beta$ -LUSO
3aox		3box	
			
$\alpha$ -HOSO	$\beta$ -HOSO	$\alpha$ -HOSO	$\beta$ -HOSO





Cartesian coordinates of DFT-optimized structure of **1a** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

Os	2.222519000	-0.045200000	0.045462000
N	-7.923901000	2.604759000	-1.745530000
N	1.667812000	-2.059780000	0.320821000
N	2.612038000	0.262951000	2.081448000
N	4.263912000	-0.153684000	0.122264000
N	2.728491000	-0.396500000	-1.957588000
N	-8.215371000	-1.502655000	1.406863000
N	1.902279000	2.017318000	-0.266390000
C	1.701868000	0.471849000	3.061826000
H	0.667278000	0.471661000	2.741752000
C	2.052347000	0.672925000	4.389151000
H	1.274342000	0.836128000	5.126834000
C	3.403614000	0.660994000	4.743736000
H	3.711972000	0.815661000	5.772314000
C	4.351923000	0.445361000	3.750452000
H	5.406925000	0.430143000	3.998207000
C	3.950713000	0.247231000	2.426146000
C	4.891047000	0.007968000	1.321528000
C	6.283388000	-0.068680000	1.394521000
H	6.798435000	0.056546000	2.340004000
C	7.011135000	-0.311704000	0.227161000
C	6.351052000	-0.474751000	-0.993202000
H	6.918856000	-0.662741000	-1.897106000
C	4.957779000	-0.390521000	-1.026823000
C	4.083075000	-0.526437000	-2.200846000
C	4.558925000	-0.767626000	-3.492963000
H	5.625060000	-0.866015000	-3.661426000
C	3.669999000	-0.880253000	-4.555801000
H	4.036131000	-1.067713000	-5.559670000
C	2.302457000	-0.746721000	-4.303180000
H	1.569079000	-0.826296000	-5.098135000
C	1.876936000	-0.508051000	-3.004344000
H	0.826965000	-0.397706000	-2.762477000
C	-8.652843000	3.688701000	-2.055743000
C	2.526980000	-3.102550000	0.398649000
H	-9.518989000	3.514139000	-2.691938000

H	3.578769000	-2.844569000	0.438798000
C	-8.369245000	4.976570000	-1.623889000
C	2.131053000	-4.422720000	0.416921000
H	-8.991342000	5.820244000	-1.902727000
H	2.858660000	-5.223289000	0.480485000
C	-7.252175000	5.167078000	-0.795635000
C	0.758929000	-4.710437000	0.315428000
C	-6.476531000	4.050717000	-0.460196000
C	-0.144703000	-3.647245000	0.243872000
H	-5.621064000	4.137162000	0.196279000
H	-1.197933000	-3.839558000	0.115118000
C	-6.842338000	2.791659000	-0.965122000
C	0.307257000	-2.317744000	0.287256000
C	-6.085145000	1.563532000	-0.581807000
C	-0.532961000	-1.115112000	0.197256000
C	-6.829429000	0.457019000	-0.169377000
C	0.232586000	0.057109000	-0.024768000
C	-6.235618000	-0.730529000	0.261423000
C	-0.392120000	1.300205000	-0.292301000
C	-7.148943000	-1.846413000	0.646585000
C	0.569229000	2.412194000	-0.327905000
C	-6.953134000	-3.148719000	0.181762000
C	0.264615000	3.774852000	-0.319912000
H	-6.116651000	-3.399935000	-0.460567000
H	-0.760033000	4.113909000	-0.271633000
C	-7.872974000	-4.152073000	0.525375000
C	1.272275000	4.747254000	-0.330688000
C	-8.968239000	-3.803952000	1.325718000
C	2.610355000	4.327396000	-0.334975000
H	-9.717391000	-4.523793000	1.630136000
H	3.442241000	5.018884000	-0.350113000
C	-9.079870000	-2.470625000	1.722279000
C	2.859719000	2.964480000	-0.286486000
H	-9.926991000	-2.171561000	2.338023000
H	3.880968000	2.602736000	-0.251611000
C	-4.819916000	-0.815947000	0.323182000
C	-1.797753000	1.347960000	-0.490845000
C	-4.022789000	0.287690000	-0.131561000
C	-2.586841000	0.205605000	-0.103789000
C	-4.669155000	1.476857000	-0.608767000
C	-1.946380000	-1.014789000	0.316695000
C	-3.844509000	2.506757000	-1.166372000
C	-2.779228000	-2.030428000	0.891953000
H	-4.314768000	3.343236000	-1.670481000
H	-2.317733000	-2.872840000	1.391787000
C	-2.484573000	2.446014000	-1.105819000
C	-4.139153000	-1.935948000	0.899602000
H	-1.909377000	3.225428000	-1.589263000
H	-4.720279000	-2.715022000	1.379232000
O	-7.017993000	6.428189000	-0.372629000
O	0.861438000	6.030602000	-0.327149000

O	0.422782000	-6.014534000	0.286245000
O	-7.624863000	-5.387185000	0.038387000
C	-8.547806000	-6.450485000	0.332599000
C	-8.060751000	-7.743604000	-0.337262000
C	-9.083192000	-8.844530000	0.005908000
C	-6.674920000	-8.133350000	0.210759000
C	-7.993188000	-7.555049000	-1.864595000
C	-0.961378000	-6.390623000	0.172687000
C	-1.068198000	-7.922535000	0.194366000
C	-2.562778000	-8.273874000	0.062430000
C	-0.286330000	-8.524314000	-0.988704000
C	-0.520746000	-8.471203000	1.525808000
C	-5.885768000	6.686539000	0.474974000
C	-5.851724000	8.180235000	0.831336000
C	-5.719779000	9.027905000	-0.448145000
C	-7.132236000	8.568857000	1.594740000
C	-4.621646000	8.403449000	1.732402000
C	1.844470000	7.082565000	-0.317099000
C	1.128925000	8.441202000	-0.307053000
C	0.252316000	8.568495000	0.953352000
C	0.263270000	8.592631000	-1.572296000
C	2.221614000	9.528060000	-0.291715000
H	-9.542920000	-6.176394000	-0.041857000
H	-8.609508000	-6.582482000	1.420910000
H	-10.083244000	-8.594351000	-0.368821000
H	-9.155386000	-9.000404000	1.089243000
H	-8.783072000	-9.794882000	-0.449866000
H	-6.706995000	-8.280826000	1.297457000
H	-5.931237000	-7.359441000	-0.004794000
H	-6.333222000	-9.069732000	-0.245375000
H	-8.976044000	-7.289357000	-2.273417000
H	-7.666816000	-8.482157000	-2.350064000
H	-7.288156000	-6.762701000	-2.135724000
H	-1.521753000	-5.954447000	1.009966000
H	-1.365461000	-5.990273000	-0.766283000
H	-2.698017000	-9.361301000	0.073228000
H	-2.982500000	-7.893339000	-0.876758000
H	-3.147716000	-7.855234000	0.890420000
H	-0.671162000	-8.152387000	-1.946406000
H	-0.378585000	-9.616583000	-0.990917000
H	0.777585000	-8.273455000	-0.929493000
H	-1.074271000	-8.060309000	2.379286000
H	0.536897000	-8.219527000	1.654190000
H	-0.616783000	-9.562671000	1.557264000
H	-4.967910000	6.395461000	-0.053100000
H	-5.970822000	6.079736000	1.385910000
H	-4.803768000	8.775028000	-0.996438000
H	-5.677219000	10.094286000	-0.197472000
H	-6.571173000	8.869941000	-1.117780000
H	-8.024306000	8.405436000	0.981690000
H	-7.102252000	9.627617000	1.877161000

H	-7.238461000	7.978905000	2.513704000
H	-3.691501000	8.138482000	1.214648000
H	-4.682557000	7.804740000	2.649464000
H	-4.553106000	9.457366000	2.024908000
H	2.478202000	6.988770000	-1.208544000
H	2.475498000	6.973375000	0.574587000
H	-0.237964000	9.548497000	0.978713000
H	0.854467000	8.470015000	1.865125000
H	-0.525893000	7.798595000	0.975536000
H	-0.508742000	7.817921000	-1.619910000
H	0.874602000	8.520262000	-2.480396000
H	-0.234049000	9.569443000	-1.579283000
H	2.856623000	9.446301000	0.598826000
H	1.763316000	10.523434000	-0.285803000
H	2.866172000	9.461557000	-1.176638000
H	-7.910793000	0.525033000	-0.179303000
H	8.093165000	-0.374223000	0.268404000

Cartesian coordinates of DFT-optimized structure of **2a** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

Os	2.194111000	-0.984051000	0.014047000
N	0.972237000	-2.694704000	0.186749000
N	2.685401000	-0.969422000	2.051781000
N	4.074634000	-1.793636000	0.018704000
N	2.528390000	-1.357594000	-2.021623000
N	2.614902000	1.075718000	-0.163155000
C	1.910069000	-0.533002000	3.072415000
H	0.935690000	-0.155757000	2.787609000
C	2.318518000	-0.561055000	4.398165000
H	1.649531000	-0.195749000	5.169593000
C	3.586111000	-1.059963000	4.707510000
H	3.936624000	-1.095356000	5.733583000
C	4.395037000	-1.514201000	3.672230000
H	5.382145000	-1.908115000	3.884659000
C	3.939691000	-1.466718000	2.351508000
C	4.731576000	-1.933928000	1.204067000
C	6.017433000	-2.477713000	1.226910000
H	6.554712000	-2.595890000	2.160741000
C	6.608220000	-2.871791000	0.023971000
C	5.919118000	-2.720488000	-1.181713000
H	6.380547000	-3.026036000	-2.113630000
C	4.635695000	-2.170798000	-1.164145000
C	3.754820000	-1.923510000	-2.315251000
C	4.107414000	-2.226301000	-3.633442000
H	5.074601000	-2.669318000	-3.840761000
C	3.222666000	-1.961177000	-4.672399000
H	3.493119000	-2.195597000	-5.696533000
C	1.985030000	-1.388898000	-4.369105000
H	1.260323000	-1.162592000	-5.143478000

C	1.679488000	-1.105061000	-3.045648000
H	0.732954000	-0.659525000	-2.765676000
C	1.412485000	-3.974607000	0.182949000
H	2.488229000	-4.102795000	0.213334000
C	0.579633000	-5.072191000	0.133266000
H	0.981793000	-6.078502000	0.132446000
C	-0.806794000	-4.856485000	0.049343000
C	-1.280941000	-3.542146000	0.063312000
H	-2.335213000	-3.347199000	-0.050678000
C	-0.392329000	-2.460157000	0.172263000
C	-5.033445000	3.405545000	-0.406461000
C	-0.760035000	-1.036775000	0.172991000
C	-6.131938000	2.622423000	-0.066631000
C	0.366398000	-0.192134000	0.005334000
C	-5.958282000	1.289266000	0.289434000
C	0.214654000	1.205771000	-0.174731000
C	1.503999000	1.913415000	-0.164085000
C	1.692401000	3.292435000	-0.059559000
H	0.850290000	3.962196000	0.039342000
C	2.976187000	3.852137000	-0.033756000
C	4.083533000	2.994391000	-0.103143000
H	5.104214000	3.353029000	-0.096624000
C	3.842599000	1.629866000	-0.149061000
H	4.673611000	0.933990000	-0.164868000
C	-4.669826000	0.711554000	0.361663000
C	-1.084232000	1.750932000	-0.348652000
C	-3.539494000	1.500451000	-0.034626000
C	-2.222111000	0.929269000	-0.020032000
C	-3.729382000	2.861285000	-0.445961000
C	-2.049554000	-0.459761000	0.322547000
C	-2.597428000	3.584461000	-0.938922000
C	-3.186843000	-1.155667000	0.851764000
H	-2.745228000	4.559921000	-1.387578000
H	-3.047402000	-2.129390000	1.303871000
C	-1.343327000	3.054236000	-0.889054000
C	-4.432401000	-0.603076000	0.873007000
H	-0.527829000	3.616083000	-1.326012000
H	-5.253221000	-1.157465000	1.313107000
O	3.038585000	5.193738000	0.067674000
O	-1.580164000	-5.955000000	-0.048006000
C	-3.009914000	-5.810686000	-0.132957000
C	-3.652896000	-7.202613000	-0.220550000
C	-5.177113000	-6.991502000	-0.308826000
C	-3.156082000	-7.935242000	-1.481258000
C	-3.313688000	-8.022833000	1.038491000
C	4.326298000	5.836930000	0.111325000
C	4.127354000	7.352550000	0.256833000
C	3.385271000	7.664457000	1.570177000
C	3.333226000	7.900010000	-0.944328000
C	5.529646000	7.991550000	0.287588000
H	-3.368156000	-5.275371000	0.756256000

H	-3.258470000	-5.218234000	-1.022970000
H	-5.689174000	-7.958014000	-0.375908000
H	-5.450188000	-6.405996000	-1.195224000
H	-5.561691000	-6.469332000	0.575733000
H	-3.400595000	-7.369296000	-2.388763000
H	-3.630168000	-8.920241000	-1.561572000
H	-2.071502000	-8.081228000	-1.453953000
H	-3.673262000	-7.521464000	1.945649000
H	-2.233394000	-8.169812000	1.137423000
H	-3.787676000	-9.010025000	0.990077000
H	4.871457000	5.607595000	-0.813418000
H	4.895866000	5.440746000	0.961907000
H	3.258018000	8.746717000	1.688932000
H	3.945949000	7.294689000	2.437656000
H	2.392974000	7.202336000	1.584727000
H	2.335686000	7.452330000	-0.998275000
H	3.851447000	7.691377000	-1.888490000
H	3.214323000	8.986345000	-0.859234000
H	6.122082000	7.617846000	1.131670000
H	5.446757000	9.079203000	0.392501000
H	6.084892000	7.784935000	-0.635504000
H	-7.124886000	3.051842000	-0.080035000
H	7.606159000	-3.296640000	0.026042000
N	-5.275133000	4.766286000	-0.744235000
C	-4.646920000	5.882138000	-0.259725000
C	-5.298619000	6.974383000	-0.791738000
C	-6.327683000	6.419695000	-1.586947000
N	-6.322558000	5.088700000	-1.555557000
N	-7.122546000	0.535989000	0.607844000
N	-8.092816000	1.084360000	1.393393000
C	-9.068068000	0.178104000	1.406924000
C	-8.750700000	-0.956429000	0.625200000
C	-7.495988000	-0.687931000	0.120917000
H	-6.859401000	-1.242607000	-0.551927000
H	-9.350694000	-1.837200000	0.448778000
H	-9.964908000	0.369106000	1.982590000
H	-7.068433000	6.935678000	-2.184651000
H	-5.069228000	8.016697000	-0.624941000
H	-3.819952000	5.806086000	0.430118000

Cartesian coordinates of DFT-optimized structure of **3a** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

C	4.055649000	2.468887000	-0.171154000
C	5.413802000	2.473468000	-0.258118000
C	6.168145000	1.262223000	-0.187373000
C	5.459823000	0.023858000	-0.033253000
C	4.024677000	0.012564000	0.043564000
C	3.300393000	1.263663000	0.008256000
C	6.197027000	-1.206554000	0.031828000

C	5.469913000	-2.437547000	0.004991000
C	4.110294000	-2.454605000	0.040359000
C	3.333919000	-1.252940000	0.142016000
C	1.893486000	1.202535000	0.117337000
C	1.206712000	-0.017315000	0.198150000
C	1.929904000	-1.216672000	0.260912000
C	7.579394000	1.234178000	-0.264935000
C	8.287532000	0.048231000	-0.114205000
C	7.608758000	-1.154884000	0.049661000
H	3.546983000	3.414364000	-0.279246000
H	5.930946000	3.417135000	-0.381395000
H	3.612688000	-3.407906000	-0.065097000
H	6.010802000	-3.371812000	-0.088486000
N	0.978508000	2.305927000	0.130526000
N	-0.370656000	1.983264000	0.037013000
C	-1.046509000	3.132967000	0.129734000
C	-0.165222000	4.210435000	0.304231000
C	1.098487000	3.654321000	0.313022000
N	1.056474000	-2.339212000	0.419233000
N	-0.303037000	-2.082988000	0.294080000
C	-0.932237000	-3.236015000	0.544794000
C	-0.008315000	-4.244979000	0.857350000
C	1.232551000	-3.643605000	0.783359000
N	8.331902000	2.428010000	-0.465342000
N	9.369135000	2.724532000	0.367722000
C	9.909402000	3.827886000	-0.147257000
C	8.236851000	3.321237000	-1.496904000
C	9.241097000	4.249996000	-1.318964000
N	8.386184000	-2.336708000	0.200684000
N	9.470046000	-2.544577000	-0.600145000
C	10.019776000	-3.666050000	-0.138956000
C	9.311532000	-4.189983000	0.966859000
C	8.271959000	-3.305551000	1.161280000
C	-0.106334000	-0.261369000	-2.943151000
C	-0.389315000	-0.358913000	-4.298825000
C	-1.722113000	-0.402451000	-4.711288000
C	-2.721696000	-0.346779000	-3.745605000
C	-2.386696000	-0.247637000	-2.393047000
N	-1.065620000	-0.204725000	-1.991606000
C	-3.387282000	-0.185758000	-1.314617000
N	-2.828776000	-0.100124000	-0.078580000
C	-3.580141000	-0.037334000	1.052741000
C	-4.973439000	-0.057916000	0.962285000
C	-5.567678000	-0.142959000	-0.298839000
C	-4.777191000	-0.207603000	-1.448304000
C	-2.766925000	0.051595000	2.277720000
N	-1.398551000	0.063266000	2.091549000
C	-0.603866000	0.151444000	3.181966000
C	-1.101209000	0.224944000	4.476246000
C	-2.483086000	0.209252000	4.672249000
C	-3.315072000	0.122992000	3.560779000

H	0.913401000	-0.226469000	-2.580300000
H	0.426722000	-0.399926000	-5.011844000
H	-1.978958000	-0.479203000	-5.762470000
H	-3.764341000	-0.381535000	-4.039087000
H	-5.590369000	-0.008125000	1.851745000
H	-5.242136000	-0.273148000	-2.424948000
H	0.460559000	0.161860000	2.982366000
H	-0.410960000	0.293079000	5.309806000
H	-2.905692000	0.264125000	5.669881000
H	-4.391416000	0.110757000	3.686530000
Os	-0.788013000	-0.060325000	0.087190000
H	-2.125584000	3.122278000	0.079358000
H	-0.412986000	5.254802000	0.419033000
H	2.048504000	4.128815000	0.476840000
H	-2.010878000	-3.276130000	0.500278000
H	-0.215185000	-5.272968000	1.113656000
H	2.204082000	-4.047089000	1.005125000
H	10.758828000	4.284749000	0.344671000
H	7.490557000	3.208998000	-2.269432000
H	9.461828000	5.101539000	-1.945941000
H	10.904421000	-4.062988000	-0.620668000
H	9.529788000	-5.077914000	1.542021000
H	7.488237000	-3.270732000	1.903197000
H	9.369519000	0.058577000	-0.133937000
H	-6.648679000	-0.158858000	-0.385770000

Cartesian coordinates of DFT-optimized structure of **4a** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

Os	1.814688000	-3.093382000	0.017988000
N	-1.564150000	6.844250000	-1.646444000
N	-0.140932000	-3.697764000	0.458508000
N	2.445760000	-3.203508000	2.017880000
N	2.853081000	-4.857221000	0.049662000
N	1.633874000	-3.750878000	-1.967627000
N	-5.229020000	4.778381000	1.386036000
N	3.301061000	-1.693293000	-0.439674000
C	2.201069000	-2.309472000	3.002840000
H	1.611162000	-1.448181000	2.714397000
C	2.664870000	-2.468435000	4.301724000
H	2.433958000	-1.714364000	5.046091000
C	3.419746000	-3.599291000	4.618091000
H	3.797555000	-3.754924000	5.623077000
C	3.680547000	-4.529229000	3.617197000
H	4.264177000	-5.415776000	3.835846000
C	3.191861000	-4.324903000	2.324377000
C	3.424617000	-5.263424000	1.214270000
C	4.138163000	-6.463122000	1.256000000
H	4.601334000	-6.804541000	2.174386000
C	4.248850000	-7.224547000	0.090381000

C	3.653621000	-6.789206000	-1.095817000
H	3.742271000	-7.382579000	-1.998273000
C	2.948956000	-5.583661000	-1.095625000
C	2.256231000	-4.955354000	-2.232872000
C	2.213326000	-5.517540000	-3.511094000
H	2.707741000	-6.463697000	-3.697903000
C	1.538820000	-4.866667000	-4.538760000
H	1.503621000	-5.300634000	-5.532441000
C	0.911689000	-3.650197000	-4.263758000
H	0.372351000	-3.104151000	-5.029908000
C	0.981760000	-3.131638000	-2.977797000
H	0.508930000	-2.191815000	-2.720308000
C	-1.066196000	8.055244000	-1.943901000
C	-0.829814000	-4.838054000	0.580907000
H	-1.678754000	8.674973000	-2.596667000
C	0.148079000	8.540928000	-1.480471000
H	0.506871000	9.528125000	-1.751169000
C	0.908782000	7.722790000	-0.630594000
C	0.408645000	6.455617000	-0.306504000
H	0.940619000	5.795873000	0.366222000
C	-0.825025000	6.053517000	-0.845330000
N	-1.075347000	-2.670566000	0.469052000
C	-1.428651000	4.737056000	-0.482001000
C	-0.567367000	-1.348681000	0.274692000
C	-2.769683000	4.734048000	-0.096307000
C	0.802104000	-1.369383000	-0.013534000
C	-3.435289000	3.574301000	0.304199000
C	1.456971000	-0.171200000	-0.321094000
C	-4.883676000	3.702593000	0.639970000
N	2.861025000	-0.377340000	-0.492318000
C	-5.831465000	2.807291000	0.139655000
H	-5.543965000	1.973627000	-0.490940000
C	-7.190440000	3.002176000	0.430983000
C	-7.550655000	4.105712000	1.214490000
H	-8.578681000	4.321043000	1.477096000
C	-6.527306000	4.948876000	1.650016000
C	4.634176000	-1.652028000	-0.544345000
H	-6.780712000	5.818690000	2.254484000
C	-2.718579000	2.351370000	0.371683000
C	0.758696000	1.046401000	-0.463067000
C	-1.350372000	2.306838000	-0.063935000
C	-0.624259000	1.065714000	-0.048059000
C	-0.713444000	3.512258000	-0.516100000
C	-1.289599000	-0.141411000	0.382417000
C	0.608866000	3.411058000	-1.057341000
C	-2.608199000	-0.022706000	0.931075000
H	1.054285000	4.280510000	-1.526344000
H	-3.065019000	-0.874277000	1.418002000
C	1.307236000	2.242636000	-1.030211000
C	-3.284448000	1.159045000	0.928246000
H	2.277279000	2.213097000	-1.508585000

H	-4.266430000	1.205322000	1.383955000
O	2.073747000	8.235585000	-0.179117000
O	-8.050120000	2.098205000	-0.086640000
C	-9.459541000	2.260765000	0.147996000
C	-10.221320000	1.118884000	-0.540721000
C	-11.721318000	1.344598000	-0.268379000
C	-9.784954000	-0.237087000	0.045901000
C	-9.960246000	1.148474000	-2.058592000
C	2.899630000	7.446301000	0.693697000
C	4.156265000	8.249082000	1.061828000
C	4.958761000	8.588748000	-0.208494000
C	3.760014000	9.541990000	1.799704000
C	5.006273000	7.360579000	1.990839000
H	-9.780351000	3.231840000	-0.251635000
H	-9.648539000	2.249639000	1.229514000
H	-12.062186000	2.304531000	-0.675260000
H	-11.940524000	1.333630000	0.806230000
H	-12.314555000	0.552281000	-0.738999000
H	-9.978115000	-0.281031000	1.125013000
H	-8.716564000	-0.413379000	-0.115003000
H	-10.339928000	-1.055047000	-0.428101000
H	-10.273488000	2.105490000	-2.494165000
H	-10.523499000	0.351710000	-2.558234000
H	-8.898095000	1.005287000	-2.281448000
H	3.175745000	6.514402000	0.182617000
H	2.329941000	7.192342000	1.597276000
H	5.259759000	7.677770000	-0.740703000
H	5.868612000	9.142075000	0.051543000
H	4.370982000	9.205050000	-0.896252000
H	3.138844000	10.184791000	1.167757000
H	4.654182000	10.107909000	2.085851000
H	3.197131000	9.318000000	2.714447000
H	5.305736000	6.430564000	1.492257000
H	4.458922000	7.096013000	2.903874000
H	5.918758000	7.889091000	2.289330000
H	-3.316810000	5.669344000	-0.107520000
H	4.799882000	-8.158638000	0.106314000
C	3.939626000	0.452197000	-0.596811000
C	5.080668000	-0.325426000	-0.645385000
C	-2.327608000	-3.204271000	0.565148000
C	-2.207141000	-4.578007000	0.651275000
H	-0.301833000	-5.780415000	0.599223000
H	5.199069000	-2.572758000	-0.527824000
H	3.833603000	1.522599000	-0.593764000
H	6.098631000	0.023026000	-0.732786000
H	-3.209429000	-2.589292000	0.530120000
H	-3.009755000	-5.294072000	0.742864000

Cartesian coordinates of DFT-optimized structure of **5a** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

Os	1.911837000	-3.000474000	0.005771000
N	-0.062718000	-3.671240000	0.306657000
N	2.425574000	-3.168181000	2.033689000
N	2.989017000	-4.741584000	0.041192000
N	1.855923000	-3.602618000	-2.003244000
N	-5.136897000	4.854166000	1.419563000
C	2.092101000	-2.318596000	3.032667000
H	1.496055000	-1.464163000	2.736916000
C	2.477603000	-2.513080000	4.351759000
H	2.178019000	-1.793811000	5.106047000
C	3.244989000	-3.633752000	4.675781000
H	3.563463000	-3.815909000	5.696702000
C	3.595487000	-4.518362000	3.661750000
H	4.189684000	-5.396565000	3.886270000
C	3.183216000	-4.280328000	2.347913000
C	3.508737000	-5.171656000	1.223197000
C	4.258848000	-6.348744000	1.265246000
H	4.682179000	-6.705712000	2.196805000
C	4.458825000	-7.066426000	0.083792000
C	3.915621000	-6.609342000	-1.119169000
H	4.073320000	-7.168703000	-2.033948000
C	3.172903000	-5.426976000	-1.120162000
C	2.524981000	-4.781323000	-2.272779000
C	2.564669000	-5.302107000	-3.568895000
H	3.095465000	-6.227779000	-3.758546000
C	1.924930000	-4.637301000	-4.609383000
H	1.953785000	-5.039080000	-5.616708000
C	1.247436000	-3.448873000	-4.329378000
H	0.731344000	-2.894206000	-5.105279000
C	1.236465000	-2.970135000	-3.026586000
H	0.722812000	-2.053151000	-2.765225000
C	-0.440871000	-4.968853000	0.375460000
H	0.365487000	-5.692243000	0.405214000
C	-1.754638000	-5.385655000	0.394427000
H	-2.005891000	-6.438398000	0.448190000
C	-2.765487000	-4.413356000	0.305894000
C	-2.395819000	-3.066728000	0.249874000
H	-3.149867000	-2.305278000	0.132814000
C	-1.043547000	-2.691067000	0.288342000
C	-1.360763000	4.786845000	-0.460493000
C	-0.524781000	-1.315797000	0.207510000
C	-2.695617000	4.813395000	-0.069915000
C	0.869790000	-1.299555000	-0.018919000
C	-3.366932000	3.649729000	0.305849000
C	1.531897000	-0.086690000	-0.272309000
C	-4.811444000	3.785880000	0.654705000
C	-5.772306000	2.907514000	0.150299000
H	-5.499561000	2.081451000	-0.496520000
C	-7.126621000	3.112800000	0.458163000
C	-7.466264000	4.206706000	1.264166000

H	-8.488751000	4.428206000	1.542718000
C	-6.430099000	5.033159000	1.701312000
H	-6.668104000	5.895834000	2.321881000
C	-2.656657000	2.419737000	0.353355000
C	0.831941000	1.121589000	-0.440150000
C	-1.285852000	2.373034000	-0.071782000
C	-0.563441000	1.131004000	-0.061775000
C	-0.638579000	3.575331000	-0.512923000
C	-1.230343000	-0.083706000	0.328193000
C	0.692008000	3.486855000	-1.035269000
C	-2.547693000	0.038817000	0.879058000
H	1.140985000	4.360523000	-1.493246000
H	-3.003400000	-0.818472000	1.357707000
C	1.391618000	2.320345000	-0.994754000
C	-3.225205000	1.222085000	0.891475000
H	2.372671000	2.290826000	-1.451001000
H	-4.206474000	1.263951000	1.349417000
O	-4.032252000	-4.868703000	0.271452000
O	-8.002256000	2.228782000	-0.066512000
C	-9.407192000	2.409663000	0.183451000
C	-10.196675000	1.296518000	-0.520914000
C	-11.688849000	1.545990000	-0.226597000
C	-9.781523000	-0.079286000	0.033904000
C	-9.950637000	1.352227000	-2.040411000
C	-5.122966000	-3.933932000	0.182501000
C	-6.448280000	-4.709566000	0.162394000
C	-7.580685000	-3.667905000	0.074418000
C	-6.498084000	-5.637155000	-1.066476000
C	-6.599737000	-5.533345000	1.455316000
H	-9.714187000	3.394319000	-0.193060000
H	-9.586758000	2.378998000	1.266122000
H	-12.014803000	2.521148000	-0.608556000
H	-11.895214000	1.516281000	0.850243000
H	-12.302883000	0.775760000	-0.706694000
H	-9.959591000	-0.138909000	1.114866000
H	-8.720013000	-0.277159000	-0.146737000
H	-10.362058000	-0.875558000	-0.446331000
H	-10.251963000	2.322772000	-2.453717000
H	-10.532324000	0.575049000	-2.549682000
H	-8.893381000	1.195835000	-2.277341000
H	-5.084889000	-3.257370000	1.046295000
H	-5.012798000	-3.339761000	-0.733986000
H	-8.554999000	-4.169270000	0.058248000
H	-7.500140000	-3.063210000	-0.837096000
H	-7.568031000	-2.988683000	0.935588000
H	-6.405474000	-5.064154000	-1.997443000
H	-7.450860000	-6.178183000	-1.098133000
H	-5.689607000	-6.374786000	-1.039698000
H	-6.575748000	-4.886525000	2.341109000
H	-5.797482000	-6.271875000	1.551957000
H	-7.556401000	-6.068438000	1.456073000

H	-3.223617000	5.758814000	-0.062897000
H	5.039068000	-7.982630000	0.100369000
N	2.944990000	-0.264005000	-0.374514000
C	4.010976000	0.587912000	-0.394609000
C	5.167432000	-0.168393000	-0.399585000
C	4.740678000	-1.505047000	-0.359106000
N	3.404673000	-1.571249000	-0.330325000
N	-0.752673000	6.022910000	-0.825118000
C	0.413354000	6.561067000	-0.352893000
C	0.535346000	7.815230000	-0.913763000
C	-0.621989000	7.958825000	-1.712425000
N	-1.405480000	6.883054000	-1.656851000
H	5.320472000	-2.416253000	-0.336513000
H	6.182126000	0.199483000	-0.419950000
H	3.882333000	1.655834000	-0.368352000
H	1.035267000	6.024421000	0.347950000
H	1.337083000	8.523326000	-0.762712000
H	-0.914143000	8.799524000	-2.329019000

Cartesian coordinates of DFT-optimized structure of **6a** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

Os	1.866360000	-2.493946000	-0.286779000
N	-0.057794000	-3.216416000	0.181507000
N	2.479813000	-2.435807000	1.718929000
N	3.030477000	-4.171475000	-0.136969000
N	1.750788000	-3.292542000	-2.223188000
C	2.147082000	-1.508532000	2.646429000
H	1.492116000	-0.718868000	2.299556000
C	2.603540000	-1.551207000	3.956471000
H	2.300899000	-0.775983000	4.651782000
C	3.445131000	-2.594678000	4.347605000
H	3.820809000	-2.657806000	5.363382000
C	3.794548000	-3.558258000	3.407898000
H	4.444346000	-4.379831000	3.685920000
C	3.308967000	-3.473109000	2.100386000
C	3.626985000	-4.456287000	1.052688000
C	4.437100000	-5.587608000	1.170537000
H	4.921108000	-5.830491000	2.109372000
C	4.618503000	-6.409148000	0.055575000
C	3.996967000	-6.099983000	-1.156516000
H	4.141544000	-6.739168000	-2.019705000
C	3.194367000	-4.960015000	-1.234141000
C	2.461539000	-4.462853000	-2.409455000
C	2.464205000	-5.109535000	-3.648204000
H	3.027413000	-6.027024000	-3.773078000
C	1.746830000	-4.579484000	-4.715085000
H	1.746711000	-5.079308000	-5.677930000
C	1.030638000	-3.396713000	-4.519821000
H	0.455285000	-2.943819000	-5.319768000

C	1.057866000	-2.790662000	-3.271460000
H	0.516730000	-1.873156000	-3.075288000
C	-0.369813000	-4.513855000	0.407820000
H	0.469877000	-5.196240000	0.468478000
C	-1.659501000	-4.980796000	0.546606000
H	-1.856265000	-6.031012000	0.727302000
C	-2.719320000	-4.067539000	0.413253000
C	-2.417668000	-2.721555000	0.188991000
H	-3.211670000	-2.009765000	0.030786000
C	-1.084788000	-2.287074000	0.114341000
C	-1.814395000	5.065493000	-1.408818000
C	-0.638128000	-0.906772000	-0.133965000
C	-3.146419000	5.035408000	-0.986649000
C	0.742336000	-0.851860000	-0.429787000
C	-3.705752000	3.889073000	-0.437962000
C	1.331146000	0.357034000	-0.836602000
C	-2.941107000	2.711705000	-0.266437000
C	0.565658000	1.509224000	-1.091727000
C	-1.593765000	2.694265000	-0.757267000
C	-0.810499000	1.494444000	-0.650747000
C	-1.036045000	3.882000000	-1.342553000
C	-1.397199000	0.298406000	-0.103978000
C	0.277482000	3.792837000	-1.911305000
C	-2.690543000	0.417060000	0.502754000
H	0.663427000	4.631696000	-2.478309000
H	-3.075721000	-0.404371000	1.093014000
C	1.038186000	2.670931000	-1.787438000
C	-3.428129000	1.560953000	0.426831000
H	1.999009000	2.641641000	-2.285043000
H	-4.388105000	1.609502000	0.927730000
O	-3.963226000	-4.574659000	0.506045000
C	-5.099520000	-3.700117000	0.378711000
C	-6.386456000	-4.517412000	0.564148000
C	-7.568214000	-3.539269000	0.415979000
C	-6.478402000	-5.611941000	-0.515894000
C	-6.410769000	-5.153327000	1.967157000
H	-5.031964000	-2.911752000	1.139708000
H	-5.081305000	-3.232086000	-0.614136000
H	-8.517712000	-4.072549000	0.538081000
H	-7.574854000	-3.065510000	-0.573278000
H	-7.529736000	-2.746265000	1.172775000
H	-6.476426000	-5.175100000	-1.522245000
H	-7.405580000	-6.185087000	-0.400215000
H	-5.637262000	-6.309078000	-0.446284000
H	-6.354344000	-4.386155000	2.749404000
H	-5.571138000	-5.841956000	2.105771000
H	-7.339831000	-5.715880000	2.114990000
H	5.245416000	-7.291013000	0.131100000
N	2.745468000	0.233918000	-0.988018000
C	3.766193000	1.126325000	-1.143949000
C	4.957383000	0.426136000	-1.126880000

C	4.599395000	-0.917128000	-0.932134000
N	3.270648000	-1.039874000	-0.834351000
H	5.224514000	-1.793924000	-0.844399000
H	5.950880000	0.835206000	-1.231791000
H	3.586127000	2.184390000	-1.219706000
N	-5.070077000	3.943888000	-0.031634000
N	-5.527604000	5.016543000	0.674117000
C	-6.835817000	4.802680000	0.803488000
C	-7.242548000	3.602383000	0.177430000
C	-6.081864000	3.080893000	-0.354519000
C	-1.298280000	6.368977000	-1.922811000
C	-0.068184000	6.883935000	-1.481760000
C	0.344452000	8.139679000	-1.944858000
C	-0.495947000	8.831330000	-2.831111000
C	-1.698656000	8.240299000	-3.190849000
N	-2.114238000	7.039338000	-2.758071000
O	1.494556000	8.754476000	-1.595796000
C	2.396403000	8.098836000	-0.687874000
C	3.608703000	9.007777000	-0.435920000
C	4.541830000	8.259171000	0.535566000
C	4.348431000	9.283563000	-1.758715000
C	3.150753000	10.333313000	0.201635000
H	-7.441240000	5.516847000	1.347300000
H	-8.235646000	3.181608000	0.116762000
H	-5.897389000	2.195879000	-0.944845000
H	0.528195000	6.321029000	-0.776139000
H	-0.205796000	9.806072000	-3.208155000
H	-2.371969000	8.761388000	-3.869304000
H	2.715884000	7.143834000	-1.125904000
H	1.872619000	7.892270000	0.254561000
H	4.040357000	8.043118000	1.486902000
H	5.426722000	8.867469000	0.754402000
H	4.885642000	7.308915000	0.108990000
H	4.695257000	8.350093000	-2.219137000
H	5.225787000	9.916361000	-1.581140000
H	3.699559000	9.795636000	-2.476347000
H	2.628239000	10.155758000	1.149925000
H	2.472787000	10.879580000	-0.461903000
H	4.014416000	10.975597000	0.409488000
H	-3.754473000	5.926392000	-1.080844000

Cartesian coordinates of DFT-optimized structure of **1b** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

Ru	1.811989000	-3.049688000	0.021685000
N	-1.652242000	6.835478000	-1.648269000
N	-0.160747000	-3.732504000	0.292898000
N	2.288687000	-3.235701000	2.054316000
N	2.871344000	-4.795240000	0.055319000
N	1.786550000	-3.617314000	-1.995610000

N	-5.207200000	4.754819000	1.513975000
N	3.354502000	-1.644481000	-0.266424000
C	1.946728000	-2.391674000	3.048666000
H	1.362647000	-1.529712000	2.748973000
C	2.309452000	-2.597436000	4.375069000
H	2.004368000	-1.881640000	5.130491000
C	3.062079000	-3.726068000	4.700832000
H	3.363775000	-3.918555000	5.725153000
C	3.421500000	-4.607340000	3.685557000
H	4.005238000	-5.491727000	3.913069000
C	3.029175000	-4.352529000	2.368795000
C	3.364025000	-5.239246000	1.237120000
C	4.099840000	-6.426494000	1.283533000
H	4.502648000	-6.799904000	2.217877000
C	4.311232000	-7.132792000	0.097200000
C	3.794999000	-6.656916000	-1.110268000
H	3.963108000	-7.207729000	-2.028368000
C	3.065611000	-5.464943000	-1.106727000
C	2.444572000	-4.795682000	-2.266715000
C	2.504728000	-5.302326000	-3.567564000
H	3.026738000	-6.232347000	-3.760922000
C	1.894115000	-4.613121000	-4.610991000
H	1.937285000	-5.001781000	-5.623085000
C	1.229403000	-3.419413000	-4.328982000
H	0.738010000	-2.846112000	-5.107423000
C	1.200017000	-2.960581000	-3.016743000
H	0.695992000	-2.039046000	-2.750964000
C	-1.163229000	8.043421000	-1.970840000
C	-0.542586000	-5.025609000	0.341381000
H	-1.799321000	8.661691000	-2.602157000
H	0.259742000	-5.753922000	0.381011000
C	0.070669000	8.527256000	-1.559801000
C	-1.859860000	-5.439440000	0.330152000
H	0.422684000	9.510601000	-1.852540000
H	-2.117136000	-6.491498000	0.369391000
C	0.861665000	7.711296000	-0.735966000
C	-2.863545000	-4.461883000	0.227795000
C	0.367547000	6.450436000	-0.379535000
C	-2.486800000	-3.115939000	0.190638000
H	0.921251000	5.795706000	0.280180000
H	-3.233467000	-2.347711000	0.066406000
C	-0.885328000	6.046984000	-0.871069000
C	-1.131821000	-2.753000000	0.262471000
C	-1.475273000	4.730890000	-0.485973000
C	-0.599480000	-1.381089000	0.204133000
C	-2.808083000	4.724892000	-0.070919000
C	0.797000000	-1.357424000	-0.012774000
C	-3.461982000	3.564077000	0.345208000
C	1.480884000	-0.145573000	-0.256848000
C	-4.897987000	3.694398000	0.730829000
C	2.942972000	-0.320886000	-0.289993000

C	-5.869970000	2.818221000	0.243505000
C	3.900614000	0.693780000	-0.243580000
H	-5.611427000	1.997444000	-0.415993000
H	3.609989000	1.731646000	-0.166358000
C	-7.216588000	3.018186000	0.586030000
C	5.270325000	0.397776000	-0.250252000
C	-7.538593000	4.103409000	1.410689000
C	5.666900000	-0.945894000	-0.292875000
H	-8.554242000	4.319844000	1.716908000
H	6.704845000	-1.251044000	-0.308273000
C	-6.493503000	4.927967000	1.829583000
C	4.670114000	-1.912752000	-0.282513000
H	-6.717825000	5.784167000	2.464207000
H	4.938011000	-2.963712000	-0.275861000
C	-2.743968000	2.340223000	0.388331000
C	0.738522000	1.052651000	-0.437695000
C	-1.382578000	2.302560000	-0.064602000
C	-0.650124000	1.064459000	-0.054145000
C	-0.755466000	3.508606000	-0.525226000
C	-1.306789000	-0.154430000	0.343321000
C	0.561312000	3.406649000	-1.080195000
C	-2.617274000	-0.041434000	0.913769000
H	0.994894000	4.270367000	-1.570806000
H	-3.061915000	-0.905394000	1.391973000
C	1.270078000	2.243827000	-1.032289000
C	-3.296804000	1.140189000	0.940826000
H	2.241502000	2.208337000	-1.509349000
H	-4.270527000	1.179279000	1.415280000
O	2.049561000	8.218279000	-0.341031000
O	6.106418000	1.453625000	-0.204806000
O	-4.132514000	-4.910085000	0.163797000
O	-8.103689000	2.137982000	0.073637000
C	-9.501845000	2.309566000	0.364334000
C	-10.306035000	1.212613000	-0.348384000
C	-11.790056000	1.438873000	0.000487000
C	-9.862671000	-0.176486000	0.148436000
C	-10.109099000	1.318781000	-1.872457000
C	-5.212722000	-3.969006000	0.028578000
C	-6.542985000	-4.734720000	-0.026646000
C	-7.661739000	-3.685628000	-0.177561000
C	-6.555643000	-5.685826000	-1.238333000
C	-6.748923000	-5.531844000	1.275393000
C	2.907943000	7.428167000	0.499402000
C	4.221693000	8.188117000	0.735907000
C	4.941841000	8.424891000	-0.605131000
C	3.938440000	9.533453000	1.430633000
C	5.097298000	7.306896000	1.648085000
C	7.527716000	1.224887000	-0.182619000
C	8.253519000	2.574790000	-0.087689000
C	7.851160000	3.300562000	1.210173000
C	7.912174000	3.447170000	-1.310471000

C	9.765194000	2.274717000	-0.067758000
H	-9.820978000	3.302149000	0.020291000
H	-9.652858000	2.251891000	1.450377000
H	-12.136076000	2.423118000	-0.337955000
H	-11.962293000	1.371090000	1.081581000
H	-12.412922000	0.679656000	-0.485964000
H	-10.003748000	-0.272238000	1.232251000
H	-8.806311000	-0.359080000	-0.073611000
H	-10.452954000	-0.962072000	-0.337546000
H	-10.434409000	2.298321000	-2.244474000
H	-10.697579000	0.551102000	-2.388220000
H	-9.058191000	1.183616000	-2.147579000
H	-5.199921000	-3.281906000	0.884848000
H	-5.067057000	-3.386356000	-0.890315000
H	-8.639601000	-4.178625000	-0.218352000
H	-7.541955000	-3.102203000	-1.098592000
H	-7.674058000	-2.986920000	0.667933000
H	-6.419635000	-5.132591000	-2.175894000
H	-7.512998000	-6.216434000	-1.296979000
H	-5.757693000	-6.431533000	-1.164830000
H	-6.755080000	-4.867484000	2.148429000
H	-5.954789000	-6.271890000	1.417287000
H	-7.707635000	-6.062752000	1.250515000
H	3.107295000	6.466308000	0.009386000
H	2.397848000	7.234631000	1.452457000
H	5.162518000	7.474830000	-1.107670000
H	5.891716000	8.947180000	-0.442459000
H	4.331382000	9.032224000	-1.281073000
H	3.301233000	10.173061000	0.811622000
H	4.875587000	10.069274000	1.621439000
H	3.435596000	9.382406000	2.393907000
H	5.313936000	6.337569000	1.182298000
H	4.608961000	7.119366000	2.612138000
H	6.053932000	7.802705000	1.848348000
H	7.818780000	0.693712000	-1.098246000
H	7.775617000	0.595307000	0.681631000
H	8.389859000	4.251087000	1.297726000
H	8.092026000	2.694790000	2.092595000
H	6.777649000	3.515014000	1.228589000
H	6.838718000	3.656078000	-1.361019000
H	8.206655000	2.951924000	-2.244027000
H	8.442687000	4.404919000	-1.256593000
H	10.037860000	1.647353000	0.789700000
H	10.334971000	3.207862000	0.006007000
H	10.083765000	1.758697000	-0.981679000
H	-3.356451000	5.659481000	-0.071504000
H	4.880183000	-8.056248000	0.113608000

Cartesian coordinates of DFT-optimized structure of **2b** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

Ru	1.958137000	-1.358021000	-0.018038000
N	0.459712000	-2.827121000	0.147701000
N	2.427155000	-1.430042000	2.024022000
N	3.650721000	-2.502142000	-0.006308000
N	2.221672000	-1.774984000	-2.055932000
N	2.763109000	0.580174000	-0.191838000
C	1.747615000	-0.849304000	3.033378000
H	0.865499000	-0.291350000	2.742752000
C	2.136691000	-0.949307000	4.364513000
H	1.548239000	-0.458811000	5.132137000
C	3.281271000	-1.682132000	4.678989000
H	3.615225000	-1.781153000	5.706577000
C	3.992784000	-2.288352000	3.647960000
H	4.885191000	-2.863178000	3.866775000
C	3.556744000	-2.155660000	2.327047000
C	4.252256000	-2.768483000	1.178151000
C	5.407160000	-3.554690000	1.211927000
H	5.904036000	-3.780228000	2.148265000
C	5.917031000	-4.052000000	0.010422000
C	5.281196000	-3.765083000	-1.199669000
H	5.679933000	-4.153985000	-2.129361000
C	4.130075000	-2.972947000	-1.182914000
C	3.318865000	-2.554650000	-2.343202000
C	3.624012000	-2.909314000	-3.659867000
H	4.493832000	-3.522255000	-3.865767000
C	2.811591000	-2.474529000	-4.702714000
H	3.043189000	-2.746829000	-5.727171000
C	1.700279000	-1.685933000	-4.404124000
H	1.036767000	-1.323081000	-5.181397000
C	1.443646000	-1.361609000	-3.076561000
H	0.593095000	-0.750823000	-2.798485000
C	0.660521000	-4.161136000	0.122195000
H	1.695154000	-4.484437000	0.147936000
C	-0.358329000	-5.090969000	0.057848000
H	-0.146408000	-6.153683000	0.041832000
C	-1.681402000	-4.625443000	-0.019456000
C	-1.908313000	-3.245972000	0.011402000
H	-2.909016000	-2.859740000	-0.099840000
C	-0.834206000	-2.350095000	0.135025000
C	-4.321307000	4.281284000	-0.297789000
C	-0.932586000	-0.880056000	0.155359000
C	-5.540928000	3.708655000	0.048116000
C	0.323929000	-0.254429000	-0.016611000
C	-5.612859000	2.359783000	0.379562000
C	0.431842000	1.145869000	-0.176884000
C	1.831855000	1.606484000	-0.168240000
C	2.270681000	2.925853000	-0.046885000
H	1.569189000	3.739357000	0.069701000
C	3.637812000	3.235438000	-0.030043000
C	4.564304000	2.187976000	-0.121559000

H	5.634058000	2.349590000	-0.121184000
C	4.069021000	0.892126000	-0.181801000
H	4.755668000	0.053276000	-0.213591000
C	-4.452825000	1.552677000	0.421666000
C	-0.746485000	1.925368000	-0.326435000
C	-3.201485000	2.126844000	0.020448000
C	-2.011924000	1.322440000	0.007026000
C	-3.140807000	3.506541000	-0.366359000
C	-2.094025000	-0.079443000	0.328727000
C	-1.900441000	4.017838000	-0.863905000
C	-3.334399000	-0.564373000	0.861701000
H	-1.870252000	5.013043000	-1.292270000
H	-3.371664000	-1.555985000	1.294722000
C	-0.765531000	3.263956000	-0.841569000
C	-4.456739000	0.207238000	0.908068000
H	0.135593000	3.674374000	-1.279028000
H	-5.361554000	-0.194764000	1.349082000
O	3.950555000	4.540739000	0.083385000
O	-2.642162000	-5.563216000	-0.126718000
C	-4.022932000	-5.162901000	-0.197369000
C	-4.907683000	-6.416517000	-0.261377000
C	-6.369430000	-5.934435000	-0.340985000
C	-4.564273000	-7.243488000	-1.514856000
C	-4.709718000	-7.267980000	1.007080000
C	5.336412000	4.931485000	0.107035000
C	5.427646000	6.457498000	0.250451000
C	4.774879000	6.903643000	1.572548000
C	4.734630000	7.143740000	-0.941902000
C	6.925487000	6.820695000	0.261135000
H	-4.268523000	-4.565888000	0.690477000
H	-4.171052000	-4.541919000	-1.090414000
H	-7.048498000	-6.793480000	-0.383839000
H	-6.542746000	-5.325589000	-1.236714000
H	-6.642466000	-5.335054000	0.536099000
H	-4.711622000	-6.654843000	-2.428899000
H	-5.209044000	-8.127782000	-1.577372000
H	-3.523689000	-7.582855000	-1.493498000
H	-4.957364000	-6.695241000	1.909488000
H	-3.674445000	-7.612290000	1.096710000
H	-5.360356000	-8.149660000	0.979831000
H	5.815782000	4.603248000	-0.824297000
H	5.833565000	4.436391000	0.951104000
H	4.854587000	7.990576000	1.689834000
H	5.267739000	6.435433000	2.433713000
H	3.713819000	6.635732000	1.601506000
H	3.670589000	6.889743000	-0.982433000
H	5.192827000	6.842193000	-1.892002000
H	4.820983000	8.233242000	-0.858135000
H	7.448633000	6.341749000	1.097850000
H	7.051368000	7.904411000	0.364115000
H	7.419006000	6.513397000	-0.668970000

H	-6.437059000	4.314882000	0.059440000
H	6.812009000	-4.664976000	0.017160000
N	-4.311589000	5.669363000	-0.610271000
C	-3.486590000	6.641742000	-0.112174000
C	-3.932049000	7.845076000	-0.616559000
C	-5.051004000	7.503580000	-1.410479000
N	-5.288685000	6.193547000	-1.403835000
N	-6.892043000	1.828652000	0.704926000
N	-7.731351000	2.528587000	1.520138000
C	-8.856325000	1.816678000	1.536988000
C	-8.766223000	0.660419000	0.728330000
C	-7.492028000	0.704699000	0.203700000
H	-6.978964000	0.057158000	-0.491399000
H	-9.520783000	-0.091352000	0.548463000
H	-9.692999000	2.156553000	2.134196000
H	-5.689588000	8.157972000	-1.990285000
H	-3.515078000	8.824537000	-0.433067000
H	-2.682038000	6.401872000	0.566680000

Cartesian coordinates of DFT-optimized structure of **3b** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

C	2.334824000	-2.455716000	-0.301344000
C	3.694698000	-2.454482000	-0.243992000
C	4.432833000	-1.237959000	-0.113385000
C	3.707160000	-0.003167000	-0.029082000
C	2.270337000	-0.001375000	-0.073893000
C	1.562801000	-1.249300000	-0.248032000
C	4.426481000	1.231189000	0.111796000
C	3.684808000	2.425796000	0.372823000
C	2.324486000	2.426393000	0.368707000
C	1.562301000	1.249027000	0.070298000
C	0.151972000	-1.190866000	-0.316031000
C	-0.548279000	0.009672000	-0.160454000
C	0.155117000	1.210354000	-0.023604000
C	5.845164000	-1.201363000	-0.061062000
C	6.534550000	0.004056000	-0.011802000
C	5.838065000	1.206249000	0.056176000
H	1.838372000	-3.412712000	-0.352317000
H	4.225834000	-3.396716000	-0.300554000
H	1.816046000	3.337094000	0.651582000
H	4.216215000	3.337112000	0.620300000
N	-0.747174000	-2.290256000	-0.510311000
N	-2.090726000	-2.015276000	-0.312215000
C	-2.755504000	-3.133645000	-0.607829000
C	-1.870073000	-4.143086000	-1.020229000
C	-0.613992000	-3.572950000	-0.959692000
N	-0.733363000	2.330624000	0.039883000
N	-2.079557000	2.032675000	0.165589000
C	-2.729995000	3.197388000	0.126749000

C	-1.830956000	4.263148000	-0.046538000
C	-0.581422000	3.678960000	-0.112531000
N	6.617020000	-2.399083000	-0.093367000
N	7.638258000	-2.524468000	-0.987439000
C	8.203914000	-3.693271000	-0.690231000
C	6.557169000	-3.464136000	0.762857000
C	7.568476000	-4.329349000	0.400337000
N	6.597568000	2.408164000	0.103169000
N	7.696986000	2.486857000	0.906037000
C	8.222277000	3.681389000	0.641981000
C	7.482483000	4.383182000	-0.337376000
C	6.449531000	3.531185000	-0.665806000
C	-1.737266000	-0.343860000	3.003713000
C	-1.975200000	-0.498561000	4.365458000
C	-3.293436000	-0.550913000	4.816557000
C	-4.324526000	-0.446424000	3.887013000
C	-4.027610000	-0.293789000	2.530744000
N	-2.724728000	-0.242534000	2.093184000
C	-5.063219000	-0.175254000	1.483830000
N	-4.547753000	-0.027026000	0.242169000
C	-5.326447000	0.102667000	-0.856767000
C	-6.717995000	0.084131000	-0.728821000
C	-7.272831000	-0.070273000	0.543389000
C	-6.448995000	-0.201703000	1.663195000
C	-4.548387000	0.250382000	-2.104406000
N	-3.180601000	0.228013000	-1.962914000
C	-2.417067000	0.351488000	-3.065769000
C	-2.949733000	0.505311000	-4.341504000
C	-4.335583000	0.532612000	-4.492865000
C	-5.137060000	0.402638000	-3.361961000
H	-0.729122000	-0.296644000	2.609744000
H	-1.137415000	-0.574865000	5.049754000
H	-3.517693000	-0.669847000	5.871423000
H	-5.357238000	-0.481838000	4.213645000
H	-7.361945000	0.185916000	-1.594331000
H	-6.884696000	-0.321970000	2.648039000
H	-1.346780000	0.323245000	-2.899396000
H	-2.283860000	0.600815000	-5.192027000
H	-4.787099000	0.651808000	-5.472214000
H	-6.216622000	0.419518000	-3.455483000
Ru	-2.520415000	-0.002630000	0.014441000
H	-3.832516000	-3.153524000	-0.522268000
H	-2.110524000	-5.148789000	-1.330264000
H	0.336465000	-3.986729000	-1.243698000
H	-3.807129000	3.211927000	0.211997000
H	-2.059431000	5.315366000	-0.123952000
H	0.378254000	4.128571000	-0.295347000
H	9.047239000	-4.040696000	-1.273620000
H	5.827948000	-3.504384000	1.558454000
H	7.814329000	-5.275746000	0.859499000
H	9.112925000	4.000021000	1.168692000

H	7.676655000	5.363087000	-0.748406000
H	5.649478000	3.617022000	-1.385826000
H	7.616780000	0.007808000	-0.016558000
H	-8.350885000	-0.088292000	0.662373000

Cartesian coordinates of DFT-optimized structure of **4b** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

Ru	3.872531000	-0.355490000	-0.005114000
N	-6.128117000	2.700728000	-1.769440000
N	3.222129000	-2.270149000	0.528422000
N	4.339971000	0.176583000	1.971314000
N	5.901867000	-0.558808000	0.019288000
N	4.270073000	-0.975171000	-1.970660000
N	-6.614810000	-1.334702000	1.448916000
N	3.631419000	1.648006000	-0.551509000
C	3.480842000	0.548450000	2.940122000
H	2.435412000	0.570411000	2.656125000
C	3.889486000	0.884571000	4.226538000
H	3.149863000	1.176494000	4.963918000
C	5.248462000	0.836459000	4.535270000
H	5.604126000	1.091362000	5.528146000
C	6.147909000	0.453380000	3.544212000
H	7.209070000	0.408304000	3.759368000
C	5.681910000	0.126613000	2.268572000
C	6.570258000	-0.289565000	1.164236000
C	7.961081000	-0.420637000	1.205198000
H	8.517762000	-0.210165000	2.110882000
C	8.630529000	-0.830875000	0.050300000
C	7.919365000	-1.103764000	-1.120225000
H	8.443628000	-1.421370000	-2.013836000
C	6.529522000	-0.957753000	-1.110997000
C	5.601835000	-1.194150000	-2.236110000
C	6.022520000	-1.614021000	-3.500146000
H	7.076082000	-1.782047000	-3.690829000
C	5.087772000	-1.816230000	-4.511758000
H	5.408401000	-2.142390000	-5.495682000
C	3.739528000	-1.592421000	-4.235033000
H	2.973592000	-1.736609000	-4.989060000
C	3.376463000	-1.175172000	-2.958751000
H	2.340982000	-0.990074000	-2.698532000
C	-6.813590000	3.802219000	-2.115591000
C	3.735763000	-3.492067000	0.688568000
H	-7.676466000	3.643348000	-2.760248000
C	-6.489484000	5.088995000	-1.710296000
H	-7.076095000	5.947612000	-2.018890000
C	-5.378634000	5.259498000	-0.869304000
C	-4.648991000	4.124359000	-0.495109000
H	-3.801241000	4.195450000	0.173525000
C	-5.052239000	2.867753000	-0.977050000

N	1.846180000	-2.419663000	0.543403000
C	-4.343698000	1.621869000	-0.558511000
C	1.081304000	-1.235516000	0.305636000
C	-5.130646000	0.555339000	-0.122222000
C	1.901765000	-0.157081000	-0.031097000
C	-4.585893000	-0.646994000	0.331826000
C	1.322485000	1.062592000	-0.386680000
C	-5.542957000	-1.724434000	0.719197000
N	2.314124000	2.069383000	-0.602733000
C	-5.379028000	-3.039820000	0.279794000
H	-4.536983000	-3.328368000	-0.339059000
C	-6.337010000	-4.008028000	0.618188000
C	-7.440011000	-3.612184000	1.385060000
H	-8.219593000	-4.302590000	1.681295000
C	-7.517565000	-2.269482000	1.757942000
C	4.383188000	2.742148000	-0.693962000
H	-8.368999000	-1.933412000	2.348087000
C	-3.175324000	-0.786285000	0.401934000
C	-0.074056000	1.211912000	-0.532260000
C	-2.334580000	0.271926000	-0.084468000
C	-0.903816000	0.126817000	-0.066676000
C	-2.932771000	1.475920000	-0.589643000
C	-0.320274000	-1.101829000	0.415629000
C	-2.072345000	2.458903000	-1.177568000
C	-1.190700000	-2.071237000	1.012006000
H	-2.513054000	3.309718000	-1.683715000
H	-0.769469000	-2.920071000	1.534780000
C	-0.716717000	2.334656000	-1.148054000
C	-2.543991000	-1.920269000	1.008248000
H	-0.120563000	3.078635000	-1.660134000
H	-3.158869000	-2.664300000	1.500596000
O	-5.105634000	6.521904000	-0.474721000
O	-6.113660000	-5.258292000	0.158760000
C	-7.074689000	-6.289347000	0.443953000
C	-6.600345000	-7.609067000	-0.182054000
C	-7.665788000	-8.674338000	0.142219000
C	-5.247284000	-8.025918000	0.425108000
C	-6.470890000	-7.453918000	-1.709175000
C	-3.979469000	6.763012000	0.385815000
C	-3.886880000	8.266341000	0.686626000
C	-3.691715000	9.057078000	-0.620939000
C	-5.163178000	8.740661000	1.407175000
C	-2.665789000	8.470959000	1.604269000
H	-8.048715000	-5.996571000	0.030217000
H	-7.176360000	-6.396386000	1.531939000
H	-8.642463000	-8.404842000	-0.278121000
H	-7.785871000	-8.805879000	1.224462000
H	-7.374516000	-9.641937000	-0.282160000
H	-5.325324000	-8.155878000	1.511729000
H	-4.475759000	-7.274749000	0.227797000
H	-4.912923000	-8.977784000	-0.003706000

H	-7.429195000	-7.165780000	-2.159005000
H	-6.157760000	-8.401024000	-2.163790000
H	-5.730477000	-6.690668000	-1.969106000
H	-3.064912000	6.414368000	-0.112083000
H	-4.108082000	6.194254000	1.316116000
H	-2.779493000	8.739997000	-1.141535000
H	-3.602269000	10.128834000	-0.408922000
H	-4.537588000	8.914535000	-1.301023000
H	-6.050254000	8.588433000	0.783993000
H	-5.093332000	9.808562000	1.644651000
H	-5.311074000	8.196223000	2.348180000
H	-1.739090000	8.143660000	1.117128000
H	-2.771802000	7.913583000	2.543049000
H	-2.554924000	9.531812000	1.855948000
H	-6.208705000	0.664352000	-0.135790000
H	9.709903000	-0.938232000	0.062405000
C	2.276340000	3.425927000	-0.744864000
C	3.576983000	3.886052000	-0.819838000
C	1.534240000	-3.740822000	0.680848000
C	2.714130000	-4.451441000	0.789795000
H	4.808317000	-3.622198000	0.710831000
H	5.460315000	2.655397000	-0.685682000
H	1.348731000	3.970995000	-0.748950000
H	3.896659000	4.910160000	-0.939999000
H	0.516664000	-4.089387000	0.658037000
H	2.819278000	-5.518455000	0.915737000

Cartesian coordinates of DFT-optimized structure of **5b** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

Ru	3.561205000	0.039823000	0.007787000
N	2.355658000	-1.664576000	0.263702000
N	4.085576000	0.133072000	2.037355000
N	5.443663000	-0.750869000	-0.001666000
N	3.837255000	-0.409492000	-2.022902000
N	-6.696511000	2.307218000	1.598039000
C	3.328679000	0.593918000	3.052778000
H	2.344644000	0.953485000	2.776638000
C	3.763921000	0.613839000	4.373506000
H	3.108291000	0.997897000	5.147251000
C	5.040513000	0.136419000	4.669263000
H	5.413804000	0.136345000	5.688016000
C	5.833300000	-0.344083000	3.631050000
H	6.828545000	-0.721435000	3.835548000
C	5.345554000	-0.340945000	2.321888000
C	6.121414000	-0.836859000	1.167196000
C	7.419028000	-1.355752000	1.183195000
H	7.980305000	-1.431959000	2.107031000
C	7.987940000	-1.778395000	-0.020186000
C	7.270148000	-1.680817000	-1.214328000

H	7.716633000	-2.009327000	-2.145564000
C	5.976530000	-1.153416000	-1.179442000
C	5.060291000	-0.964273000	-2.322117000
C	5.387437000	-1.317160000	-3.633673000
H	6.355978000	-1.752739000	-3.849962000
C	4.468687000	-1.110347000	-4.658661000
H	4.716872000	-1.382519000	-5.679255000
C	3.229845000	-0.550492000	-4.347280000
H	2.480200000	-0.371237000	-5.110111000
C	2.956832000	-0.217030000	-3.024966000
H	2.007807000	0.219666000	-2.737380000
C	2.801794000	-2.937753000	0.277744000
H	3.878892000	-3.059742000	0.301446000
C	1.974439000	-4.042718000	0.250140000
H	2.380672000	-5.047353000	0.261201000
C	0.587869000	-3.834173000	0.170294000
C	0.106368000	-2.520878000	0.169549000
H	-0.949788000	-2.332974000	0.061409000
C	0.993728000	-1.436570000	0.253590000
C	-3.594851000	4.504970000	-0.231609000
C	0.622364000	-0.008932000	0.231003000
C	-4.695242000	3.740219000	0.141024000
C	1.745037000	0.817509000	0.025729000
C	-4.567059000	2.389437000	0.465745000
C	1.584588000	2.195132000	-0.173405000
C	-5.821305000	1.652905000	0.799285000
C	-6.103041000	0.400686000	0.249989000
H	-5.409618000	-0.090937000	-0.422784000
C	-7.323926000	-0.225869000	0.546554000
C	-8.225110000	0.439528000	1.387239000
H	-9.184833000	0.018984000	1.659655000
C	-7.852605000	1.695511000	1.868383000
H	-8.539127000	2.238082000	2.516651000
C	-3.276192000	1.795598000	0.479427000
C	0.312482000	2.783410000	-0.309532000
C	-2.135179000	2.566422000	0.072461000
C	-0.827330000	1.971453000	0.049014000
C	-2.305371000	3.936883000	-0.316702000
C	-0.665592000	0.581455000	0.385695000
C	-1.173097000	4.653135000	-0.822638000
C	-1.806024000	-0.102532000	0.919870000
H	-1.315713000	5.642052000	-1.242529000
H	-1.677451000	-1.084098000	1.358010000
C	0.072488000	4.104581000	-0.813226000
C	-3.042751000	0.469818000	0.965283000
H	0.887202000	4.664271000	-1.254543000
H	-3.863800000	-0.080877000	1.409055000
O	-0.180381000	-4.937189000	0.090085000
O	-7.533058000	-1.432688000	-0.022088000
C	-8.781538000	-2.106411000	0.215329000
C	-8.790007000	-3.443384000	-0.540327000

C	-10.148806000	-4.113248000	-0.256891000
C	-7.650365000	-4.346314000	-0.031440000
C	-8.637428000	-3.198018000	-2.053275000
C	-1.610915000	-4.804528000	0.003412000
C	-2.240687000	-6.202828000	-0.077786000
C	-3.767231000	-6.007300000	-0.159642000
C	-1.741529000	-6.933863000	-1.338521000
C	-1.888226000	-7.016712000	1.181798000
H	-9.604949000	-1.466707000	-0.128665000
H	-8.899162000	-2.276260000	1.293606000
H	-10.982311000	-3.491934000	-0.606611000
H	-10.288649000	-4.297715000	0.815238000
H	-10.210042000	-5.077723000	-0.773449000
H	-7.749694000	-4.538683000	1.044137000
H	-6.671629000	-3.887577000	-0.205334000
H	-7.669227000	-5.312786000	-0.548425000
H	-9.448482000	-2.565064000	-2.434250000
H	-8.668434000	-4.148347000	-2.598845000
H	-7.686724000	-2.705703000	-2.281721000
H	-1.974498000	-4.268657000	0.889916000
H	-1.863766000	-4.218149000	-0.889493000
H	-4.270127000	-6.979179000	-0.218489000
H	-4.050996000	-5.429160000	-1.047474000
H	-4.152112000	-5.484247000	0.724343000
H	-1.997535000	-6.374077000	-2.246658000
H	-2.203379000	-7.925133000	-1.413251000
H	-0.655067000	-7.066379000	-1.316102000
H	-2.244442000	-6.514086000	2.089572000
H	-0.806541000	-7.157782000	1.273665000
H	-2.357847000	-8.006261000	1.139587000
H	-5.672626000	4.205306000	0.174417000
H	8.993916000	-2.184190000	-0.027677000
N	2.837979000	2.874589000	-0.257580000
C	3.210631000	4.186598000	-0.213869000
C	4.591305000	4.239948000	-0.227773000
C	5.014059000	2.899981000	-0.258403000
N	3.964713000	2.074265000	-0.263497000
N	-3.816983000	5.877403000	-0.544027000
C	-3.173061000	6.972947000	-0.036713000
C	-3.803706000	8.086237000	-0.551764000
C	-4.837573000	7.563347000	-1.361452000
N	-4.854015000	6.231454000	-1.354567000
H	-2.349439000	6.869457000	0.653864000
H	-3.557972000	9.121425000	-0.364680000
H	-5.567341000	8.102203000	-1.952540000
H	6.014868000	2.492541000	-0.264658000
H	5.206499000	5.126882000	-0.208855000
H	2.486831000	4.979813000	-0.142617000

Cartesian coordinates of DFT-optimized structure of **6b** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 1, multiplicity = 1

Ru	-2.701375000	-1.586957000	-0.041974000
N	-3.359705000	0.385480000	0.286522000
N	-2.834636000	-2.107424000	1.985878000
N	-4.443044000	-2.650419000	0.011433000
N	-3.321972000	-1.509563000	-2.044308000
C	-1.969629000	-1.783178000	2.967190000
H	-1.118294000	-1.186843000	2.661398000
C	-2.141769000	-2.177854000	4.289559000
H	-1.409720000	-1.886338000	5.034624000
C	-3.258678000	-2.943437000	4.623983000
H	-3.425786000	-3.269699000	5.645192000
C	-4.162210000	-3.283787000	3.621488000
H	-5.038911000	-3.875930000	3.856594000
C	-3.939912000	-2.860366000	2.308904000
C	-4.851594000	-3.175449000	1.190568000
C	-6.029538000	-3.925428000	1.247836000
H	-6.374927000	-4.355986000	2.180502000
C	-6.762375000	-4.115189000	0.074150000
C	-6.321776000	-3.564388000	-1.131343000
H	-6.893369000	-3.715638000	-2.039565000
C	-5.137534000	-2.822469000	-1.137976000
C	-4.503532000	-2.166569000	-2.299498000
C	-5.045389000	-2.196460000	-3.586847000
H	-5.977297000	-2.719097000	-3.768528000
C	-4.387518000	-1.555244000	-4.632532000
H	-4.803258000	-1.574759000	-5.634529000
C	-3.190078000	-0.891475000	-4.366235000
H	-2.640553000	-0.377287000	-5.147052000
C	-2.695867000	-0.893258000	-3.066273000
H	-1.769694000	-0.390901000	-2.813192000
C	-4.648984000	0.772768000	0.378048000
H	-5.380189000	-0.026553000	0.424604000
C	-5.056136000	2.092039000	0.401671000
H	-6.105323000	2.352956000	0.476407000
C	-4.077435000	3.093062000	0.289804000
C	-2.734713000	2.710407000	0.204720000
H	-1.968223000	3.456193000	0.067729000
C	-2.376345000	1.353983000	0.243647000
C	5.118369000	1.592724000	-0.609783000
C	-1.005983000	0.817141000	0.141453000
C	5.130199000	2.943566000	-0.252315000
C	-1.006439000	-0.572909000	-0.088997000
C	3.973410000	3.594403000	0.156264000
C	0.192174000	-1.247413000	-0.357303000
C	2.740607000	2.907390000	0.247268000
C	1.408631000	-0.560899000	-0.537053000
C	2.687257000	1.540791000	-0.183570000
C	1.437354000	0.832159000	-0.157759000

C	3.887653000	0.888041000	-0.626958000
C	0.234235000	1.510510000	0.249103000
C	3.771269000	-0.443427000	-1.146650000
C	0.373392000	2.824615000	0.804634000
H	4.634036000	-0.903008000	-1.614105000
H	-0.475200000	3.284710000	1.294399000
C	2.597680000	-1.131617000	-1.099527000
C	1.561591000	3.492735000	0.804361000
H	2.555108000	-2.111929000	-1.556696000
H	1.621344000	4.473164000	1.262601000
O	-4.519197000	4.364934000	0.265407000
C	-3.574003000	5.444101000	0.146099000
C	-4.329194000	6.780947000	0.174746000
C	-3.275397000	7.897637000	0.041293000
C	-5.318182000	6.855423000	-1.004036000
C	-5.082579000	6.934012000	1.509772000
H	-2.860047000	5.388792000	0.978150000
H	-3.023195000	5.334803000	-0.797170000
H	-3.761415000	8.879681000	0.055438000
H	-2.718434000	7.812940000	-0.899842000
H	-2.554301000	7.868661000	0.867223000
H	-4.796108000	6.760534000	-1.964290000
H	-5.843632000	7.817434000	-1.001038000
H	-6.067351000	6.059376000	-0.944505000
H	-4.390813000	6.893215000	2.360312000
H	-5.826862000	6.141721000	1.639143000
H	-5.602688000	7.898204000	1.545855000
H	-7.679013000	-4.694767000	0.098812000
N	0.001600000	-2.659365000	-0.457415000
C	0.844676000	-3.732340000	-0.474991000
C	0.076047000	-4.880624000	-0.473574000
C	-1.256271000	-4.435335000	-0.431741000
N	-1.307069000	-3.101221000	-0.408955000
H	-2.173477000	-5.006160000	-0.404039000
H	0.432227000	-5.899607000	-0.491087000
H	1.914033000	-3.614247000	-0.453244000
N	4.073255000	4.972221000	0.504194000
N	5.099157000	5.403187000	1.291416000
C	4.955224000	6.726407000	1.339254000
C	3.848296000	7.168473000	0.579381000
C	3.309741000	6.013760000	0.051475000
C	6.430409000	0.975124000	-0.965729000
C	6.818680000	-0.259170000	-0.419248000
C	8.084557000	-0.769533000	-0.733165000
C	8.912907000	-0.019045000	-1.582145000
C	8.439347000	1.196771000	-2.054144000
N	7.231093000	1.705431000	-1.764635000
O	8.586439000	-1.934571000	-0.271356000
C	7.789418000	-2.746333000	0.608085000
C	8.587539000	-3.999008000	0.999532000
C	7.691579000	-4.833227000	1.935654000

C	8.933284000	-4.820291000	-0.257088000
C	9.876523000	-3.593743000	1.739497000
H	5.649783000	7.317088000	1.923191000
H	3.497622000	8.179572000	0.432138000
H	2.476186000	5.850003000	-0.614962000
H	6.151297000	-0.783344000	0.251802000
H	9.899169000	-0.386167000	-1.844735000
H	9.067258000	1.801744000	-2.706019000
H	6.860316000	-3.027384000	0.094611000
H	7.531368000	-2.163296000	1.501786000
H	7.423783000	-4.272256000	2.839420000
H	8.215896000	-5.742863000	2.249713000
H	6.763280000	-5.136988000	1.436508000
H	8.024603000	-5.130605000	-0.787842000
H	9.486984000	-5.725515000	0.017993000
H	9.551133000	-4.241726000	-0.951196000
H	9.647828000	-3.015552000	2.643470000
H	10.525298000	-2.984345000	1.102288000
H	10.438250000	-4.484449000	2.044092000
H	6.062014000	3.494173000	-0.285115000

Cartesian coordinates of DFT-optimized structure of **1a<sub>ox</sub>** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

Os	2.191900000	-0.046596000	0.031683000
N	-7.886651000	2.597263000	-1.795872000
N	1.675118000	-2.076997000	0.312582000
N	2.651903000	0.205856000	2.068977000
N	4.297253000	-0.132922000	0.094845000
N	2.745932000	-0.439111000	-1.958566000
N	-8.195490000	-1.469563000	1.400422000
N	1.917681000	2.039303000	-0.283978000
C	1.731624000	0.368597000	3.045442000
H	0.695952000	0.334499000	2.733587000
C	2.083138000	0.570233000	4.373971000
H	1.302491000	0.698076000	5.114905000
C	3.432940000	0.599164000	4.721028000
H	3.740087000	0.752879000	5.749749000
C	4.387377000	0.423716000	3.723191000
H	5.442358000	0.438372000	3.968127000
C	3.986147000	0.228563000	2.402098000
C	4.923060000	0.027059000	1.283735000
C	6.316961000	-0.020171000	1.351033000
H	6.835679000	0.103345000	2.293901000
C	7.037392000	-0.235168000	0.175072000
C	6.372654000	-0.406214000	-1.039885000
H	6.934659000	-0.580641000	-1.949185000
C	4.977266000	-0.351639000	-1.054275000
C	4.093840000	-0.521827000	-2.219786000
C	4.555792000	-0.763256000	-3.513403000

H	5.620801000	-0.824352000	-3.701441000
C	3.648968000	-0.925434000	-4.556535000
H	4.003145000	-1.112728000	-5.564329000
C	2.284784000	-0.844621000	-4.280821000
H	1.539327000	-0.965426000	-5.058334000
C	1.872216000	-0.603689000	-2.976785000
H	0.823227000	-0.531344000	-2.720997000
C	-8.614619000	3.677713000	-2.120032000
C	2.534701000	-3.116007000	0.379736000
H	-9.475363000	3.497487000	-2.761543000
H	3.587047000	-2.861269000	0.416238000
C	-8.335959000	4.968605000	-1.693578000
C	2.134510000	-4.436017000	0.394394000
H	-8.958037000	5.809034000	-1.981898000
H	2.861279000	-5.237452000	0.451011000
C	-7.226480000	5.167797000	-0.857334000
C	0.762919000	-4.722467000	0.300155000
C	-6.449998000	4.054883000	-0.509500000
C	-0.142046000	-3.653425000	0.236272000
H	-5.600397000	4.147021000	0.153901000
H	-1.196456000	-3.842581000	0.114257000
C	-6.811995000	2.793864000	-1.009905000
C	0.318037000	-2.333166000	0.281184000
C	-6.057031000	1.568019000	-0.614470000
C	-0.527018000	-1.124221000	0.194726000
C	-6.803713000	0.465151000	-0.194432000
C	0.220534000	0.054536000	-0.035331000
C	-6.215757000	-0.721059000	0.246541000
C	-0.380970000	1.303384000	-0.313001000
C	-7.133694000	-1.829518000	0.642640000
C	0.585530000	2.425412000	-0.337534000
C	-6.944322000	-3.136019000	0.189536000
C	0.265205000	3.776140000	-0.307638000
H	-6.111690000	-3.398655000	-0.453310000
H	-0.761803000	4.107323000	-0.257008000
C	-7.870180000	-4.130601000	0.545107000
C	1.271644000	4.760397000	-0.299253000
C	-8.960957000	-3.766949000	1.344553000
C	2.610827000	4.350088000	-0.307939000
H	-9.714001000	-4.478959000	1.657631000
H	3.437957000	5.046927000	-0.310226000
C	-9.064712000	-2.429084000	1.728280000
C	2.869648000	2.987126000	-0.283442000
H	-9.908614000	-2.118796000	2.342479000
H	3.893129000	2.632482000	-0.254671000
C	-4.800741000	-0.808569000	0.312438000
C	-1.780695000	1.347487000	-0.523886000
C	-4.002186000	0.289318000	-0.152489000
C	-2.568075000	0.203772000	-0.122022000
C	-4.643005000	1.476404000	-0.641252000
C	-1.938102000	-1.017823000	0.317442000

C	-3.819460000	2.501742000	-1.209885000
C	-2.769993000	-2.028420000	0.898803000
H	-4.291533000	3.332932000	-1.720240000
H	-2.310461000	-2.867143000	1.405612000
C	-2.460816000	2.443537000	-1.148082000
C	-4.128677000	-1.925841000	0.902632000
H	-1.881664000	3.216832000	-1.635889000
H	-4.715891000	-2.696876000	1.386845000
O	-6.999372000	6.430742000	-0.439844000
O	0.849404000	6.030168000	-0.275454000
O	0.422445000	-6.018099000	0.271025000
O	-7.630449000	-5.370619000	0.070028000
C	-8.558856000	-6.426833000	0.375928000
C	-8.080577000	-7.727843000	-0.284688000
C	-9.107972000	-8.820289000	0.070833000
C	-6.695198000	-8.120621000	0.262362000
C	-8.017013000	-7.552340000	-1.813749000
C	-0.965791000	-6.396214000	0.160794000
C	-1.069224000	-7.927818000	0.180635000
C	-2.564279000	-8.279174000	0.051866000
C	-0.290071000	-8.526582000	-1.005752000
C	-0.518000000	-8.477575000	1.510074000
C	-5.879074000	6.697062000	0.421973000
C	-5.858494000	8.191373000	0.776482000
C	-5.715075000	9.038188000	-0.502331000
C	-7.150891000	8.573363000	1.523018000
C	-4.641369000	8.422667000	1.693051000
C	1.819046000	7.101022000	-0.245314000
C	1.080984000	8.446171000	-0.206413000
C	0.207573000	8.534409000	1.059545000
C	0.209000000	8.609196000	-1.465848000
C	2.158440000	9.548054000	-0.173014000
H	-9.553044000	-6.149748000	0.001664000
H	-8.617662000	-6.548768000	1.465457000
H	-10.107828000	-8.567789000	-0.302804000
H	-9.177500000	-8.967018000	1.155594000
H	-8.814431000	-9.775889000	-0.378151000
H	-6.724709000	-8.259226000	1.350283000
H	-5.947794000	-7.352696000	0.038234000
H	-6.360223000	-9.062526000	-0.187264000
H	-8.999630000	-7.284203000	-2.221474000
H	-7.697932000	-8.485511000	-2.292317000
H	-7.308101000	-6.766648000	-2.094081000
H	-1.520382000	-5.960477000	1.001368000
H	-1.368929000	-5.993617000	-0.776901000
H	-2.697997000	-9.366666000	0.061464000
H	-2.986368000	-7.897893000	-0.885887000
H	-3.147512000	-7.862532000	0.881988000
H	-0.677316000	-8.152939000	-1.961725000
H	-0.382711000	-9.618663000	-1.009388000
H	0.774205000	-8.276655000	-0.948610000

H	-1.068661000	-8.067418000	2.365665000
H	0.540440000	-8.227627000	1.635624000
H	-0.614959000	-9.568863000	1.540107000
H	-4.953296000	6.410486000	-0.094524000
H	-5.972766000	6.091001000	1.332448000
H	-4.790281000	8.790762000	-1.038216000
H	-5.682838000	10.105063000	-0.252388000
H	-6.556568000	8.873991000	-1.182897000
H	-8.034176000	8.404872000	0.898738000
H	-7.130192000	9.632426000	1.804970000
H	-7.265823000	7.983492000	2.440979000
H	-3.703098000	8.161991000	1.187924000
H	-4.710977000	7.825348000	2.610409000
H	-4.582478000	9.477428000	1.984447000
H	2.449785000	7.030311000	-1.140000000
H	2.449775000	6.979225000	0.643987000
H	-0.295676000	9.506824000	1.106620000
H	0.814285000	8.425176000	1.966959000
H	-0.560820000	7.754310000	1.068329000
H	-0.554172000	7.826454000	-1.525088000
H	0.817525000	8.561597000	-2.377351000
H	-0.300322000	9.579582000	-1.452362000
H	2.797998000	9.457721000	0.713339000
H	1.685051000	10.535800000	-0.145212000
H	2.799976000	9.509145000	-1.061659000
H	-7.884769000	0.536058000	-0.206819000
H	8.120607000	-0.274600000	0.206616000

Cartesian coordinates of DFT-optimized structure of **2aox** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

Os	2.165957000	-0.971767000	0.012002000
N	0.967734000	-2.698114000	0.209981000
N	2.712098000	-1.057154000	2.041885000
N	4.116145000	-1.762367000	-0.021330000
N	2.489032000	-1.439216000	-2.013042000
N	2.638744000	1.092842000	-0.192092000
C	1.909142000	-0.694685000	3.066565000
H	0.910073000	-0.376101000	2.798957000
C	2.332769000	-0.721115000	4.389080000
H	1.648063000	-0.415089000	5.171502000
C	3.628852000	-1.146279000	4.676447000
H	3.988756000	-1.180976000	5.698945000
C	4.458984000	-1.533302000	3.627914000
H	5.467733000	-1.874194000	3.826965000
C	3.990732000	-1.484678000	2.315571000
C	4.788791000	-1.890317000	1.145510000
C	6.096848000	-2.378463000	1.146735000
H	6.650773000	-2.489837000	2.070855000
C	6.681954000	-2.729528000	-0.071148000

C	5.965757000	-2.603473000	-1.262090000
H	6.418521000	-2.888547000	-2.203929000
C	4.659573000	-2.111243000	-1.209776000
C	3.733832000	-1.925926000	-2.339593000
C	4.054727000	-2.231511000	-3.661741000
H	5.039300000	-2.613884000	-3.901629000
C	3.109797000	-2.046585000	-4.666804000
H	3.354956000	-2.281586000	-5.696821000
C	1.848790000	-1.560381000	-4.324820000
H	1.078538000	-1.402612000	-5.070819000
C	1.574454000	-1.272842000	-2.994063000
H	0.609674000	-0.891396000	-2.686078000
C	1.409887000	-3.975075000	0.207109000
H	2.485168000	-4.106042000	0.231438000
C	0.573033000	-5.070360000	0.167450000
H	0.973879000	-6.076890000	0.167132000
C	-0.813458000	-4.854716000	0.093247000
C	-1.287137000	-3.536170000	0.107777000
H	-2.342029000	-3.339993000	0.004529000
C	-0.394242000	-2.462726000	0.202910000
C	-5.001180000	3.422595000	-0.459293000
C	-0.762722000	-1.033901000	0.196031000
C	-6.105293000	2.644618000	-0.120943000
C	0.349398000	-0.181875000	0.015913000
C	-5.943756000	1.313961000	0.246417000
C	0.225425000	1.210664000	-0.186617000
C	1.525099000	1.922185000	-0.175889000
C	1.698300000	3.293234000	-0.052885000
H	0.853083000	3.957596000	0.055288000
C	2.986767000	3.861573000	-0.019757000
C	4.097852000	3.011965000	-0.103961000
H	5.116266000	3.375880000	-0.094608000
C	3.863369000	1.646789000	-0.170964000
H	4.697459000	0.955676000	-0.201039000
C	-4.655992000	0.733276000	0.338099000
C	-1.067419000	1.754065000	-0.378511000
C	-3.522603000	1.513214000	-0.063022000
C	-2.208111000	0.935385000	-0.035400000
C	-3.701395000	2.869190000	-0.491747000
C	-2.050669000	-0.447520000	0.337232000
C	-2.567409000	3.581091000	-0.997771000
C	-3.188486000	-1.132285000	0.872819000
H	-2.713318000	4.548685000	-1.462887000
H	-3.053932000	-2.097445000	1.343200000
C	-1.315399000	3.050360000	-0.938769000
C	-4.430432000	-0.571031000	0.876669000
H	-0.495410000	3.599672000	-1.382555000
H	-5.256642000	-1.111980000	1.322368000
O	3.035799000	5.191924000	0.100209000
O	-1.586457000	-5.945945000	0.005670000
C	-3.020721000	-5.805752000	-0.078263000

C	-3.656085000	-7.200004000	-0.175609000
C	-5.181326000	-6.993822000	-0.260626000
C	-3.157643000	-7.920196000	-1.442876000
C	-3.311797000	-8.028279000	1.076737000
C	4.318054000	5.857698000	0.154940000
C	4.092092000	7.365553000	0.328933000
C	3.347095000	7.640280000	1.648992000
C	3.287742000	7.921867000	-0.861308000
C	5.484773000	8.025350000	0.369986000
H	-3.376954000	-5.277897000	0.815561000
H	-3.268034000	-5.208721000	-0.964841000
H	-5.688517000	-7.962178000	-0.335672000
H	-5.457830000	-6.402210000	-1.141827000
H	-5.567402000	-6.481355000	0.628837000
H	-3.404817000	-7.347911000	-2.345591000
H	-3.629103000	-8.905696000	-1.530158000
H	-2.072688000	-8.063998000	-1.417782000
H	-3.671941000	-7.535603000	1.988295000
H	-2.230909000	-8.172939000	1.172954000
H	-3.782504000	-9.016478000	1.020580000
H	4.860466000	5.650668000	-0.775593000
H	4.889910000	5.451142000	0.997968000
H	3.204506000	8.717992000	1.788075000
H	3.913935000	7.262314000	2.508765000
H	2.361011000	7.164632000	1.655718000
H	2.297278000	7.459545000	-0.922995000
H	3.808244000	7.740439000	-1.809721000
H	3.151146000	9.004003000	-0.754431000
H	6.084005000	7.645887000	1.206565000
H	5.383920000	9.109222000	0.495015000
H	6.041944000	7.845059000	-0.557348000
H	-7.095585000	3.079217000	-0.144832000
H	7.697217000	-3.109926000	-0.090914000
N	-5.235725000	4.779349000	-0.803799000
C	-4.587551000	5.896481000	-0.344109000
C	-5.245212000	6.986594000	-0.869972000
C	-6.297899000	6.431625000	-1.635113000
N	-6.302317000	5.102100000	-1.591229000
N	-7.112090000	0.571150000	0.559333000
N	-8.103583000	1.149287000	1.297241000
C	-9.080460000	0.246516000	1.314082000
C	-8.744974000	-0.915457000	0.580023000
C	-7.476582000	-0.669083000	0.102745000
H	-6.826227000	-1.247305000	-0.536184000
H	-9.343756000	-1.799344000	0.416057000
H	-9.992329000	0.458486000	1.857708000
H	-7.049055000	6.947816000	-2.219308000
H	-5.006178000	8.028871000	-0.717710000
H	-3.747036000	5.822495000	0.329325000

Cartesian coordinates of DFT-optimized structure of **3a<sub>ox</sub>** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

C	4.065967000	2.476116000	-0.136506000
C	5.422778000	2.470428000	-0.231096000
C	6.166686000	1.252520000	-0.186931000
C	5.455415000	0.016791000	-0.038811000
C	4.020171000	0.012803000	0.047942000
C	3.307714000	1.272169000	0.026407000
C	6.183763000	-1.218436000	0.014353000
C	5.454331000	-2.448405000	-0.034664000
C	4.096678000	-2.463536000	0.006080000
C	3.331930000	-1.257668000	0.137707000
C	1.899719000	1.220570000	0.139174000
C	1.228847000	-0.009628000	0.236749000
C	1.934804000	-1.221578000	0.284635000
C	7.578196000	1.218079000	-0.278770000
C	8.277673000	0.027389000	-0.131338000
C	7.595084000	-1.174593000	0.034695000
H	3.564942000	3.427251000	-0.216917000
H	5.946502000	3.412106000	-0.336576000
H	3.590005000	-3.409739000	-0.118320000
H	5.993540000	-3.380610000	-0.151782000
N	0.984549000	2.315792000	0.139808000
N	-0.365423000	1.987021000	0.043768000
C	-1.045376000	3.131248000	0.115128000
C	-0.168400000	4.215834000	0.275397000
C	1.096311000	3.668218000	0.299072000
N	1.063892000	-2.343458000	0.448930000
N	-0.294127000	-2.103205000	0.304114000
C	-0.915903000	-3.254942000	0.581848000
C	0.012415000	-4.244895000	0.930457000
C	1.248236000	-3.632328000	0.853388000
N	8.336014000	2.403876000	-0.482521000
N	9.412655000	2.661901000	0.314205000
C	9.951859000	3.765919000	-0.197504000
C	8.217943000	3.322213000	-1.491874000
C	9.245913000	4.226405000	-1.333125000
N	8.367029000	-2.355304000	0.186778000
N	9.478916000	-2.540897000	-0.582232000
C	10.019434000	-3.667094000	-0.125241000
C	9.279535000	-4.216249000	0.948411000
C	8.228922000	-3.343642000	1.126922000
C	-0.095024000	-0.098929000	-2.911658000
C	-0.361185000	-0.192575000	-4.271952000
C	-1.682702000	-0.317859000	-4.695803000
C	-2.696156000	-0.342664000	-3.741397000
C	-2.379089000	-0.247271000	-2.387323000
N	-1.071561000	-0.130809000	-1.979286000
C	-3.383924000	-0.249710000	-1.310457000
N	-2.839780000	-0.155542000	-0.077633000

C	-3.592890000	-0.112160000	1.043390000
C	-4.984338000	-0.183145000	0.951610000
C	-5.567047000	-0.291855000	-0.311667000
C	-4.770748000	-0.321061000	-1.457080000
C	-2.791445000	0.028937000	2.271642000
N	-1.431628000	0.109641000	2.086195000
C	-0.631005000	0.266178000	3.162340000
C	-1.130119000	0.334016000	4.457226000
C	-2.506302000	0.245686000	4.656953000
C	-3.339570000	0.094856000	3.551652000
H	0.917060000	-0.002513000	-2.541263000
H	0.462391000	-0.165614000	-4.975956000
H	-1.924099000	-0.393508000	-5.750379000
H	-3.730934000	-0.438383000	-4.046597000
H	-5.605236000	-0.148830000	1.838173000
H	-5.226239000	-0.390987000	-2.437100000
H	0.430763000	0.329014000	2.963757000
H	-0.441587000	0.455266000	5.285328000
H	-2.927923000	0.295847000	5.654896000
H	-4.412730000	0.028620000	3.682558000
Os	-0.745640000	-0.063962000	0.101224000
H	-2.124194000	3.117811000	0.059050000
H	-0.423015000	5.260057000	0.371643000
H	2.042056000	4.153481000	0.455045000
H	-1.993350000	-3.309336000	0.524419000
H	-0.187814000	-5.267407000	1.210789000
H	2.222753000	-4.019421000	1.094443000
H	10.827935000	4.196931000	0.270179000
H	7.443997000	3.239828000	-2.240555000
H	9.459381000	5.086877000	-1.950181000
H	10.921168000	-4.050333000	-0.585646000
H	9.486826000	-5.112680000	1.514169000
H	7.425486000	-3.326112000	1.847987000
H	9.359407000	0.031419000	-0.155277000
H	-6.646051000	-0.346372000	-0.404116000

Cartesian coordinates of DFT-optimized structure of **4a<sub>ox</sub>** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

Os	1.790862000	-3.056808000	0.026577000
N	-1.561513000	6.817513000	-1.668648000
N	-0.164209000	-3.703618000	0.439352000
N	2.418142000	-3.263811000	2.027576000
N	2.849307000	-4.879283000	0.043162000
N	1.683125000	-3.726837000	-1.968596000
N	-5.213434000	4.776221000	1.374500000
N	3.318876000	-1.677811000	-0.390527000
C	2.157521000	-2.372578000	3.008852000
H	1.583634000	-1.500702000	2.723556000

C	2.593014000	-2.554635000	4.315480000
H	2.353761000	-1.806364000	5.062171000
C	3.326084000	-3.696504000	4.632404000
H	3.679865000	-3.868494000	5.643079000
C	3.599472000	-4.619664000	3.627040000
H	4.168394000	-5.514582000	3.847082000
C	3.141184000	-4.392568000	2.330021000
C	3.385938000	-5.311011000	1.205212000
C	4.087192000	-6.517824000	1.244523000
H	4.524053000	-6.880738000	2.166740000
C	4.217412000	-7.254734000	0.066895000
C	3.655329000	-6.790305000	-1.122771000
H	3.758243000	-7.363526000	-2.035838000
C	2.962899000	-5.577822000	-1.107790000
C	2.300423000	-4.922463000	-2.248347000
C	2.278534000	-5.451185000	-3.538276000
H	2.770472000	-6.394630000	-3.741180000
C	1.625650000	-4.766394000	-4.559366000
H	1.605641000	-5.173556000	-5.564373000
C	1.002768000	-3.555079000	-4.265414000
H	0.481468000	-2.983891000	-5.024838000
C	1.052389000	-3.068292000	-2.965146000
H	0.581902000	-2.131587000	-2.696777000
C	-1.069600000	8.027441000	-1.979649000
C	-0.858471000	-4.839929000	0.531166000
H	-1.685383000	8.637413000	-2.638141000
C	0.142835000	8.522713000	-1.521245000
H	0.496575000	9.508870000	-1.801963000
C	0.908484000	7.718074000	-0.663114000
C	0.414599000	6.451105000	-0.325440000
H	0.949176000	5.802361000	0.355970000
C	-0.816710000	6.040482000	-0.860902000
N	-1.092118000	-2.671681000	0.455158000
C	-1.417027000	4.724837000	-0.488027000
C	-0.580930000	-1.353682000	0.285126000
C	-2.759338000	4.720708000	-0.105964000
C	0.796142000	-1.356019000	0.004989000
C	-3.427794000	3.563460000	0.297921000
C	1.472656000	-0.161536000	-0.294842000
C	-4.875997000	3.695337000	0.633853000
N	2.874086000	-0.364076000	-0.438738000
C	-5.825051000	2.798907000	0.140295000
H	-5.542579000	1.962606000	-0.489158000
C	-7.183051000	2.998377000	0.436863000
C	-7.536242000	4.106643000	1.216700000
H	-8.562623000	4.325679000	1.482448000
C	-6.509978000	4.950799000	1.643776000
C	4.651369000	-1.629686000	-0.449528000
H	-6.759015000	5.824296000	2.244303000
C	-2.710579000	2.342962000	0.374148000
C	0.769779000	1.047450000	-0.450744000

C	-1.341927000	2.298742000	-0.058952000
C	-0.616547000	1.058890000	-0.036461000
C	-0.702693000	3.500847000	-0.515865000
C	-1.292411000	-0.144689000	0.398614000
C	0.620141000	3.402402000	-1.057757000
C	-2.610631000	-0.026872000	0.947009000
H	1.060618000	4.271239000	-1.531578000
H	-3.065220000	-0.876468000	1.438417000
C	1.322659000	2.238536000	-1.023327000
C	-3.280918000	1.156303000	0.939365000
H	2.292973000	2.203695000	-1.500487000
H	-4.261653000	1.210318000	1.395886000
O	2.070148000	8.240673000	-0.218336000
O	-8.045919000	2.094195000	-0.071587000
C	-9.454471000	2.257163000	0.173208000
C	-10.220427000	1.110878000	-0.503138000
C	-11.718277000	1.336825000	-0.219242000
C	-9.777779000	-0.241513000	0.087065000
C	-9.972182000	1.132847000	-2.023290000
C	2.903656000	7.464055000	0.659590000
C	4.156405000	8.277945000	1.016023000
C	4.951671000	8.612224000	-0.260278000
C	3.754594000	9.574160000	1.745022000
C	5.015711000	7.402426000	1.948842000
H	-9.778349000	3.225765000	-0.229544000
H	-9.634096000	2.251887000	1.256245000
H	-12.063334000	2.294469000	-0.627909000
H	-11.928404000	1.330856000	0.857190000
H	-12.314651000	0.541738000	-0.681066000
H	-9.961493000	-0.279794000	1.168031000
H	-8.710699000	-0.417951000	-0.082332000
H	-10.336242000	-1.062412000	-0.377611000
H	-10.289625000	2.087420000	-2.461117000
H	-10.539281000	0.333262000	-2.513929000
H	-8.911898000	0.988941000	-2.254530000
H	3.183465000	6.529451000	0.155604000
H	2.337843000	7.215418000	1.566971000
H	5.255740000	7.698902000	-0.786708000
H	5.859335000	9.172673000	-0.008146000
H	4.357714000	9.219947000	-0.950332000
H	3.127166000	10.208127000	1.110355000
H	4.646250000	10.147857000	2.023245000
H	3.196571000	9.353850000	2.663618000
H	5.319059000	6.470228000	1.456727000
H	4.473953000	7.142200000	2.866436000
H	5.925997000	7.939257000	2.238939000
H	-3.306870000	5.655524000	-0.123229000
H	4.758788000	-8.194251000	0.076186000
C	3.951563000	0.472746000	-0.494649000
C	5.094969000	-0.298603000	-0.517904000
C	-2.349137000	-3.200251000	0.523946000

C	-2.236312000	-4.573640000	0.588022000
H	-0.337358000	-5.786263000	0.542545000
H	5.221800000	-2.547030000	-0.429398000
H	3.839186000	1.542840000	-0.481390000
H	6.113789000	0.053363000	-0.568300000
H	-3.227678000	-2.580082000	0.490150000
H	-3.042181000	-5.287922000	0.657101000

Cartesian coordinates of DFT-optimized structure of **5a<sub>ox</sub>** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

Os	1.883703000	-2.975778000	0.009239000
N	-0.081111000	-3.668440000	0.311749000
N	2.339809000	-3.289725000	2.041168000
N	3.062340000	-4.713196000	-0.004756000
N	1.777721000	-3.636564000	-1.985557000
N	-5.131675000	4.877333000	1.362798000
C	1.882964000	-2.528689000	3.059358000
H	1.204983000	-1.729384000	2.789779000
C	2.261385000	-2.746176000	4.378163000
H	1.869721000	-2.101292000	5.156195000
C	3.134681000	-3.793407000	4.666971000
H	3.447727000	-3.990845000	5.686418000
C	3.598233000	-4.592923000	3.625305000
H	4.270210000	-5.417997000	3.827818000
C	3.194178000	-4.332709000	2.316943000
C	3.611244000	-5.137576000	1.155408000
C	4.462904000	-6.243967000	1.159200000
H	4.912706000	-6.600195000	2.077772000
C	4.724604000	-6.891402000	-0.049617000
C	4.134233000	-6.446144000	-1.233298000
H	4.330065000	-6.958207000	-2.167486000
C	3.288023000	-5.336221000	-1.182871000
C	2.549982000	-4.729951000	-2.304155000
C	2.584165000	-5.219690000	-3.608880000
H	3.194263000	-6.083261000	-3.843992000
C	1.830962000	-4.600512000	-4.602776000
H	1.855730000	-4.976630000	-5.619758000
C	1.044271000	-3.499738000	-4.267412000
H	0.437252000	-2.988536000	-5.005555000
C	1.038773000	-3.050962000	-2.952906000
H	0.442586000	-2.200512000	-2.648411000
C	-0.456839000	-4.965906000	0.370727000
H	0.346551000	-5.692324000	0.384872000
C	-1.771672000	-5.377106000	0.401551000
H	-2.024601000	-6.429453000	0.448900000
C	-2.782394000	-4.402791000	0.335830000
C	-2.409779000	-3.053503000	0.285434000
H	-3.163175000	-2.289467000	0.185303000
C	-1.059029000	-2.687464000	0.310231000

C	-1.336507000	4.788597000	-0.468379000
C	-0.537131000	-1.308685000	0.236878000
C	-2.676230000	4.816557000	-0.092710000
C	0.853841000	-1.281824000	0.003733000
C	-3.353347000	3.657532000	0.285434000
C	1.538117000	-0.084841000	-0.252453000
C	-4.801513000	3.797751000	0.617431000
C	-5.755604000	2.912014000	0.114855000
H	-5.477620000	2.077701000	-0.519052000
C	-7.113442000	3.123060000	0.405820000
C	-7.459176000	4.228401000	1.193238000
H	-8.484217000	4.454753000	1.458057000
C	-6.427303000	5.060850000	1.629690000
H	-6.670917000	5.932178000	2.235446000
C	-2.643289000	2.428993000	0.354054000
C	0.841621000	1.123426000	-0.426853000
C	-1.271712000	2.378097000	-0.063960000
C	-0.553278000	1.133982000	-0.042551000
C	-0.618305000	3.573978000	-0.510698000
C	-1.232217000	-0.072902000	0.360044000
C	0.710725000	3.480165000	-1.035064000
C	-2.548260000	0.055410000	0.909853000
H	1.159311000	4.349133000	-1.501436000
H	-3.005247000	-0.794929000	1.398369000
C	1.408421000	2.313591000	-0.989249000
C	-3.218498000	1.241757000	0.907448000
H	2.387372000	2.275593000	-1.448899000
H	-4.200095000	1.295163000	1.362714000
O	-4.044361000	-4.851782000	0.317615000
O	-7.983454000	2.233128000	-0.115233000
C	-9.391762000	2.418018000	0.116564000
C	-10.173358000	1.296054000	-0.582326000
C	-11.668646000	1.549316000	-0.307459000
C	-9.764675000	-0.072617000	-0.005518000
C	-9.910674000	1.332568000	-2.099626000
C	-5.142024000	-3.916718000	0.257253000
C	-6.463730000	-4.697708000	0.263812000
C	-7.600226000	-3.658526000	0.201543000
C	-6.536427000	-5.623166000	-0.965523000
C	-6.584776000	-5.523633000	1.558605000
H	-9.693076000	3.397846000	-0.276402000
H	-9.582914000	2.401394000	1.197452000
H	-11.990475000	2.519250000	-0.705791000
H	-11.886589000	1.533716000	0.767384000
H	-12.277271000	0.772670000	-0.784029000
H	-9.955010000	-0.118686000	1.074001000
H	-8.701253000	-0.272969000	-0.171696000
H	-10.339944000	-0.874761000	-0.482254000
H	-10.207139000	2.297854000	-2.528419000
H	-10.487140000	0.549179000	-2.605228000
H	-8.850956000	1.172891000	-2.323043000

H	-5.083335000	-3.246550000	1.124149000
H	-5.050851000	-3.320486000	-0.659360000
H	-8.572852000	-4.163142000	0.205518000
H	-7.541112000	-3.052647000	-0.710752000
H	-7.571319000	-2.980688000	1.063307000
H	-6.463300000	-5.048728000	-1.897244000
H	-7.489198000	-6.164672000	-0.978347000
H	-5.727468000	-6.360727000	-0.956194000
H	-6.545469000	-4.878039000	2.444658000
H	-5.778316000	-6.259715000	1.637814000
H	-7.539086000	-6.062305000	1.577680000
H	-3.203407000	5.762232000	-0.097683000
H	5.385338000	-7.750998000	-0.067776000
N	2.952234000	-0.269976000	-0.353222000
C	4.014636000	0.579765000	-0.340384000
C	5.175136000	-0.174313000	-0.352157000
C	4.750733000	-1.508009000	-0.347529000
N	3.412066000	-1.575475000	-0.334342000
N	-0.725437000	6.020353000	-0.829348000
C	0.453658000	6.547768000	-0.372574000
C	0.568851000	7.807540000	-0.919172000
C	-0.604246000	7.966980000	-1.692987000
N	-1.391805000	6.895666000	-1.635515000
H	5.332666000	-2.418379000	-0.344717000
H	6.188725000	0.195623000	-0.356038000
H	3.884606000	1.647350000	-0.292354000
H	1.085693000	6.002422000	0.312177000
H	1.375765000	8.510889000	-0.774318000
H	-0.903997000	8.816950000	-2.292814000

Cartesian coordinates of DFT-optimized structure of **6a<sub>ox</sub>** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

Os	1.841355000	-2.463836000	-0.313701000
N	-0.063457000	-3.210305000	0.185598000
N	2.424576000	-2.505241000	1.709002000
N	3.102170000	-4.138093000	-0.191372000
N	1.667660000	-3.360851000	-2.208633000
C	1.990249000	-1.642866000	2.653784000
H	1.263715000	-0.908722000	2.330597000
C	2.448369000	-1.683248000	3.964524000
H	2.071075000	-0.963068000	4.681160000
C	3.380762000	-2.654526000	4.325313000
H	3.756253000	-2.714472000	5.341046000
C	3.822429000	-3.557229000	3.361440000
H	4.538985000	-4.326702000	3.621730000
C	3.337917000	-3.473680000	2.057120000
C	3.728136000	-4.398279000	0.978271000
C	4.625436000	-5.464449000	1.065677000
H	5.137099000	-5.690198000	1.993278000

C	4.849620000	-6.245575000	-0.069377000
C	4.180274000	-5.968775000	-1.262251000
H	4.345830000	-6.585607000	-2.137045000
C	3.293602000	-4.890300000	-1.297989000
C	2.476353000	-4.449448000	-2.441600000
C	2.475106000	-5.082374000	-3.683813000
H	3.118718000	-5.936924000	-3.853670000
C	1.644976000	-4.615785000	-4.699630000
H	1.641458000	-5.103875000	-5.668132000
C	0.818825000	-3.521510000	-4.448229000
H	0.151208000	-3.127056000	-5.205416000
C	0.853862000	-2.924691000	-3.194466000
H	0.230886000	-2.072272000	-2.955942000
C	-0.367027000	-4.507421000	0.417244000
H	0.472674000	-5.189926000	0.471375000
C	-1.655703000	-4.972314000	0.568952000
H	-1.849792000	-6.022105000	0.753186000
C	-2.718871000	-4.061770000	0.442431000
C	-2.420368000	-2.712620000	0.212838000
H	-3.215687000	-2.001010000	0.061743000
C	-1.091095000	-2.284108000	0.124763000
C	-1.806018000	5.070106000	-1.398715000
C	-0.648343000	-0.899976000	-0.132318000
C	-3.134522000	5.042002000	-0.967919000
C	0.723604000	-0.833069000	-0.453672000
C	-3.697029000	3.895690000	-0.420133000
C	1.327291000	0.360480000	-0.874955000
C	-2.931850000	2.718192000	-0.252085000
C	0.559752000	1.511946000	-1.123992000
C	-1.590352000	2.698373000	-0.756015000
C	-0.809297000	1.496566000	-0.656893000
C	-1.033276000	3.882746000	-1.345758000
C	-1.399036000	0.307343000	-0.092708000
C	0.270355000	3.792639000	-1.935050000
C	-2.683783000	0.428147000	0.529597000
H	0.649038000	4.632583000	-2.504828000
H	-3.061834000	-0.389190000	1.129304000
C	1.029411000	2.668804000	-1.826794000
C	-3.415692000	1.574350000	0.455050000
H	1.980841000	2.633514000	-2.341029000
H	-4.368588000	1.631120000	0.967661000
O	-3.955432000	-4.566533000	0.545406000
C	-5.100648000	-3.697900000	0.411178000
C	-6.380947000	-4.524806000	0.595099000
C	-7.568327000	-3.554574000	0.438455000
C	-6.460786000	-5.623487000	-0.481789000
C	-6.405906000	-5.155417000	2.000491000
H	-5.037891000	-2.908388000	1.170610000
H	-5.079127000	-3.235784000	-0.583722000
H	-8.514188000	-4.094290000	0.559256000
H	-7.574531000	-3.085127000	-0.552783000

H	-7.538004000	-2.758618000	1.192362000
H	-6.457043000	-5.190212000	-1.489614000
H	-7.385153000	-6.201268000	-0.367940000
H	-5.616497000	-6.316261000	-0.406024000
H	-6.358481000	-4.385068000	2.780100000
H	-5.562466000	-5.838151000	2.145338000
H	-7.331575000	-5.723884000	2.145998000
H	5.542961000	-7.077957000	-0.021524000
N	2.741814000	0.231785000	-1.039616000
C	3.757588000	1.125853000	-1.182722000
C	4.953659000	0.429896000	-1.179955000
C	4.600856000	-0.913087000	-1.004185000
N	3.270289000	-1.040925000	-0.905535000
H	5.230066000	-1.788794000	-0.936432000
H	5.944684000	0.843725000	-1.284290000
H	3.575558000	2.184885000	-1.245841000
N	-5.056978000	3.953574000	-0.011429000
N	-5.515166000	5.045535000	0.665463000
C	-6.821708000	4.833066000	0.802505000
C	-7.228423000	3.615593000	0.208454000
C	-6.069654000	3.080577000	-0.311023000
C	-1.288298000	6.373594000	-1.911451000
C	-0.056032000	6.882968000	-1.472411000
C	0.356154000	8.140459000	-1.933249000
C	-0.486512000	8.833675000	-2.816036000
C	-1.691315000	8.245588000	-3.174155000
N	-2.107550000	7.044937000	-2.741285000
O	1.506204000	8.753561000	-1.585419000
C	2.406822000	8.099826000	-0.673959000
C	3.616369000	9.011296000	-0.418465000
C	4.547350000	8.264722000	0.556755000
C	4.360213000	9.287669000	-1.738795000
C	3.153727000	10.336177000	0.217018000
H	-7.427387000	5.560154000	1.328405000
H	-8.221581000	3.193683000	0.159431000
H	-5.887404000	2.182459000	-0.881859000
H	0.541403000	6.318026000	-0.769192000
H	-0.196772000	9.809181000	-3.191280000
H	-2.365763000	8.768903000	-3.849414000
H	2.729388000	7.145473000	-1.110970000
H	1.879782000	7.892965000	0.266526000
H	4.043463000	8.049823000	1.507086000
H	5.431081000	8.874096000	0.777085000
H	4.893208000	7.314103000	0.132623000
H	4.709438000	8.354569000	-2.198145000
H	5.236301000	9.921203000	-1.557960000
H	3.713418000	9.799355000	-2.458564000
H	2.628827000	10.158059000	1.163880000
H	2.476650000	10.880887000	-0.448700000
H	4.015443000	10.980293000	0.427057000
H	-3.740115000	5.935145000	-1.055910000

Cartesian coordinates of DFT-optimized structure of **1box** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

Ru	1.784655000	-3.014718000	0.016152000
N	-1.637184000	6.819290000	-1.660949000
N	-0.174306000	-3.736029000	0.291244000
N	2.249667000	-3.289295000	2.049453000
N	2.904102000	-4.800980000	0.041808000
N	1.758493000	-3.655396000	-1.987596000
N	-5.184153000	4.757752000	1.511248000
N	3.370115000	-1.640525000	-0.282687000
C	1.852450000	-2.465907000	3.038743000
H	1.232331000	-1.628814000	2.744325000
C	2.214314000	-2.667705000	4.366769000
H	1.869104000	-1.972779000	5.123515000
C	3.012512000	-3.762761000	4.688810000
H	3.313183000	-3.949550000	5.714110000
C	3.419844000	-4.623096000	3.671830000
H	4.037760000	-5.483234000	3.899170000
C	3.029476000	-4.374559000	2.356581000
C	3.400140000	-5.236939000	1.216350000
C	4.168939000	-6.402922000	1.259518000
H	4.575858000	-6.774071000	2.192198000
C	4.403042000	-7.089771000	0.067119000
C	3.874373000	-6.622334000	-1.136889000
H	4.055061000	-7.161862000	-2.058443000
C	3.111483000	-5.451671000	-1.119605000
C	2.457739000	-4.800414000	-2.272161000
C	2.516127000	-5.296040000	-3.574165000
H	3.071769000	-6.202103000	-3.783541000
C	1.856976000	-4.624077000	-4.600716000
H	1.898742000	-5.003696000	-5.615908000
C	1.146254000	-3.464471000	-4.300162000
H	0.616016000	-2.907493000	-5.063986000
C	1.119084000	-3.013507000	-2.984441000
H	0.580404000	-2.116180000	-2.708116000
C	-1.148826000	8.025515000	-1.990428000
C	-0.547907000	-5.029694000	0.333366000
H	-1.786400000	8.641465000	-2.622109000
H	0.253847000	-5.757973000	0.370404000
C	0.086415000	8.509880000	-1.583657000
C	-1.865773000	-5.442207000	0.321939000
H	0.437313000	9.492427000	-1.880174000
H	-2.121115000	-6.494511000	0.357635000
C	0.880118000	7.698093000	-0.758434000
C	-2.872012000	-4.467267000	0.225958000
C	0.387343000	6.437376000	-0.396609000
C	-2.496020000	-3.116483000	0.193962000
H	0.942225000	5.785870000	0.265460000

H	-3.243574000	-2.348323000	0.076727000
C	-0.866593000	6.035353000	-0.884344000
C	-1.144979000	-2.760393000	0.263652000
C	-1.458191000	4.720895000	-0.495505000
C	-0.611700000	-1.383939000	0.207611000
C	-2.790683000	4.717562000	-0.076955000
C	0.781238000	-1.341564000	-0.018162000
C	-3.448680000	3.560276000	0.341247000
C	1.485390000	-0.145334000	-0.271068000
C	-4.883673000	3.695176000	0.729219000
C	2.955010000	-0.320991000	-0.298677000
C	-5.857645000	2.821275000	0.244036000
C	3.898848000	0.696063000	-0.238812000
H	-5.604376000	2.000235000	-0.417259000
H	3.604600000	1.732481000	-0.158744000
C	-7.203141000	3.026683000	0.590523000
C	5.275770000	0.402695000	-0.237248000
C	-7.517343000	4.113227000	1.416310000
C	5.676282000	-0.938553000	-0.284349000
H	-8.531171000	4.333482000	1.725676000
H	6.714951000	-1.240258000	-0.294286000
C	-6.468617000	4.935164000	1.831796000
C	4.683302000	-1.909698000	-0.287692000
H	-6.687996000	5.792380000	2.466386000
H	4.955803000	-2.958962000	-0.286641000
C	-2.732847000	2.335798000	0.387472000
C	0.742571000	1.046650000	-0.459917000
C	-1.374307000	2.294973000	-0.072347000
C	-0.646284000	1.056343000	-0.061991000
C	-0.744657000	3.496923000	-0.539066000
C	-1.310714000	-0.155590000	0.351026000
C	0.567440000	3.393958000	-1.105384000
C	-2.617205000	-0.041885000	0.926182000
H	0.996087000	4.257098000	-1.600485000
H	-3.059858000	-0.902874000	1.410222000
C	1.276680000	2.232826000	-1.060418000
C	-3.289568000	1.143030000	0.950116000
H	2.244251000	2.191801000	-1.543806000
H	-4.260862000	1.190520000	1.427825000
O	2.067369000	8.206800000	-0.368115000
O	6.098552000	1.457158000	-0.181702000
O	-4.134573000	-4.912092000	0.164071000
O	-8.093928000	2.150353000	0.081194000
C	-9.491401000	2.324988000	0.377297000
C	-10.300354000	1.231623000	-0.335345000
C	-11.782430000	1.459388000	0.020839000
C	-9.857144000	-0.159855000	0.154993000
C	-10.109918000	1.342570000	-1.859919000
C	-5.222896000	-3.972747000	0.035888000
C	-6.547772000	-4.746162000	-0.024585000
C	-7.671222000	-3.700372000	-0.165382000

C	-6.556489000	-5.686204000	-1.244918000
C	-6.748303000	-5.555383000	1.270827000
C	2.927563000	7.422639000	0.476979000
C	4.237862000	8.188598000	0.712668000
C	4.958980000	8.423834000	-0.628095000
C	3.948090000	9.534982000	1.402664000
C	5.115446000	7.313818000	1.629183000
C	7.527513000	1.245280000	-0.156617000
C	8.233591000	2.603882000	-0.049456000
C	7.818602000	3.314002000	1.253130000
C	7.884639000	3.480810000	-1.266851000
C	9.748818000	2.321270000	-0.027742000
H	-9.808438000	3.319176000	0.036358000
H	-9.637832000	2.265179000	1.463734000
H	-12.128079000	2.445442000	-0.312568000
H	-11.950185000	1.387869000	1.102368000
H	-12.408583000	0.703037000	-0.465787000
H	-9.993438000	-0.258966000	1.239095000
H	-8.802165000	-0.343763000	-0.072601000
H	-10.451062000	-0.942723000	-0.330878000
H	-10.435299000	2.323840000	-2.227212000
H	-10.702000000	0.577557000	-2.375445000
H	-9.060474000	1.206518000	-2.140283000
H	-5.210124000	-3.294618000	0.898517000
H	-5.077468000	-3.384917000	-0.879001000
H	-8.646314000	-4.198272000	-0.209077000
H	-7.555560000	-3.109108000	-1.081847000
H	-7.686174000	-3.008969000	0.685981000
H	-6.423729000	-5.124116000	-2.177580000
H	-7.511666000	-6.220003000	-1.307113000
H	-5.755878000	-6.429799000	-1.178706000
H	-6.755852000	-4.899096000	2.149832000
H	-5.951943000	-6.294539000	1.405046000
H	-7.705146000	-6.089150000	1.241820000
H	3.130833000	6.459900000	-0.009680000
H	2.416155000	7.231282000	1.429665000
H	5.184027000	7.473101000	-1.127398000
H	5.906568000	8.950189000	-0.465488000
H	4.347362000	9.026921000	-1.306783000
H	3.309493000	10.170238000	0.780628000
H	4.882870000	10.074918000	1.593194000
H	3.444362000	9.385013000	2.365626000
H	5.337480000	6.344090000	1.166763000
H	4.626099000	7.127209000	2.592903000
H	6.069402000	7.814553000	1.829741000
H	7.822293000	0.724506000	-1.076130000
H	7.775135000	0.612510000	0.704450000
H	8.346201000	4.269746000	1.349052000
H	8.064098000	2.704386000	2.131513000
H	6.742746000	3.516930000	1.270268000
H	6.809241000	3.679759000	-1.318053000

H	8.186208000	2.995681000	-2.203317000
H	8.405101000	4.443351000	-1.204366000
H	10.027011000	1.691060000	0.825728000
H	10.306019000	3.261084000	0.054730000
H	10.076140000	1.816620000	-0.944804000
H	-3.336144000	5.653720000	-0.077287000
H	4.997789000	-7.996647000	0.077042000

Cartesian coordinates of DFT-optimized structure of **2box** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

Ru	1.918634000	-1.340919000	-0.028594000
N	0.442683000	-2.826641000	0.119495000
N	2.389380000	-1.556379000	2.011970000
N	3.695080000	-2.470973000	-0.038243000
N	2.196990000	-1.818291000	-2.057014000
N	2.780904000	0.588128000	-0.195738000
C	1.639333000	-1.076763000	3.022912000
H	0.720130000	-0.578608000	2.742615000
C	2.016081000	-1.204468000	4.355930000
H	1.377281000	-0.796618000	5.130720000
C	3.208169000	-1.857826000	4.659221000
H	3.531590000	-1.975413000	5.687868000
C	3.983117000	-2.366687000	3.619365000
H	4.910344000	-2.884425000	3.832876000
C	3.560983000	-2.208933000	2.300079000
C	4.304223000	-2.730373000	1.135172000
C	5.507893000	-3.439578000	1.154149000
H	6.015985000	-3.660140000	2.084872000
C	6.047504000	-3.867185000	-0.060325000
C	5.392280000	-3.597108000	-1.262638000
H	5.810431000	-3.939435000	-2.201264000
C	4.191833000	-2.882817000	-1.220922000
C	3.339425000	-2.510920000	-2.367507000
C	3.636605000	-2.840914000	-3.689236000
H	4.542751000	-3.388176000	-3.919315000
C	2.763856000	-2.467041000	-4.708357000
H	2.988828000	-2.719822000	-5.738903000
C	1.602507000	-1.770975000	-4.381087000
H	0.891665000	-1.461804000	-5.138593000
C	1.352996000	-1.467747000	-3.046610000
H	0.463663000	-0.926958000	-2.749170000
C	0.652982000	-4.157300000	0.077386000
H	1.688134000	-4.477992000	0.083908000
C	-0.366231000	-5.086614000	0.024114000
H	-0.151929000	-6.148289000	-0.002566000
C	-1.692597000	-4.625895000	-0.022849000
C	-1.923869000	-3.243724000	0.016749000
H	-2.927237000	-2.859959000	-0.074760000
C	-0.850281000	-2.352660000	0.125005000

C	-4.285386000	4.304590000	-0.330453000
C	-0.947697000	-0.879712000	0.152591000
C	-5.512235000	3.736748000	0.002239000
C	0.299023000	-0.242789000	-0.017719000
C	-5.599599000	2.388380000	0.328763000
C	0.439236000	1.150316000	-0.183377000
C	1.847811000	1.609733000	-0.162308000
C	2.275255000	2.923137000	-0.023147000
H	1.572028000	3.734334000	0.097585000
C	3.648613000	3.236068000	0.002048000
C	4.577300000	2.191916000	-0.094075000
H	5.646298000	2.355612000	-0.086816000
C	4.085823000	0.896031000	-0.172050000
H	4.774538000	0.060029000	-0.211902000
C	-4.442591000	1.575119000	0.386059000
C	-0.732974000	1.929493000	-0.349311000
C	-3.187051000	2.141746000	-0.008684000
C	-2.003132000	1.328934000	-0.013260000
C	-3.112403000	3.519139000	-0.397569000
C	-2.103275000	-0.068742000	0.322348000
C	-1.869958000	4.020970000	-0.900300000
C	-3.345322000	-0.546030000	0.851697000
H	-1.836022000	5.012021000	-1.336993000
H	-3.389627000	-1.532921000	1.293227000
C	-0.738597000	3.264256000	-0.872547000
C	-4.460786000	0.235980000	0.885313000
H	0.165758000	3.664181000	-1.312190000
H	-5.370776000	-0.154442000	1.325076000
O	3.951473000	4.533072000	0.123955000
O	-2.648171000	-5.560810000	-0.110111000
C	-4.037867000	-5.171683000	-0.139187000
C	-4.910590000	-6.434224000	-0.171618000
C	-6.378355000	-5.964956000	-0.207837000
C	-4.598167000	-7.262321000	-1.432456000
C	-4.665824000	-7.278404000	1.093560000
C	5.338061000	4.941370000	0.142662000
C	5.410143000	6.467983000	0.281700000
C	4.756687000	6.910062000	1.604816000
C	4.706326000	7.142617000	-0.911006000
C	6.904534000	6.846267000	0.286497000
H	-4.257406000	-4.575245000	0.755125000
H	-4.215373000	-4.556158000	-1.029900000
H	-7.049656000	-6.830774000	-0.227288000
H	-6.584839000	-5.360975000	-1.099722000
H	-6.630197000	-5.365725000	0.675585000
H	-4.775745000	-6.677276000	-2.343346000
H	-5.239535000	-8.150159000	-1.473240000
H	-3.555665000	-7.596487000	-1.440648000
H	-4.890753000	-6.704260000	2.000951000
H	-3.625529000	-7.614252000	1.152746000
H	-5.309475000	-8.165456000	1.089318000

H	5.812793000	4.613945000	-0.790378000
H	5.837849000	4.451251000	0.987027000
H	4.825807000	7.997962000	1.718270000
H	5.257042000	6.449538000	2.465685000
H	3.698198000	6.632284000	1.637975000
H	3.644244000	6.879591000	-0.947004000
H	5.164082000	6.842229000	-1.861568000
H	4.783074000	8.232930000	-0.830774000
H	7.435396000	6.375709000	1.122993000
H	7.018212000	7.931504000	0.385941000
H	7.398154000	6.541910000	-0.644419000
H	-6.403740000	4.349488000	0.006280000
H	6.981157000	-4.418965000	-0.069045000
N	-4.264615000	5.691212000	-0.632049000
C	-3.414552000	6.652373000	-0.149194000
C	-3.862986000	7.862542000	-0.630504000
C	-5.008901000	7.538829000	-1.394612000
N	-5.260693000	6.232653000	-1.391395000
N	-6.883377000	1.867276000	0.636392000
N	-7.742031000	2.595382000	1.407214000
C	-8.869215000	1.889035000	1.414067000
C	-8.763317000	0.708845000	0.641019000
C	-7.476531000	0.730878000	0.150142000
H	-6.951629000	0.062917000	-0.516094000
H	-9.517536000	-0.043241000	0.461583000
H	-9.719896000	2.248867000	1.978719000
H	-5.656717000	8.204851000	-1.950238000
H	-3.432226000	8.836562000	-0.450496000
H	-2.595502000	6.401011000	0.507723000

Cartesian coordinates of DFT-optimized structure of **3box** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

C	2.339396000	-2.461287000	-0.334656000
C	3.697547000	-2.452446000	-0.269761000
C	4.427820000	-1.234003000	-0.117720000
C	3.701018000	-0.001318000	-0.030661000
C	2.264554000	-0.002821000	-0.083875000
C	1.566537000	-1.256903000	-0.270203000
C	4.413823000	1.234978000	0.118711000
C	3.672716000	2.426173000	0.399440000
C	2.314221000	2.427720000	0.393465000
C	1.560600000	1.251692000	0.070361000
C	0.157356000	-1.207741000	-0.344818000
C	-0.528766000	0.008616000	-0.198536000
C	0.158994000	1.221758000	-0.044128000
C	5.840086000	-1.195467000	-0.051508000
C	6.523027000	0.013520000	-0.002722000
C	5.824967000	1.216047000	0.060148000
H	1.847588000	-3.418351000	-0.405930000

H	4.233745000	-3.390405000	-0.339062000
H	1.799846000	3.329777000	0.691958000
H	4.204675000	3.331528000	0.665371000
N	-0.740027000	-2.300181000	-0.526543000
N	-2.081131000	-2.022645000	-0.313422000
C	-2.752716000	-3.137835000	-0.591157000
C	-1.873206000	-4.153150000	-1.005232000
C	-0.616493000	-3.588523000	-0.966134000
N	-0.724689000	2.337612000	0.022317000
N	-2.067661000	2.045856000	0.172345000
C	-2.717275000	3.209765000	0.124398000
C	-1.818200000	4.269899000	-0.077736000
C	-0.571899000	3.683041000	-0.154862000
N	6.615941000	-2.386586000	-0.074902000
N	7.677078000	-2.483550000	-0.926532000
C	8.241179000	-3.651422000	-0.628047000
C	6.532353000	-3.469557000	0.759715000
C	7.567225000	-4.315223000	0.423317000
N	6.580763000	2.415804000	0.102669000
N	7.708625000	2.478107000	0.868401000
C	8.226387000	3.675110000	0.607161000
C	7.455524000	4.395231000	-0.335768000
C	6.410127000	3.553141000	-0.643899000
C	-1.732716000	-0.424866000	2.965297000
C	-1.959981000	-0.581800000	4.328760000
C	-3.271711000	-0.592217000	4.796212000
C	-4.314220000	-0.448079000	3.883662000
C	-4.031007000	-0.295398000	2.527127000
N	-2.736266000	-0.281192000	2.079151000
C	-5.066884000	-0.145673000	1.486798000
N	-4.558441000	-0.002173000	0.248063000
C	-5.335903000	0.138523000	-0.842553000
C	-6.726868000	0.145580000	-0.712073000
C	-7.276552000	0.000548000	0.562264000
C	-6.450979000	-0.149171000	1.677136000
C	-4.562298000	0.263187000	-2.093538000
N	-3.200226000	0.206256000	-1.953504000
C	-2.422619000	0.298088000	-3.049024000
C	-2.950968000	0.457554000	-4.326085000
C	-4.333485000	0.521707000	-4.479649000
C	-5.143521000	0.421697000	-3.350797000
H	-0.728622000	-0.408787000	2.561586000
H	-1.115263000	-0.691914000	4.998832000
H	-3.484634000	-0.710781000	5.853086000
H	-5.342387000	-0.452284000	4.224324000
H	-7.371084000	0.257016000	-1.575353000
H	-6.881536000	-0.268384000	2.663668000
H	-1.354106000	0.244651000	-2.885861000
H	-2.279759000	0.528373000	-5.174070000
H	-4.778956000	0.645973000	-5.460733000
H	-6.221475000	0.466603000	-3.447060000

Ru	-2.470085000	-0.002339000	0.011055000
H	-3.828498000	-3.156546000	-0.491790000
H	-2.121918000	-5.160099000	-1.303064000
H	0.328616000	-4.010217000	-1.256096000
H	-3.792554000	3.230612000	0.228600000
H	-2.047062000	5.320736000	-0.165733000
H	0.387125000	4.126595000	-0.358091000
H	9.111380000	-3.979664000	-1.182122000
H	5.775317000	-3.532009000	1.527363000
H	7.805374000	-5.267033000	0.875050000
H	9.134694000	3.983650000	1.108895000
H	7.640029000	5.380690000	-0.737584000
H	5.590213000	3.652270000	-1.339368000
H	7.605023000	0.020780000	-0.003253000
H	-8.353873000	0.000966000	0.686591000

Cartesian coordinates of DFT-optimized structure of **4box** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

Ru	3.823308000	-0.349980000	0.002511000
N	-6.109727000	2.687708000	-1.779831000
N	3.212639000	-2.284486000	0.516991000
N	4.363873000	0.125382000	1.980829000
N	5.915388000	-0.559277000	0.013458000
N	4.277743000	-0.935575000	-1.967944000
N	-6.603466000	-1.327749000	1.440217000
N	3.624172000	1.668640000	-0.517449000
C	3.493849000	0.472931000	2.948277000
H	2.449096000	0.503023000	2.666905000
C	3.901692000	0.777712000	4.242985000
H	3.158934000	1.051486000	4.983307000
C	5.258076000	0.721127000	4.553185000
H	5.610257000	0.951609000	5.552859000
C	6.162978000	0.361651000	3.557170000
H	7.222894000	0.311154000	3.774213000
C	5.700847000	0.066759000	2.275260000
C	6.583435000	-0.321367000	1.157899000
C	7.973922000	-0.452645000	1.194840000
H	8.531788000	-0.266711000	2.104404000
C	8.637694000	-0.831442000	0.027311000
C	7.923786000	-1.074113000	-1.146887000
H	8.442551000	-1.368497000	-2.050840000
C	6.534402000	-0.928190000	-1.124068000
C	5.603083000	-1.141550000	-2.249130000
C	6.009445000	-1.531489000	-3.524564000
H	7.060720000	-1.690229000	-3.731906000
C	5.060289000	-1.715714000	-4.527233000
H	5.369326000	-2.019065000	-5.521716000
C	3.716264000	-1.504885000	-4.230027000
H	2.940493000	-1.635922000	-4.975519000

C	3.364843000	-1.115868000	-2.941347000
H	2.331719000	-0.941932000	-2.669318000
C	-6.797438000	3.784611000	-2.135481000
C	3.727045000	-3.505746000	0.655941000
H	-7.657016000	3.619295000	-2.782502000
C	-6.478575000	5.074363000	-1.735064000
H	-7.067138000	5.929131000	-2.050348000
C	-5.372359000	5.254487000	-0.890132000
C	-4.639604000	4.123460000	-0.506563000
H	-3.796753000	4.201302000	0.167592000
C	-5.038330000	2.865162000	-0.985213000
N	1.837147000	-2.431058000	0.538371000
C	-4.328560000	1.621453000	-0.561368000
C	1.076649000	-1.250744000	0.317857000
C	-5.115040000	0.552977000	-0.127691000
C	1.887158000	-0.154311000	-0.016359000
C	-4.573414000	-0.650700000	0.327468000
C	1.321530000	1.080381000	-0.371155000
C	-5.532992000	-1.726099000	0.714903000
N	2.306650000	2.085968000	-0.566315000
C	-5.369690000	-3.042206000	0.280174000
H	-4.529072000	-3.335703000	-0.338378000
C	-6.331403000	-4.006598000	0.622301000
C	-7.433349000	-3.603056000	1.386494000
H	-8.215338000	-4.289760000	1.684802000
C	-7.508808000	-2.258460000	1.753434000
C	4.373896000	2.765205000	-0.625336000
H	-8.359978000	-1.917399000	2.340637000
C	-3.164495000	-0.788029000	0.403933000
C	-0.070253000	1.217738000	-0.527994000
C	-2.324131000	0.270672000	-0.081469000
C	-0.895404000	0.126118000	-0.059018000
C	-2.919278000	1.474506000	-0.590356000
C	-0.319489000	-1.107222000	0.430822000
C	-2.061840000	2.458462000	-1.182466000
C	-1.188546000	-2.077377000	1.027330000
H	-2.506045000	3.304097000	-1.693331000
H	-0.767439000	-2.922406000	1.555227000
C	-0.707584000	2.340043000	-1.149753000
C	-2.539524000	-1.921728000	1.018303000
H	-0.108432000	3.079771000	-1.663922000
H	-3.159415000	-2.660463000	1.511415000
O	-5.105761000	6.518783000	-0.501881000
O	-6.111077000	-5.258346000	0.169492000
C	-7.073820000	-6.287216000	0.461363000
C	-6.600757000	-7.611174000	-0.156250000
C	-7.667282000	-8.673074000	0.175621000
C	-5.247905000	-8.025407000	0.453171000
C	-6.471934000	-7.466197000	-1.684419000
C	-3.981618000	6.770887000	0.359224000
C	-3.895624000	8.276817000	0.648296000

C	-3.703228000	9.058180000	-0.665316000
C	-5.174150000	8.751166000	1.364847000
C	-2.675691000	8.493473000	1.564764000
H	-8.047050000	-5.995270000	0.045551000
H	-7.175008000	-6.386490000	1.550006000
H	-8.643838000	-8.405326000	-0.246024000
H	-7.786893000	-8.797414000	1.258735000
H	-7.377132000	-9.643643000	-0.242604000
H	-5.325461000	-8.147554000	1.540713000
H	-4.475362000	-7.276833000	0.249934000
H	-4.915241000	-8.980753000	0.030926000
H	-7.430178000	-7.180288000	-2.135724000
H	-6.159847000	-8.416605000	-2.132735000
H	-5.730919000	-6.705415000	-1.949880000
H	-3.065293000	6.421882000	-0.135023000
H	-4.110287000	6.208646000	1.293368000
H	-2.789913000	8.740437000	-1.183587000
H	-3.617552000	10.131739000	-0.461252000
H	-4.548633000	8.907713000	-1.344241000
H	-6.060450000	8.590476000	0.742700000
H	-5.108794000	9.821132000	1.593939000
H	-5.319866000	8.213491000	2.310054000
H	-1.747361000	8.166830000	1.080293000
H	-2.779587000	7.942750000	2.507687000
H	-2.569799000	9.556645000	1.808491000
H	-6.192930000	0.661721000	-0.144650000
H	9.716863000	-0.938829000	0.032602000
C	2.265678000	3.446949000	-0.672891000
C	3.563877000	3.909921000	-0.728287000
C	1.524882000	-3.755191000	0.659907000
C	2.703677000	-4.465324000	0.751906000
H	4.799259000	-3.638859000	0.671492000
H	5.451315000	2.683374000	-0.614150000
H	1.335956000	3.989028000	-0.670321000
H	3.883402000	4.936417000	-0.821564000
H	0.506905000	-4.103229000	0.640993000
H	2.810741000	-5.533250000	0.864004000

Cartesian coordinates of DFT-optimized structure of **5box** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

Ru	3.512508000	0.038942000	0.008739000
N	2.333041000	-1.671329000	0.272136000
N	4.091112000	-0.000304000	2.031093000
N	5.477444000	-0.697434000	-0.051659000
N	3.782630000	-0.489703000	-2.008322000
N	-6.711598000	2.330284000	1.535086000
C	3.292682000	0.335511000	3.062199000
H	2.274635000	0.604801000	2.811380000
C	3.741984000	0.344812000	4.378758000

H	3.059817000	0.627220000	5.172201000
C	5.062050000	-0.013256000	4.641948000
H	5.444483000	-0.018332000	5.656939000
C	5.890085000	-0.373093000	3.580703000
H	6.917637000	-0.662914000	3.763837000
C	5.390523000	-0.362640000	2.279468000
C	6.182873000	-0.748350000	1.094476000
C	7.521414000	-1.148141000	1.071571000
H	8.109033000	-1.196647000	1.980051000
C	8.093074000	-1.488049000	-0.155860000
C	7.338966000	-1.436541000	-1.329280000
H	7.785537000	-1.707712000	-2.278111000
C	6.004353000	-1.030880000	-1.245300000
C	5.035900000	-0.926222000	-2.354682000
C	5.333215000	-1.262006000	-3.674563000
H	6.326161000	-1.608593000	-3.933960000
C	4.348269000	-1.154681000	-4.653936000
H	4.572918000	-1.413072000	-5.683176000
C	3.076802000	-0.718124000	-4.289288000
H	2.277680000	-0.622885000	-5.015257000
C	2.831948000	-0.398876000	-2.957719000
H	1.858907000	-0.055553000	-2.630017000
C	2.788417000	-2.940458000	0.282221000
H	3.865408000	-3.060479000	0.288120000
C	1.960760000	-4.044304000	0.275095000
H	2.369149000	-5.047716000	0.284611000
C	0.571668000	-3.840712000	0.220504000
C	0.085267000	-2.525831000	0.219445000
H	-0.972835000	-2.341202000	0.129944000
C	0.972193000	-1.445531000	0.281113000
C	-3.575653000	4.524508000	-0.230641000
C	0.601404000	-0.015509000	0.260871000
C	-4.682023000	3.758517000	0.122880000
C	1.716749000	0.818023000	0.046432000
C	-4.562981000	2.406331000	0.444868000
C	1.586670000	2.197729000	-0.156057000
C	-5.823888000	1.671219000	0.755661000
C	-6.094530000	0.419053000	0.202442000
H	-5.390229000	-0.074452000	-0.457565000
C	-7.322904000	-0.204746000	0.476201000
C	-8.237911000	0.464363000	1.298628000
H	-9.203574000	0.046221000	1.553052000
C	-7.873333000	1.720833000	1.785128000
H	-8.571222000	2.265597000	2.418892000
C	-3.273922000	1.811707000	0.479933000
C	0.316826000	2.788219000	-0.294649000
C	-2.128428000	2.579089000	0.083175000
C	-0.823568000	1.978385000	0.070047000
C	-2.288198000	3.949501000	-0.307816000
C	-0.677445000	0.585932000	0.418300000
C	-1.153687000	4.660330000	-0.814681000

C	-1.821833000	-0.092224000	0.949400000
H	-1.292790000	5.646798000	-1.240487000
H	-1.699780000	-1.069485000	1.397267000
C	0.089591000	4.108418000	-0.802753000
C	-3.053675000	0.488540000	0.979082000
H	0.907872000	4.659607000	-1.247447000
H	-3.882794000	-0.052559000	1.418841000
O	-0.191633000	-4.939782000	0.164700000
O	-7.522723000	-1.410819000	-0.094404000
C	-8.777443000	-2.083004000	0.118068000
C	-8.772537000	-3.419027000	-0.639019000
C	-10.137172000	-4.087869000	-0.382148000
C	-7.643733000	-4.323693000	-0.109445000
C	-8.590988000	-3.172209000	-2.148552000
C	-1.629068000	-4.818694000	0.111545000
C	-2.246760000	-6.223268000	0.062530000
C	-3.776266000	-6.039894000	0.011874000
C	-1.769230000	-6.966403000	-1.199505000
C	-1.859805000	-7.016892000	1.324943000
H	-9.592220000	-1.441163000	-0.241704000
H	-8.915822000	-2.253216000	1.193710000
H	-10.963270000	-3.465771000	-0.747615000
H	-10.297725000	-4.272770000	0.686990000
H	-10.188959000	-5.051958000	-0.900383000
H	-7.763973000	-4.517544000	0.963712000
H	-6.661307000	-3.865818000	-0.263852000
H	-7.653676000	-5.289366000	-0.628110000
H	-9.393991000	-2.538038000	-2.544203000
H	-8.612748000	-4.122007000	-2.695406000
H	-7.635565000	-2.680739000	-2.358413000
H	-1.970715000	-4.275542000	1.001633000
H	-1.904404000	-4.245027000	-0.782289000
H	-4.271917000	-7.016503000	-0.022890000
H	-4.084157000	-5.476367000	-0.877241000
H	-4.145778000	-5.508304000	0.897216000
H	-2.047791000	-6.419807000	-2.108939000
H	-2.226846000	-7.960906000	-1.251572000
H	-0.681846000	-7.093289000	-1.198463000
H	-2.201836000	-6.506101000	2.233516000
H	-0.775214000	-7.147659000	1.395831000
H	-2.320942000	-8.010960000	1.304763000
H	-5.658564000	4.225567000	0.145164000
H	9.131155000	-1.799189000	-0.197416000
N	2.842359000	2.869223000	-0.240842000
C	3.218142000	4.176327000	-0.161402000
C	4.599781000	4.228446000	-0.180308000
C	5.019529000	2.892174000	-0.248388000
N	3.965879000	2.069321000	-0.272825000
N	-3.790475000	5.896518000	-0.533509000
C	-3.126721000	6.988127000	-0.038360000
C	-3.765165000	8.104803000	-0.532619000

C	-4.823593000	7.590169000	-1.317088000
N	-4.848348000	6.259573000	-1.314142000
H	-2.288745000	6.879605000	0.633776000
H	-3.510263000	9.138070000	-0.347786000
H	-5.565056000	8.135515000	-1.887095000
H	6.020106000	2.484619000	-0.273387000
H	5.216469000	5.113123000	-0.142816000
H	2.495979000	4.969185000	-0.066560000

Cartesian coordinates of DFT-optimized structure of **6box** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 2

Ru	-2.671352000	-1.551615000	-0.037221000
N	-3.353087000	0.404798000	0.280176000
N	-2.935753000	-2.008415000	1.998456000
N	-4.424501000	-2.706193000	-0.011491000
N	-3.358485000	-1.455961000	-2.022089000
C	-2.139997000	-1.566610000	2.991113000
H	-1.333514000	-0.905681000	2.700058000
C	-2.331207000	-1.936465000	4.318402000
H	-1.659139000	-1.556320000	5.078958000
C	-3.387825000	-2.787156000	4.634813000
H	-3.566206000	-3.094134000	5.659748000
C	-4.222292000	-3.237873000	3.614178000
H	-5.055349000	-3.892875000	3.838817000
C	-3.984514000	-2.839397000	2.299719000
C	-4.825641000	-3.245089000	1.155926000
C	-5.942987000	-4.083105000	1.189136000
H	-6.284750000	-4.527602000	2.115801000
C	-6.620706000	-4.335829000	-0.004818000
C	-6.191430000	-3.758384000	-1.200710000
H	-6.726254000	-3.949888000	-2.122865000
C	-5.066052000	-2.930419000	-1.174133000
C	-4.462069000	-2.215390000	-2.316049000
C	-4.964730000	-2.267670000	-3.615377000
H	-5.835659000	-2.873334000	-3.834727000
C	-4.344679000	-1.536453000	-4.626257000
H	-4.729920000	-1.572881000	-5.639539000
C	-3.232448000	-0.758469000	-4.313298000
H	-2.720443000	-0.168707000	-5.064771000
C	-2.771140000	-0.742058000	-3.001084000
H	-1.909112000	-0.153514000	-2.713605000
C	-4.644892000	0.782749000	0.363499000
H	-5.375419000	-0.016939000	0.400136000
C	-5.050090000	2.101611000	0.392921000
H	-6.099807000	2.360596000	0.461782000
C	-4.073009000	3.106578000	0.295592000
C	-2.725800000	2.726567000	0.216426000
H	-1.958992000	3.473914000	0.091677000
C	-2.371983000	1.373548000	0.247802000

C	5.119478000	1.570749000	-0.610517000
C	-0.999772000	0.835433000	0.152222000
C	5.134587000	2.922190000	-0.259160000
C	-0.988380000	-0.553565000	-0.083132000
C	3.980554000	3.581919000	0.147344000
C	0.195497000	-1.252582000	-0.350967000
C	2.747976000	2.896874000	0.247661000
C	1.411370000	-0.566795000	-0.533815000
C	2.691047000	1.530050000	-0.179359000
C	1.439535000	0.825663000	-0.148624000
C	3.886033000	0.871000000	-0.624799000
C	0.242360000	1.516094000	0.266204000
C	3.767819000	-0.458873000	-1.145778000
C	0.384836000	2.828904000	0.822508000
H	4.629410000	-0.918714000	-1.614300000
H	-0.459343000	3.288990000	1.318837000
C	2.593881000	-1.145316000	-1.098006000
C	1.576350000	3.488009000	0.815457000
H	2.544636000	-2.124068000	-1.556959000
H	1.645897000	4.466266000	1.276038000
O	-4.513732000	4.371267000	0.279047000
C	-3.572117000	5.460449000	0.171438000
C	-4.336927000	6.790880000	0.208558000
C	-3.288332000	7.914158000	0.087395000
C	-5.322165000	6.868756000	-0.973155000
C	-5.095065000	6.928464000	1.542582000
H	-2.863034000	5.399859000	1.006476000
H	-3.020310000	5.358661000	-0.771372000
H	-3.780581000	8.892835000	0.108217000
H	-2.728312000	7.840651000	-0.852811000
H	-2.569755000	7.882753000	0.915347000
H	-4.796662000	6.783113000	-1.932333000
H	-5.851354000	7.828513000	-0.964544000
H	-6.068831000	6.069737000	-0.921710000
H	-4.406098000	6.883697000	2.395090000
H	-5.836926000	6.132390000	1.662815000
H	-5.619326000	7.890004000	1.584505000
H	-7.491330000	-4.982552000	-0.002081000
N	-0.000025000	-2.662542000	-0.442246000
C	0.842011000	-3.733813000	-0.425826000
C	0.074784000	-4.883744000	-0.417420000
C	-1.255718000	-4.440761000	-0.404287000
N	-1.306646000	-3.104793000	-0.407084000
H	-2.171242000	-5.014447000	-0.386488000
H	0.431744000	-5.902058000	-0.414486000
H	1.911367000	-3.615168000	-0.391254000
N	4.086596000	4.958885000	0.482046000
N	5.139721000	5.394704000	1.231366000
C	4.998062000	6.717178000	1.274209000
C	3.867216000	7.155521000	0.546411000
C	3.309428000	5.999486000	0.045263000

C	6.428599000	0.949767000	-0.972185000
C	6.817687000	-0.283645000	-0.426253000
C	8.081639000	-0.794936000	-0.749682000
C	8.902558000	-0.045309000	-1.606439000
C	8.426929000	1.170552000	-2.076594000
N	7.221664000	1.680236000	-1.777151000
O	8.586410000	-1.958654000	-0.291287000
C	7.797750000	-2.770284000	0.596720000
C	8.600105000	-4.022496000	0.980565000
C	7.713563000	-4.856421000	1.925959000
C	8.933296000	-4.844102000	-0.279236000
C	9.896283000	-3.616699000	1.707508000
H	5.711288000	7.311590000	1.831020000
H	3.514795000	8.166318000	0.401998000
H	2.457110000	5.833994000	-0.596494000
H	6.156246000	-0.806079000	0.252125000
H	9.886566000	-0.413172000	-1.876136000
H	9.049878000	1.774331000	-2.733903000
H	6.864074000	-3.051574000	0.091879000
H	7.548775000	-2.186355000	1.492320000
H	7.455509000	-4.295483000	2.832582000
H	8.240967000	-5.766151000	2.234408000
H	6.780022000	-5.160012000	1.436544000
H	8.019450000	-5.154503000	-0.801010000
H	9.489577000	-5.749230000	-0.009276000
H	9.544455000	-4.265887000	-0.979539000
H	9.676579000	-3.038502000	2.613693000
H	10.538632000	-3.007303000	1.063818000
H	10.461227000	-4.507236000	2.006462000
H	6.067656000	3.469981000	-0.297639000

Cartesian coordinates of DFT-optimized structure of **7a** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Os	-5.552880000	-0.049698000	0.032965000
Os	5.543806000	0.094285000	0.000328000
N	-5.081891000	-2.089341000	0.290784000
N	5.072890000	2.134032000	-0.256985000
N	-6.014375000	0.241079000	2.055692000
N	6.003229000	-0.196598000	-2.022826000
N	-7.597146000	-0.080488000	0.023406000
N	7.588113000	0.124734000	0.007854000
N	-5.986108000	-0.351662000	-1.995803000
N	5.979145000	0.396220000	2.028648000
N	-5.141320000	2.003401000	-0.220231000
N	5.132162000	-1.958734000	0.253926000
C	-5.138178000	0.404028000	3.074985000
C	5.125982000	-0.359410000	-3.041244000
H	4.079959000	-0.329750000	-2.762120000
C	-5.535314000	0.596683000	4.390275000

C	5.521763000	-0.552221000	-4.356919000
H	4.768623000	-0.676914000	-5.127219000
C	-6.899542000	0.626338000	4.690006000
C	6.885685000	-0.582218000	-4.658004000
C	-7.813693000	0.461156000	3.655819000
C	7.800897000	-0.417171000	-3.624735000
H	-8.877807000	0.480668000	3.860621000
C	-7.365940000	0.269303000	2.345453000
C	7.354501000	-0.225116000	-2.313941000
C	-8.267537000	0.084735000	1.198779000
C	8.257285000	-0.040641000	-1.168192000
C	-9.663488000	0.061623000	1.212459000
C	9.653224000	-0.017705000	-1.183284000
H	-10.212921000	0.190746000	2.137815000
H	10.201714000	-0.146909000	-2.109190000
C	-10.350574000	-0.132349000	0.011645000
C	10.341553000	0.176212000	0.016829000
C	-9.646599000	-0.300285000	-1.183207000
C	9.638814000	0.344272000	1.212389000
C	-8.250833000	-0.271075000	-1.157300000
C	8.243020000	0.315269000	1.187883000
C	-7.333699000	-0.424443000	-2.296081000
C	7.327047000	0.468827000	2.327573000
C	-7.765014000	-0.628769000	-3.609988000
C	7.759726000	0.673161000	3.641029000
H	-8.826369000	-0.683291000	-3.822500000
C	-6.838305000	-0.761893000	-4.637575000
C	6.834084000	0.806450000	4.669552000
C	-5.478233000	-0.686097000	-4.327507000
C	5.473689000	0.730810000	4.360868000
H	4.712533000	0.828546000	5.127200000
C	-5.097584000	-0.482231000	-3.008929000
C	5.091674000	0.526949000	3.042683000
H	4.048845000	0.461553000	2.758029000
C	-5.979308000	-3.102057000	0.323996000
C	5.970365000	3.146687000	-0.290453000
H	-7.022450000	-2.808149000	0.334872000
H	7.013476000	2.852696000	-0.301940000
C	-5.631982000	-4.436331000	0.332702000
C	5.623128000	4.480989000	-0.298711000
H	-6.390252000	-5.210075000	0.360707000
H	6.381440000	5.254684000	-0.326952000
C	-4.268623000	-4.772965000	0.268836000
C	4.259826000	4.817716000	-0.234107000
C	-3.326662000	-3.741783000	0.240455000
C	3.317803000	3.786596000	-0.205438000
H	-2.277913000	-3.970009000	0.138647000
H	2.269116000	4.014859000	-0.103048000
C	-3.730919000	-2.397447000	0.293090000
C	3.721950000	2.442246000	-0.258512000
C	-2.843339000	-1.227333000	0.249900000

C	2.834291000	1.272208000	-0.214947000
C	-3.557619000	-0.023480000	0.035636000
C	3.548546000	0.068300000	-0.000889000
C	-2.876373000	1.197367000	-0.186295000
C	2.867274000	-1.152495000	0.221232000
C	-3.792130000	2.346395000	-0.226822000
C	3.782940000	-2.301606000	0.261352000
C	-3.433585000	3.695116000	-0.175476000
C	3.424256000	-3.650308000	0.210421000
H	-2.397919000	3.989117000	-0.084159000
H	2.388514000	-3.944244000	0.119777000
C	-4.400701000	4.707674000	-0.196016000
C	4.391298000	-4.662943000	0.230546000
C	-5.753361000	4.341726000	-0.254365000
C	5.744025000	-4.297105000	0.288037000
H	-6.556551000	5.065932000	-0.279495000
H	6.547167000	-5.021376000	0.312799000
C	-6.058655000	2.989491000	-0.248119000
C	6.049429000	-2.944898000	0.281414000
H	-7.094478000	2.670267000	-0.255393000
H	7.085284000	-2.625762000	0.288017000
C	-1.463300000	1.195122000	-0.344655000
C	1.454226000	-1.150148000	0.379883000
C	-0.724643000	0.012630000	0.021123000
C	0.715571000	0.032363000	0.014172000
C	-1.428196000	-1.188346000	0.394866000
C	1.419127000	1.233323000	-0.359618000
C	-0.651659000	-2.248665000	0.961822000
C	0.642591000	2.293707000	-0.926455000
H	-1.154458000	-3.063333000	1.468484000
H	1.145399000	3.108427000	-1.433025000
C	0.712758000	-2.231337000	0.953366000
C	-0.721822000	2.276370000	-0.918020000
H	1.243719000	-3.034103000	1.450066000
H	-1.252778000	3.079172000	-1.414666000
O	-3.976122000	-6.087651000	0.230525000
O	3.931449000	-5.928776000	0.182491000
O	3.967441000	6.132414000	-0.195395000
O	-3.940980000	5.973532000	-0.147481000
C	-4.884019000	7.061854000	-0.147151000
C	-4.121592000	8.392727000	-0.075958000
C	-5.176361000	9.516575000	-0.072331000
C	-3.205962000	8.544306000	-1.305416000
C	-3.289010000	8.458555000	1.218371000
C	2.592634000	6.550619000	-0.118188000
C	2.530402000	8.085106000	-0.132206000
C	1.043992000	8.478123000	-0.027164000
C	3.305512000	8.658313000	1.069292000
C	3.119402000	8.624282000	-1.449609000
C	-2.601263000	-6.505773000	0.153867000
C	-2.538936000	-8.040255000	0.168168000

C	-3.128312000	-8.579233000	1.485486000
C	-3.313645000	-8.613721000	-1.033465000
C	-1.052474000	-8.433206000	0.063655000
C	4.874418000	-7.017158000	0.181795000
C	4.111868000	-8.348008000	0.111498000
C	3.278413000	-8.414165000	-1.182251000
C	3.197067000	-8.499187000	1.341622000
C	5.166579000	-9.471909000	0.107481000
H	-5.552752000	6.955185000	0.716771000
H	-5.485484000	7.014088000	-1.064171000
H	-5.844997000	9.435380000	0.793268000
H	-5.790624000	9.492966000	-0.980671000
H	-4.685646000	10.495241000	-0.025607000
H	-3.785754000	8.509792000	-2.236215000
H	-2.455646000	7.747718000	-1.343367000
H	-2.679706000	9.505320000	-1.273012000
H	-3.928759000	8.364126000	2.104650000
H	-2.762886000	9.417865000	1.284696000
H	-2.542344000	7.658559000	1.252208000
H	2.043488000	6.137345000	-0.974280000
H	2.150147000	6.155759000	0.805758000
H	0.939956000	9.568950000	-0.038076000
H	0.596076000	8.108416000	0.903344000
H	0.462562000	8.078355000	-0.866960000
H	2.894673000	8.289085000	2.017161000
H	3.239697000	9.752469000	1.078035000
H	4.363885000	8.381862000	1.027233000
H	2.567731000	8.238344000	-2.315923000
H	4.170053000	8.337360000	-1.560682000
H	3.061258000	9.718530000	-1.474678000
H	-2.052438000	-6.092323000	1.010080000
H	-2.158485000	-6.111029000	-0.769991000
H	-2.576919000	-8.193120000	2.351899000
H	-3.070121000	-9.673474000	1.510758000
H	-4.179009000	-8.292340000	1.596190000
H	-4.372051000	-8.337342000	-0.991766000
H	-3.247745000	-9.707874000	-1.042005000
H	-2.902554000	-8.244622000	-1.981275000
H	-0.471313000	-8.033224000	0.903535000
H	-0.604302000	-8.063676000	-0.866800000
H	-0.948376000	-9.524024000	0.074834000
H	5.476523000	-6.969188000	1.098383000
H	5.542556000	-6.910756000	-0.682620000
H	2.752172000	-9.373454000	-1.247938000
H	3.917579000	-8.320047000	-2.068984000
H	2.531784000	-7.614122000	-1.215828000
H	2.446818000	-7.702551000	1.379859000
H	3.777497000	-8.464435000	2.272015000
H	2.670739000	-9.460184000	1.309856000
H	5.834632000	-9.390990000	-0.758594000
H	4.675786000	-10.450565000	0.061366000

H	5.781456000	-9.448073000	1.015400000
H	-4.782957000	0.721505000	5.161334000
H	-7.243948000	0.775159000	5.707956000
H	-4.091863000	0.374607000	2.796880000
H	-10.182285000	-0.449986000	-2.113565000
H	-11.434977000	-0.152566000	0.007113000
H	-7.169910000	-0.920868000	-5.658239000
H	-4.716274000	-0.783711000	-5.093073000
H	-4.055049000	-0.416690000	-2.723172000
H	7.229052000	-0.731199000	-5.676282000
H	8.864815000	-0.436976000	-3.830590000
H	11.425962000	0.196288000	0.020256000
H	10.175450000	0.493896000	2.142210000
H	8.821317000	0.727561000	3.852458000
H	7.166750000	0.965431000	5.689870000

Cartesian coordinates of DFT-optimized structure of **8a** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Os	5.467858000	0.958425000	0.034981000
N	5.331113000	-1.103713000	0.373277000
N	5.881237000	1.398070000	2.046569000
N	7.487346000	1.284181000	0.000963000
N	5.932627000	0.657012000	-1.991054000
C	5.000725000	1.439116000	3.072286000
H	3.973340000	1.213896000	2.813640000
C	5.370093000	1.745618000	4.374970000
H	4.614990000	1.762590000	5.153158000
C	6.709480000	2.025824000	4.651360000
H	7.032447000	2.269509000	5.657945000
C	7.628862000	1.986407000	3.608405000
H	8.674886000	2.198731000	3.796358000
C	7.208491000	1.672850000	2.313340000
C	8.120954000	1.608889000	1.159410000
C	9.498508000	1.837658000	1.156692000
H	10.021740000	2.097257000	2.069509000
C	10.200149000	1.726078000	-0.045752000
C	9.530300000	1.390838000	-1.224568000
H	10.078033000	1.306294000	-2.155891000
C	8.152141000	1.170373000	-1.179742000
C	7.269418000	0.812580000	-2.302559000
C	7.725189000	0.635459000	-3.611351000
H	8.778190000	0.761798000	-3.834345000
C	6.832187000	0.297874000	-4.622886000
H	7.183030000	0.158831000	-5.639983000
C	5.482517000	0.143393000	-4.301258000
H	4.746752000	-0.118785000	-5.053565000
C	5.077548000	0.330250000	-2.986552000
H	4.040684000	0.221609000	-2.692872000
N	4.034848000	-1.601731000	0.403409000

C	-3.005598000	0.779702000	-0.179813000
C	2.983524000	-0.640510000	0.292540000
C	-3.512164000	-0.504904000	0.040960000
C	3.492025000	0.641438000	0.061046000
C	-2.622824000	-1.558077000	0.276461000
C	2.603613000	1.697734000	-0.163718000
C	-1.233511000	-1.349238000	0.411573000
C	1.212253000	1.493814000	-0.283889000
C	-0.720249000	-0.043172000	0.063733000
C	0.698499000	0.189031000	0.067805000
C	-1.621176000	1.030078000	-0.292021000
C	1.599390000	-0.885588000	0.419698000
C	-1.053962000	2.244847000	-0.791606000
C	1.032015000	-2.097846000	0.925168000
H	-1.693828000	2.987895000	-1.249438000
H	1.671785000	-2.838982000	1.386131000
C	0.290181000	2.464838000	-0.787748000
C	-0.312117000	-2.317835000	0.921312000
H	0.662333000	3.373520000	-1.242674000
H	-0.684804000	-3.224678000	1.379368000
H	11.270464000	1.900699000	-0.064226000
N	-3.313474000	-2.804398000	0.382347000
N	-4.700682000	-2.745564000	0.344551000
C	-5.134439000	-4.010577000	0.382079000
C	-4.052162000	-4.903215000	0.423284000
C	-2.920300000	-4.110954000	0.409431000
H	-6.195882000	-4.210785000	0.364748000
H	-4.087566000	-5.981802000	0.450424000
H	-1.881796000	-4.390253000	0.382552000
Os	-5.485784000	-0.834304000	0.003612000
C	-5.668234000	-0.060947000	4.343349000
C	-5.213182000	-0.232522000	3.043023000
N	-6.028941000	-0.551216000	2.012462000
C	-7.376003000	-0.714155000	2.271597000
C	-7.881602000	-0.552143000	3.564017000
C	-7.028579000	-0.222617000	4.612031000
C	-8.214026000	-1.064637000	1.112671000
N	-7.503527000	-1.169334000	-0.041940000
C	-8.090768000	-1.488080000	-1.226217000
C	-9.467021000	-1.718479000	-1.278907000
C	-10.215341000	-1.615373000	-0.104140000
C	-9.592589000	-1.287008000	1.102084000
C	-7.133812000	-1.544737000	-2.343788000
N	-5.818934000	-1.266298000	-2.024712000
C	-4.898779000	-1.302473000	-3.015145000
C	-5.215732000	-1.607458000	-4.331918000
C	-6.542417000	-1.891020000	-4.661189000
C	-7.502053000	-1.856695000	-3.654939000
H	-4.166182000	-0.118221000	2.790301000
H	-4.962284000	0.195171000	5.125709000
H	-7.417975000	-0.095519000	5.616581000

H	-8.941763000	-0.684549000	3.745950000
H	-10.176347000	-1.208610000	2.011743000
H	-11.285352000	-1.791100000	-0.128719000
H	-9.954031000	-1.972401000	-2.213182000
H	-8.539130000	-2.072438000	-3.883902000
H	-6.824967000	-2.133704000	-5.680100000
H	-4.430606000	-1.620686000	-5.079886000
H	-3.883034000	-1.075160000	-2.715600000
N	-4.059145000	1.735974000	-0.309265000
N	-5.352893000	1.230925000	-0.317577000
C	-6.171455000	2.287923000	-0.368841000
C	-5.435698000	3.483182000	-0.373200000
C	-4.109293000	3.099629000	-0.321937000
N	4.685323000	2.873825000	-0.288825000
H	-3.218127000	3.699053000	-0.259305000
H	-5.817589000	4.492510000	-0.400702000
H	-7.240562000	2.133692000	-0.386928000
N	3.298047000	2.940089000	-0.288171000
C	5.124495000	4.136669000	-0.336459000
C	4.046132000	5.035024000	-0.345976000
C	2.910937000	4.248595000	-0.301768000
C	4.078552000	-2.965487000	0.429484000
C	5.403826000	-3.355603000	0.450371000
C	6.145289000	-2.164484000	0.414373000
H	4.086488000	6.113460000	-0.372233000
H	1.874843000	4.532600000	-0.244664000
H	6.187073000	4.331318000	-0.348443000
H	7.215257000	-2.015865000	0.403145000
H	5.781076000	-4.366652000	0.478692000
H	3.183428000	-3.561242000	0.397079000

Cartesian coordinates of DFT-optimized structure of **9a** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Os	5.546537000	0.888252000	-0.247746000
N	5.423105000	-1.175463000	0.171897000
N	5.966133000	1.407112000	1.738836000
N	7.569334000	1.190367000	-0.291846000
N	6.012967000	0.506669000	-2.255093000
C	5.081098000	1.505440000	2.758781000
H	4.051790000	1.286137000	2.503205000
C	5.449215000	1.861475000	4.048236000
H	4.690913000	1.922818000	4.821128000
C	6.792137000	2.134134000	4.319964000
H	7.113707000	2.415211000	5.317232000
C	7.714820000	2.039193000	3.284549000
H	8.762705000	2.246769000	3.467714000
C	7.296639000	1.676325000	2.000897000
C	8.210036000	1.552370000	0.855354000
C	9.591029000	1.758169000	0.845649000

H	10.116823000	2.045930000	1.748695000
C	10.293810000	1.587143000	-0.349540000
C	9.620022000	1.216075000	-1.515657000
H	10.167859000	1.084301000	-2.441586000
C	8.238429000	1.019868000	-1.466842000
C	7.352109000	0.633476000	-2.574372000
C	7.802703000	0.404890000	-3.877851000
H	8.856975000	0.510358000	-4.106009000
C	6.904140000	0.044478000	-4.875402000
H	7.250752000	-0.133408000	-5.887910000
C	5.552476000	-0.082604000	-4.545874000
H	4.812371000	-0.362404000	-5.287580000
C	5.151960000	0.154307000	-3.238814000
H	4.115076000	0.067130000	-2.938687000
C	6.477135000	-2.019488000	0.263518000
H	7.456025000	-1.554887000	0.239480000
C	6.357108000	-3.388784000	0.370098000
H	7.233476000	-4.022410000	0.439844000
C	5.068512000	-3.950447000	0.349940000
C	3.967068000	-3.094844000	0.269454000
H	2.969878000	-3.500082000	0.204154000
C	4.142520000	-1.701880000	0.220305000
C	-2.922919000	0.731188000	-0.513190000
C	3.073417000	-0.700508000	0.108858000
C	-3.441379000	-0.505409000	-0.115572000
C	3.575571000	0.584582000	-0.209847000
C	-2.562099000	-1.523144000	0.267087000
C	2.699089000	1.655296000	-0.508337000
C	-1.169169000	-1.312189000	0.367785000
C	1.306426000	1.406199000	-0.643413000
C	-0.645198000	-0.069582000	-0.149279000
C	0.776561000	0.150574000	-0.169126000
C	-1.534717000	0.953748000	-0.647127000
C	1.674122000	-0.882984000	0.285850000
C	-0.950094000	2.087228000	-1.294649000
C	1.095217000	-2.006125000	0.958052000
H	-1.576511000	2.765092000	-1.859902000
H	1.736474000	-2.684580000	1.506882000
C	0.396140000	2.302264000	-1.289279000
C	-0.252396000	-2.209699000	0.999443000
H	0.786922000	3.145210000	-1.845316000
H	-0.628963000	-3.039809000	1.582992000
O	5.000019000	-5.294988000	0.401991000
C	3.714713000	-5.941326000	0.371663000
C	3.913272000	-7.461589000	0.460126000
C	2.513347000	-8.104476000	0.414563000
C	4.751247000	-7.956727000	-0.733945000
C	4.609857000	-7.826701000	1.784728000
H	3.113067000	-5.582454000	1.217072000
H	3.201686000	-5.674630000	-0.561573000
H	2.596696000	-9.195187000	0.478968000

H	1.991579000	-7.863050000	-0.519526000
H	1.889154000	-7.766185000	1.250631000
H	4.267873000	-7.707105000	-1.686680000
H	4.868133000	-9.045836000	-0.691794000
H	5.749651000	-7.507835000	-0.731859000
H	4.018261000	-7.493522000	2.646572000
H	5.599727000	-7.364213000	1.852765000
H	4.735436000	-8.912779000	1.863159000
H	11.366884000	1.743202000	-0.372197000
N	-3.264910000	-2.733406000	0.552402000
N	-4.652045000	-2.665180000	0.512970000
C	-5.098667000	-3.906143000	0.736033000
C	-4.025523000	-4.795557000	0.901911000
C	-2.885564000	-4.026765000	0.768229000
H	-6.162234000	-4.094599000	0.752259000
H	-4.072308000	-5.858306000	1.085460000
H	-1.850442000	-4.319039000	0.778000000
Os	-5.418819000	-0.816810000	-0.099183000
C	-5.566172000	0.595527000	4.077872000
C	-5.120837000	0.227278000	2.815520000
N	-5.945416000	-0.235781000	1.848608000
C	-7.292278000	-0.344796000	2.135843000
C	-7.788373000	0.013987000	3.391692000
C	-6.926033000	0.488066000	4.374626000
C	-8.141172000	-0.855735000	1.046817000
N	-7.439999000	-1.135655000	-0.084016000
C	-8.038040000	-1.620322000	-1.204710000
C	-9.416314000	-1.844616000	-1.214597000
C	-10.155232000	-1.563340000	-0.063226000
C	-9.521363000	-1.065812000	1.077645000
C	-7.089516000	-1.847630000	-2.307361000
N	-5.770389000	-1.536404000	-2.040292000
C	-4.858187000	-1.724077000	-3.021163000
C	-5.187617000	-2.213397000	-4.277917000
C	-6.518788000	-2.530547000	-4.554074000
C	-7.470135000	-2.343522000	-3.556861000
H	-4.074996000	0.295961000	2.542402000
H	-4.853211000	0.960008000	4.809240000
H	-7.308104000	0.767472000	5.350804000
H	-8.848584000	-0.078850000	3.596107000
H	-10.098123000	-0.849691000	1.969325000
H	-11.226602000	-1.732203000	-0.054949000
H	-9.911915000	-2.230009000	-2.097976000
H	-8.510430000	-2.581817000	-3.744948000
H	-6.810987000	-2.915338000	-5.525425000
H	-4.408334000	-2.341180000	-5.021182000
H	-3.838082000	-1.466143000	-2.764434000
N	-3.968046000	1.667848000	-0.779382000
N	-5.266719000	1.177717000	-0.716726000
C	-6.075780000	2.222327000	-0.925343000
C	-5.329732000	3.397880000	-1.104006000

C	-4.006892000	3.015358000	-0.993790000
C	3.410032000	2.934071000	-0.649145000
N	4.797542000	2.821001000	-0.645787000
C	5.537927000	3.940318000	-0.761515000
C	5.011638000	5.219787000	-0.853848000
C	3.617511000	5.359267000	-0.790525000
C	2.832434000	4.204661000	-0.683209000
O	2.952908000	6.531122000	-0.814664000
C	3.697506000	7.760552000	-0.899320000
C	2.719681000	8.944415000	-0.878184000
C	3.564920000	10.229904000	-0.971116000
C	1.917064000	8.944354000	0.436699000
C	1.763716000	8.863093000	-2.083305000
H	4.281962000	7.761771000	-1.828597000
H	4.390050000	7.818853000	-0.049657000
H	4.153335000	10.256906000	-1.896413000
H	4.257406000	10.317137000	-0.124934000
H	2.914170000	11.111597000	-0.962769000
H	2.583142000	9.009454000	1.306047000
H	1.317766000	8.033645000	0.535778000
H	1.237827000	9.804031000	0.468886000
H	2.318908000	8.873655000	-3.029458000
H	1.079328000	9.719337000	-2.085734000
H	1.163168000	7.948351000	-2.052089000
H	5.682006000	6.064008000	-0.946366000
H	6.612159000	3.795021000	-0.769083000
H	1.762985000	4.329466000	-0.591209000
H	-3.111233000	3.610698000	-1.018372000
H	-5.703141000	4.395267000	-1.280400000
H	-7.146183000	2.076200000	-0.923652000

Cartesian coordinates of DFT-optimized structure of **10a** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Os	-2.325683000	-1.311965000	0.059560000
N	-3.061700000	0.652485000	0.276067000
N	-2.570052000	-1.778548000	2.090816000
N	-4.033096000	-2.438454000	0.044052000
N	-2.831183000	-1.329170000	-1.976380000
C	-1.778314000	-1.394390000	3.118739000
H	-0.931349000	-0.776320000	2.847462000
C	-2.019740000	-1.757093000	4.436473000
H	-1.345371000	-1.417199000	5.214812000
C	-3.128538000	-2.554302000	4.728302000
H	-3.346071000	-2.856526000	5.747280000
C	-3.955191000	-2.955204000	3.684562000
H	-4.823805000	-3.571969000	3.883614000
C	-3.671414000	-2.564299000	2.373284000
C	-4.500865000	-2.943294000	1.218586000
C	-5.655856000	-3.728105000	1.226542000

H	-6.043190000	-4.138951000	2.151696000
C	-6.311924000	-3.979818000	0.019294000
C	-5.816051000	-3.452807000	-1.175514000
H	-6.326630000	-3.651665000	-2.110622000
C	-4.658151000	-2.673269000	-1.142295000
C	-3.977286000	-2.038310000	-2.281507000
C	-4.433964000	-2.129126000	-3.599220000
H	-5.334895000	-2.690903000	-3.816588000
C	-3.736502000	-1.501405000	-4.625517000
H	-4.088235000	-1.569880000	-5.649495000
C	-2.579835000	-0.785206000	-4.309855000
H	-2.001109000	-0.277851000	-5.073887000
C	-2.165089000	-0.723966000	-2.986863000
H	-1.274021000	-0.180767000	-2.697098000
C	-4.369742000	1.000294000	0.269247000
H	-5.075354000	0.177778000	0.282088000
C	-4.818450000	2.303636000	0.236422000
H	-5.878475000	2.528795000	0.231381000
C	-3.867613000	3.336758000	0.174831000
C	-2.511791000	2.998837000	0.194818000
H	-1.762608000	3.767867000	0.097912000
C	-2.106255000	1.657830000	0.285260000
C	5.436941000	2.134756000	0.150680000
C	-0.716004000	1.174528000	0.291363000
C	5.373186000	3.531634000	0.349579000
C	-0.652217000	-0.222357000	0.092508000
C	4.131114000	4.161857000	0.510936000
C	0.589832000	-0.852516000	-0.069204000
C	2.927987000	3.433411000	0.601419000
C	1.792931000	-0.124025000	-0.159860000
C	2.973040000	2.030939000	0.252443000
C	1.747870000	1.278442000	0.189149000
C	4.233973000	1.394005000	-0.032991000
C	0.486951000	1.915360000	0.474709000
C	4.190320000	0.066633000	-0.567673000
C	0.530611000	3.242786000	1.009272000
H	5.085960000	-0.361209000	-0.999687000
H	-0.365021000	3.670651000	1.441280000
C	3.036387000	-0.657294000	-0.622846000
C	1.684526000	3.966741000	1.064328000
H	3.060429000	-1.631451000	-1.094768000
H	1.660505000	4.940962000	1.536128000
O	-4.348370000	4.591983000	0.090771000
C	-3.431815000	5.700582000	0.034343000
C	-4.229641000	7.010380000	-0.042047000
C	-3.205426000	8.160846000	-0.097497000
C	-5.098843000	7.026187000	-1.313773000
C	-5.115580000	7.163713000	1.208754000
H	-2.799081000	5.687019000	0.931651000
H	-2.789990000	5.590656000	-0.849397000
H	-3.723318000	9.124889000	-0.153792000

H	-2.555613000	8.077544000	-0.977255000
H	-2.568998000	8.174350000	0.795790000
H	-4.481565000	6.928145000	-2.215479000
H	-5.651950000	7.969722000	-1.386258000
H	-5.824379000	6.206431000	-1.308153000
H	-4.509772000	7.164786000	2.123395000
H	-5.842029000	6.348189000	1.283508000
H	-5.668870000	8.109194000	1.171103000
H	-7.210045000	-4.587825000	0.009467000
N	0.457431000	-2.271464000	-0.155067000
C	1.337948000	-3.313542000	-0.117781000
C	0.614370000	-4.490859000	-0.139255000
C	-0.733706000	-4.101383000	-0.169920000
N	-0.837438000	-2.767184000	-0.167390000
H	-1.628847000	-4.706235000	-0.180766000
H	1.010399000	-5.495037000	-0.125400000
H	2.399460000	-3.154454000	-0.045130000
N	4.263537000	5.580781000	0.596920000
N	5.558427000	6.076447000	0.609928000
C	5.454730000	7.410650000	0.612045000
C	4.106684000	7.800169000	0.580423000
C	3.383076000	6.622878000	0.558813000
C	6.827158000	1.651348000	0.157269000
C	7.232594000	0.310294000	0.247455000
C	8.588387000	-0.027707000	0.267882000
C	9.539308000	1.005379000	0.207072000
C	9.090684000	2.308759000	0.174497000
N	7.782664000	2.656635000	0.167188000
O	9.069019000	-1.282995000	0.351713000
C	8.152358000	-2.391562000	0.407015000
C	8.950043000	-3.701475000	0.482863000
C	7.925704000	-4.851889000	0.537185000
C	9.836442000	-3.854074000	-0.767699000
C	9.818759000	-3.718184000	1.754910000
H	6.349879000	8.015484000	0.623278000
H	3.710700000	8.804358000	0.566102000
H	2.321596000	6.463781000	0.485629000
H	6.483341000	-0.458734000	0.343827000
H	10.599319000	0.780161000	0.212499000
H	9.796351000	3.131234000	0.162253000
H	7.519994000	-2.377343000	-0.490546000
H	7.510166000	-2.282178000	1.290558000
H	7.275555000	-4.769094000	1.416746000
H	8.443494000	-5.816009000	0.593072000
H	7.289612000	-4.864775000	-0.356353000
H	9.230986000	-3.854471000	-1.682574000
H	10.389621000	-4.799635000	-0.730464000
H	10.562994000	-3.038569000	-0.841629000
H	9.201143000	-3.620675000	2.656440000
H	10.544361000	-2.898481000	1.750096000
H	10.371764000	-4.661808000	1.826991000

Os	7.046718000	4.621100000	0.383769000
C	7.297495000	4.092867000	4.753169000
C	6.883799000	4.032061000	3.429827000
N	7.550699000	4.637608000	2.420079000
C	8.696585000	5.346610000	2.726336000
C	9.152188000	5.437025000	4.044449000
C	8.453891000	4.808986000	5.069984000
C	9.378377000	5.981850000	1.587848000
N	8.754232000	5.747422000	0.400944000
C	9.222967000	6.252551000	-0.773071000
C	10.378049000	7.037239000	-0.779915000
C	11.033202000	7.288546000	0.427919000
C	10.536335000	6.761251000	1.622186000
C	8.394395000	5.873962000	-1.928536000
N	7.292743000	5.088232000	-1.647166000
C	6.501824000	4.704376000	-2.675828000
C	6.744356000	5.067398000	-3.993277000
C	7.853438000	5.864614000	-4.283989000
C	8.679266000	6.265191000	-3.239475000
H	5.992957000	3.488963000	3.139179000
H	6.718168000	3.585250000	5.516572000
H	8.804790000	4.877167000	6.094268000
H	10.052944000	5.998730000	4.262727000
H	11.046196000	6.959803000	2.557753000
H	11.931379000	7.896454000	0.438623000
H	10.766131000	7.448292000	-1.704663000
H	9.548083000	6.881952000	-3.437656000
H	8.071821000	6.167099000	-5.302708000
H	6.070607000	4.727738000	-4.772255000
H	5.654599000	4.086289000	-2.405408000

Cartesian coordinates of DFT-optimized structure of **11a** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Os	2.896711000	0.434224000	0.036746000
N	1.753851000	-1.326503000	0.235599000
N	3.356598000	0.535523000	2.081363000
N	4.822511000	-0.257040000	0.086082000
N	3.273668000	0.017709000	-1.984110000
N	-7.804107000	2.417875000	0.024858000
C	2.543617000	0.949674000	3.080764000
H	1.552420000	1.260782000	2.774763000
C	2.935937000	0.980905000	4.411628000
H	2.236241000	1.324565000	5.165569000
C	4.227171000	0.568739000	4.747970000
H	4.566060000	0.580478000	5.778476000
C	5.076148000	0.140045000	3.733625000
H	6.083015000	-0.185867000	3.967331000
C	4.635467000	0.125893000	2.407405000
C	5.471697000	-0.317319000	1.280958000

C	6.793426000	-0.764819000	1.332094000
H	7.327058000	-0.817458000	2.273939000
C	7.425605000	-1.145741000	0.146219000
C	6.742088000	-1.077729000	-1.070064000
H	7.236302000	-1.372511000	-1.988453000
C	5.421472000	-0.624221000	-1.079887000
C	4.537632000	-0.475464000	-2.246852000
C	4.921933000	-0.803524000	-3.549813000
H	5.917715000	-1.189791000	-3.733732000
C	4.030834000	-0.637708000	-4.604374000
H	4.326238000	-0.891338000	-5.616961000
C	2.754210000	-0.141925000	-4.331393000
H	2.022342000	0.003403000	-5.118377000
C	2.418086000	0.169870000	-3.021385000
H	1.438976000	0.555025000	-2.764462000
C	2.257896000	-2.581898000	0.276979000
H	3.337681000	-2.652940000	0.338211000
C	1.484255000	-3.722313000	0.234770000
H	1.937414000	-4.706022000	0.270817000
C	0.091530000	-3.580826000	0.108437000
C	-0.449786000	-2.293154000	0.076220000
H	-1.508956000	-2.155468000	-0.070213000
C	0.377121000	-1.162967000	0.180595000
C	-4.481265000	4.564948000	-0.306666000
C	-0.066382000	0.238874000	0.143428000
C	-5.589109000	3.716457000	-0.146222000
C	1.022387000	1.122786000	-0.006293000
C	-5.396940000	2.331016000	0.026641000
C	0.793130000	2.495175000	-0.198741000
C	-6.674176000	1.601109000	0.022037000
C	-6.837460000	0.218542000	-0.075721000
H	-5.982273000	-0.433914000	-0.176070000
C	-8.109521000	-0.366998000	-0.092848000
C	-9.233573000	0.468175000	-0.019736000
H	-10.246959000	0.089192000	-0.018001000
C	-9.019761000	1.837669000	0.020146000
H	-9.864711000	2.516582000	0.038269000
C	-4.075873000	1.814697000	0.181130000
C	-0.500476000	3.019029000	-0.374456000
C	-2.956418000	2.671871000	-0.113376000
C	-1.617603000	2.146055000	-0.085000000
C	-3.170936000	4.067377000	-0.428930000
C	-1.391348000	0.761276000	0.240845000
C	-2.051082000	4.831802000	-0.892519000
C	-2.510696000	0.016472000	0.724867000
H	-2.213461000	5.806026000	-1.335898000
H	-2.347146000	-0.946964000	1.191048000
C	-0.784484000	4.334317000	-0.867256000
C	-3.782096000	0.514304000	0.694609000
H	0.012580000	4.931797000	-1.291360000
H	-4.576650000	-0.075081000	1.134597000

O	-0.621214000	-4.720261000	0.018873000
O	-8.144462000	-1.710240000	-0.189166000
C	-9.418225000	-2.380841000	-0.225420000
C	-9.187471000	-3.892597000	-0.365223000
C	-10.576267000	-4.560384000	-0.395701000
C	-8.383959000	-4.419772000	0.838653000
C	-8.437165000	-4.194324000	-1.676409000
C	-2.053244000	-4.653972000	-0.109284000
C	-2.621343000	-6.079894000	-0.154805000
C	-4.150709000	-5.953285000	-0.299110000
C	-2.046800000	-6.840861000	-1.364717000
C	-2.282544000	-6.825124000	1.150116000
H	-9.999308000	-2.000505000	-1.075478000
H	-9.965194000	-2.159450000	0.700266000
H	-11.173987000	-4.205389000	-1.244151000
H	-11.138370000	-4.358756000	0.524356000
H	-10.471145000	-5.646900000	-0.492144000
H	-8.908441000	-4.221495000	1.781607000
H	-7.396905000	-3.949233000	0.893442000
H	-8.240029000	-5.503238000	0.755621000
H	-8.999088000	-3.831324000	-2.545952000
H	-8.296199000	-5.274843000	-1.794929000
H	-7.450683000	-3.719675000	-1.687626000
H	-2.464057000	-4.104045000	0.747528000
H	-2.306035000	-4.110349000	-1.028911000
H	-4.610415000	-6.947467000	-0.332204000
H	-4.423936000	-5.427094000	-1.221910000
H	-4.590191000	-5.409043000	0.545874000
H	-2.283664000	-6.326206000	-2.304212000
H	-2.472571000	-7.849569000	-1.417680000
H	-0.958459000	-6.935212000	-1.294111000
H	-2.697142000	-6.303262000	2.021611000
H	-1.199985000	-6.910485000	1.288374000
H	-2.704282000	-7.836698000	1.132197000
H	8.452144000	-1.495093000	0.169785000
N	2.012917000	3.236636000	-0.231423000
C	2.319742000	4.565297000	-0.173253000
C	3.695586000	4.689283000	-0.138154000
C	4.190221000	3.375705000	-0.155485000
N	3.183906000	2.494943000	-0.198238000
N	-4.870074000	5.937517000	-0.366936000
C	-4.193805000	7.121402000	-0.303995000
C	-5.119119000	8.147639000	-0.309756000
C	-6.373874000	7.520071000	-0.356433000
N	-6.233538000	6.189554000	-0.377701000
H	5.209762000	3.019728000	-0.126535000
H	4.262630000	5.606920000	-0.095858000
H	1.554965000	5.320510000	-0.125281000
H	-3.121376000	7.156740000	-0.225314000
H	-4.912420000	9.206625000	-0.274983000
H	-7.363549000	7.953167000	-0.363276000

Os	-7.432977000	4.486056000	-0.169640000
C	-7.225188000	4.911689000	4.214602000
C	-6.917655000	4.621197000	2.892811000
N	-7.761843000	4.874359000	1.866016000
C	-8.985836000	5.447990000	2.153379000
C	-9.340301000	5.758838000	3.469029000
C	-8.459980000	5.492488000	4.511890000
C	-9.863736000	5.695117000	0.998861000
C	-11.135262000	6.272210000	1.010340000
C	-11.820110000	6.425555000	-0.197345000
C	-11.237777000	6.006466000	-1.395880000
C	-9.964524000	5.434128000	-1.365927000
N	-9.312249000	5.294210000	-0.179299000
C	-9.182489000	4.936470000	-2.508790000
N	-7.931328000	4.433455000	-2.206651000
C	-7.171249000	3.957658000	-3.219966000
C	-7.589699000	3.955952000	-4.543286000
C	-8.851836000	4.465313000	-4.855993000
C	-9.647557000	4.955911000	-3.826504000
H	-6.503832000	4.684662000	4.991926000
H	-5.972256000	4.170982000	2.616410000
H	-10.305565000	6.207893000	3.671921000
H	-8.732193000	5.732383000	5.534284000
H	-11.589674000	6.599011000	1.938482000
H	-12.808307000	6.872532000	-0.204590000
H	-11.771765000	6.128153000	-2.331144000
H	-6.201153000	3.571417000	-2.932146000
H	-6.932368000	3.560214000	-5.309700000
H	-9.209873000	4.479204000	-5.879983000
H	-10.632421000	5.353891000	-4.041418000

Cartesian coordinates of DFT-optimized structure of **7b** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Ru	-5.528947000	-0.048614000	0.031325000
Ru	5.519871000	0.093238000	0.002517000
N	-5.076800000	-2.087723000	0.301778000
N	5.067737000	2.132368000	-0.267859000
N	-5.983851000	0.247450000	2.054640000
N	5.974280000	-0.202880000	-2.020890000
N	-7.569508000	-0.076491000	0.018706000
N	7.560441000	0.121056000	0.014648000
N	-5.950729000	-0.357291000	-1.999260000
N	5.942158000	0.401910000	2.032999000
N	-5.134994000	2.002972000	-0.234019000
N	5.125900000	-1.958317000	0.268004000
C	-5.108893000	0.408645000	3.067901000
C	5.099073000	-0.364087000	-3.033934000
H	4.052270000	-0.332824000	-2.755968000
C	-5.504589000	0.602553000	4.386522000

C	5.494443000	-0.558064000	-4.352643000
H	4.742379000	-0.682118000	-5.124090000
C	-6.867421000	0.633104000	4.683909000
C	6.857201000	-0.588676000	-4.650360000
C	-7.782766000	0.467982000	3.648811000
C	7.772800000	-0.423537000	-3.615489000
H	-8.846788000	0.487513000	3.853965000
C	-7.329971000	0.276158000	2.340709000
C	7.320331000	-0.231638000	-2.307287000
C	-8.233637000	0.090918000	1.188334000
C	8.224282000	-0.046381000	-1.155140000
C	-9.630826000	0.071590000	1.205243000
C	9.621467000	-0.027036000	-1.172395000
H	-10.181878000	0.203278000	2.129202000
H	10.172295000	-0.158731000	-2.096487000
C	-10.315264000	-0.122786000	0.003189000
C	10.306201000	0.167374000	0.029486000
C	-9.611303000	-0.294463000	-1.190940000
C	9.602535000	0.339068000	1.223786000
C	-8.214388000	-0.267466000	-1.157888000
C	8.205612000	0.312058000	1.191078000
C	-7.292291000	-0.426611000	-2.299495000
C	7.283793000	0.471209000	2.332908000
C	-7.725502000	-0.633450000	-3.611825000
C	7.717331000	0.678021000	3.645134000
H	-8.786300000	-0.685625000	-3.827611000
C	-6.795090000	-0.772412000	-4.637256000
C	6.787175000	0.816973000	4.670798000
C	-5.437090000	-0.699507000	-4.325849000
C	5.429097000	0.744082000	4.359724000
H	4.665950000	0.845780000	5.123550000
C	-5.061090000	-0.491993000	-3.003403000
C	5.052768000	0.536599000	3.037365000
H	4.010236000	0.472279000	2.749399000
C	-5.975305000	-3.093795000	0.332035000
C	5.966249000	3.138431000	-0.298206000
H	-7.018045000	-2.796527000	0.344451000
H	7.008984000	2.841154000	-0.310759000
C	-5.633001000	-4.431762000	0.336128000
C	5.623960000	4.476403000	-0.302227000
H	-6.392752000	-5.204178000	0.363342000
H	6.383717000	5.248810000	-0.329520000
C	-4.271432000	-4.770695000	0.269172000
C	4.262403000	4.815355000	-0.235106000
C	-3.326093000	-3.741026000	0.240560000
C	3.317055000	3.785696000	-0.206393000
H	-2.277921000	-3.971350000	0.135886000
H	2.268896000	4.016025000	-0.101593000
C	-3.732056000	-2.397699000	0.298179000
C	3.723000000	2.442367000	-0.264075000
C	-2.843792000	-1.223874000	0.255006000

C	2.834720000	1.268562000	-0.220790000
C	-3.554356000	-0.022727000	0.037562000
C	3.545280000	0.067407000	-0.003379000
C	-2.876264000	1.195129000	-0.187957000
C	2.867182000	-1.150434000	0.222199000
C	-3.792026000	2.347869000	-0.230321000
C	3.782924000	-2.303190000	0.264505000
C	-3.431696000	3.695620000	-0.171725000
C	3.422564000	-3.650940000	0.206054000
H	-2.396926000	3.991541000	-0.074636000
H	2.387776000	-3.946852000	0.109131000
C	-4.402385000	4.706359000	-0.193126000
C	4.393238000	-4.661693000	0.227403000
C	-5.753111000	4.338199000	-0.259785000
C	5.743978000	-4.293552000	0.293859000
H	-6.557868000	5.060744000	-0.285278000
H	6.548726000	-5.016109000	0.319301000
C	-6.053146000	2.982445000	-0.261457000
C	6.044037000	-2.937804000	0.295390000
H	-7.088722000	2.660602000	-0.275433000
H	7.079621000	-2.615979000	0.309204000
C	-1.462667000	1.193898000	-0.347210000
C	1.453590000	-1.149181000	0.381509000
C	-0.724526000	0.012696000	0.021401000
C	0.715449000	0.032023000	0.012906000
C	-1.427857000	-1.186761000	0.399286000
C	1.418780000	1.231474000	-0.364994000
C	-0.651502000	-2.247380000	0.966267000
C	0.642426000	2.292113000	-0.931939000
H	-1.154566000	-3.062329000	1.472331000
H	1.145492000	3.107080000	-1.437971000
C	0.712958000	-2.230319000	0.956409000
C	-0.722034000	2.275055000	-0.922075000
H	1.245190000	-3.033455000	1.451271000
H	-1.254265000	3.078206000	-1.416913000
O	-3.980564000	-6.085824000	0.229460000
O	3.935788000	-5.928160000	0.172389000
O	3.971556000	6.130487000	-0.195342000
O	-3.944961000	5.972828000	-0.137951000
C	-4.890123000	7.059192000	-0.136005000
C	-4.130494000	8.391266000	-0.058102000
C	-5.187121000	9.513341000	-0.053575000
C	-3.211532000	8.548524000	-1.284403000
C	-3.301709000	8.454096000	1.238852000
C	2.597564000	6.551314000	-0.117127000
C	2.537644000	8.085640000	-0.143386000
C	1.052112000	8.481778000	-0.035614000
C	3.318507000	8.667815000	1.050004000
C	3.121945000	8.612901000	-1.467683000
C	-2.606564000	-6.506635000	0.151322000
C	-2.546632000	-8.040961000	0.177539000

C	-3.131013000	-8.568265000	1.501783000
C	-3.327413000	-8.623108000	-1.015918000
C	-1.061090000	-8.437084000	0.069852000
C	4.880937000	-7.014536000	0.170435000
C	4.121285000	-8.346612000	0.092777000
C	3.292349000	-8.409589000	-1.204073000
C	3.202467000	-8.503718000	1.319206000
C	5.177903000	-9.468696000	0.088260000
H	-5.560667000	6.947851000	0.725914000
H	-5.489408000	7.013553000	-1.054554000
H	-5.858637000	9.427104000	0.809277000
H	-5.798061000	9.492374000	-0.964181000
H	-4.698240000	10.492609000	-0.000929000
H	-3.788520000	8.515785000	-2.217022000
H	-2.459490000	7.753569000	-1.322737000
H	-2.687272000	9.510472000	-1.247467000
H	-3.944215000	8.358347000	2.123001000
H	-2.775182000	9.412952000	1.308759000
H	-2.555454000	7.653720000	1.273526000
H	2.045085000	6.132583000	-0.968282000
H	2.157359000	6.164355000	0.811222000
H	0.949211000	9.572618000	-0.056065000
H	0.607524000	8.121137000	0.900074000
H	0.466473000	8.075263000	-0.869267000
H	2.909004000	8.309660000	2.002664000
H	3.257158000	9.762259000	1.047998000
H	4.375620000	8.386650000	1.007546000
H	2.566584000	8.219935000	-2.328472000
H	4.171889000	8.324021000	-1.580442000
H	3.064793000	9.706939000	-1.501948000
H	-2.054144000	-6.087924000	1.002525000
H	-2.166302000	-6.119643000	-0.776987000
H	-2.575708000	-8.175324000	2.362619000
H	-3.073859000	-9.662304000	1.536017000
H	-4.180966000	-8.279393000	1.614486000
H	-4.384532000	-8.341955000	-0.973516000
H	-3.266052000	-9.717551000	-1.013942000
H	-2.917855000	-8.264919000	-1.968541000
H	-0.475505000	-8.030585000	0.903551000
H	-0.616444000	-8.076418000	-0.865799000
H	-0.958180000	-9.527924000	0.090283000
H	5.480343000	-6.968804000	1.088900000
H	5.551369000	-6.903294000	-0.691584000
H	2.765804000	-9.368446000	-1.273803000
H	3.934755000	-8.313954000	-2.088307000
H	2.546100000	-7.609208000	-1.238759000
H	2.450434000	-7.708754000	1.357534000
H	3.779565000	-8.470871000	2.251752000
H	2.678197000	-9.465668000	1.282447000
H	5.849315000	-9.382568000	-0.774684000
H	4.689008000	-10.447967000	0.035790000

H	5.788952000	-9.447624000	0.998789000
H	-4.752717000	0.726597000	5.158154000
H	-7.212835000	0.782198000	5.701619000
H	-4.062024000	0.377429000	2.790183000
H	-10.146584000	-0.444723000	-2.121348000
H	-11.399848000	-0.140662000	-0.002855000
H	-7.125350000	-0.933645000	-5.658147000
H	-4.673753000	-0.801216000	-5.089482000
H	-4.018631000	-0.427660000	-2.715172000
H	7.202365000	-0.737832000	-5.668145000
H	8.836772000	-0.443117000	-3.820898000
H	11.390786000	0.185269000	0.035259000
H	10.138043000	0.489352000	2.154060000
H	8.778183000	0.730177000	3.860657000
H	7.117688000	0.978185000	5.691611000

Cartesian coordinates of DFT-optimized structure of **8b** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Ru	4.983738000	-0.359031000	-0.208774000
N	5.472466000	0.158341000	1.766846000
N	7.020202000	-0.457726000	-0.237979000
N	5.363386000	-0.918401000	-2.196774000
C	4.620147000	0.466566000	2.763512000
H	3.567970000	0.437026000	2.506207000
C	5.043437000	0.802280000	4.045244000
H	4.308709000	1.041683000	4.806079000
C	6.410614000	0.822101000	4.318944000
H	6.777866000	1.079491000	5.306923000
C	7.303179000	0.503985000	3.299130000
H	8.370357000	0.511346000	3.487834000
C	6.822439000	0.174556000	2.029548000
C	7.702596000	-0.175534000	0.895806000
C	9.098815000	-0.236320000	0.900933000
H	9.666163000	-0.015056000	1.797302000
C	9.759475000	-0.590750000	-0.277218000
C	9.034203000	-0.877903000	-1.435505000
H	9.551591000	-1.151881000	-2.347405000
C	7.639369000	-0.803164000	-1.390397000
C	6.697391000	-1.064851000	-2.498005000
C	7.107447000	-1.437512000	-3.780368000
H	8.163065000	-1.547863000	-3.999524000
C	6.159474000	-1.666313000	-4.773785000
H	6.471656000	-1.956678000	-5.771510000
C	4.809032000	-1.514595000	-4.461097000
H	4.033103000	-1.680695000	-5.200255000
C	4.457076000	-1.141263000	-3.168255000
H	3.420496000	-1.010328000	-2.881004000
C	-3.323694000	1.204830000	-0.408935000
C	2.249032000	-1.388353000	0.153318000

C	-4.078685000	0.079949000	-0.075265000
C	3.003951000	-0.263327000	-0.180097000
C	-3.426548000	-1.113283000	0.237273000
C	2.351719000	0.929773000	-0.492844000
C	-2.020281000	-1.192969000	0.343298000
C	0.945467000	1.009250000	-0.599307000
C	-1.255332000	-0.057095000	-0.117445000
C	0.180565000	-0.126691000	-0.138669000
C	-1.920089000	1.148142000	-0.556950000
C	0.845382000	-1.331870000	0.300897000
C	-1.124975000	2.171558000	-1.163105000
C	0.050216000	-2.355379000	0.906852000
H	-1.607708000	2.991072000	-1.679672000
H	0.532897000	-3.175031000	1.423251000
C	0.235518000	2.105633000	-1.183188000
C	-1.310272000	-2.289446000	0.926963000
H	0.779831000	2.875394000	-1.714865000
H	-1.854506000	-3.059347000	1.458506000
H	10.842855000	-0.643354000	-0.292726000
N	-4.357252000	-2.175108000	0.456919000
N	-5.696063000	-1.823468000	0.452385000
C	-6.383992000	-2.959232000	0.591627000
C	-5.515040000	-4.060994000	0.667710000
C	-4.243386000	-3.530411000	0.565746000
H	-7.463896000	-2.929926000	0.617505000
H	-5.776518000	-5.103042000	0.773564000
H	-3.287905000	-4.023973000	0.530568000
Ru	-6.058426000	0.176120000	-0.045124000
C	-5.879763000	1.332519000	4.206890000
C	-5.529000000	0.959024000	2.913766000
N	-6.436224000	0.735738000	1.943251000
C	-7.769952000	0.881927000	2.245758000
C	-8.178838000	1.254745000	3.528448000
C	-7.229935000	1.483959000	4.520883000
C	-8.712973000	0.619791000	1.139141000
N	-8.094866000	0.274590000	-0.013910000
C	-8.778332000	-0.008108000	-1.146928000
C	-10.174592000	0.051940000	-1.150551000
C	-10.834161000	0.406203000	0.028258000
C	-10.107789000	0.693850000	1.185736000
C	-7.899212000	-0.357950000	-2.281549000
N	-6.548968000	-0.341324000	-2.020177000
C	-5.697553000	-0.649232000	-3.017727000
C	-6.122017000	-0.985038000	-4.299042000
C	-7.489460000	-1.005302000	-4.571378000
C	-8.381104000	-0.687502000	-3.550661000
H	-4.492672000	0.828320000	2.625500000
H	-5.103149000	1.498938000	4.945256000
H	-7.541200000	1.774441000	5.518861000
H	-9.234264000	1.364936000	3.748603000
H	-10.624334000	0.967649000	2.098170000

H	-11.917551000	0.458251000	0.044932000
H	-10.742794000	-0.169816000	-2.046256000
H	-9.448466000	-0.695164000	-3.738320000
H	-7.857615000	-1.262765000	-5.559000000
H	-5.387966000	-1.224171000	-5.060615000
H	-4.645129000	-0.619349000	-2.761474000
N	-4.153337000	2.352167000	-0.602028000
N	-5.519174000	2.131912000	-0.556364000
C	-6.097712000	3.329175000	-0.676609000
C	-5.128805000	4.341642000	-0.780771000
C	-3.912040000	3.690194000	-0.716505000
H	-2.912618000	4.088823000	-0.711100000
H	-5.291154000	5.404261000	-0.880384000
H	-7.175662000	3.404680000	-0.669742000
N	3.078826000	-2.535501000	0.346819000
C	2.837736000	-3.873559000	0.461327000
C	4.054601000	-4.524745000	0.526434000
C	5.023364000	-3.512085000	0.422749000
N	4.444639000	-2.314962000	0.302020000
N	3.282291000	1.991810000	-0.712004000
N	4.621189000	1.640462000	-0.706547000
C	5.308970000	2.776401000	-0.845174000
C	4.439827000	3.877974000	-0.921719000
C	3.168210000	3.347094000	-0.820730000
H	1.838399000	-4.272393000	0.455289000
H	4.217120000	-5.587319000	0.626245000
H	6.101334000	-3.587367000	0.416512000
H	2.212583000	3.840424000	-0.786216000
H	4.701128000	4.920096000	-1.027278000
H	6.388897000	2.747327000	-0.870373000

Cartesian coordinates of DFT-optimized structure of **9b** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Ru	4.987462000	-0.190361000	-0.000082000
N	4.491808000	-2.214312000	0.306807000
N	5.460984000	0.129319000	2.016428000
N	7.027722000	-0.271676000	-0.020971000
N	5.392324000	-0.540980000	-2.026566000
C	4.596303000	0.334121000	3.030588000
H	3.547501000	0.327640000	2.758634000
C	5.004064000	0.541589000	4.343531000
H	4.259877000	0.701233000	5.116076000
C	6.368640000	0.539543000	4.633948000
H	6.723450000	0.698075000	5.646988000
C	7.273543000	0.330105000	3.597716000
H	8.338797000	0.325117000	3.797402000
C	6.808812000	0.126288000	2.295649000
C	7.701642000	-0.103808000	1.142752000
C	9.097911000	-0.161170000	1.154142000

H	9.656510000	-0.029965000	2.073576000
C	9.771045000	-0.392868000	-0.047661000
C	9.056959000	-0.563035000	-1.235985000
H	9.583485000	-0.742788000	-2.166119000
C	7.661511000	-0.496864000	-1.197380000
C	6.730081000	-0.647697000	-2.332472000
C	7.151034000	-0.882133000	-3.644248000
H	8.209085000	-0.962527000	-3.864943000
C	6.212007000	-1.011600000	-4.663041000
H	6.532740000	-1.193562000	-5.683479000
C	4.857808000	-0.902753000	-4.345527000
H	4.088092000	-0.996793000	-5.103714000
C	4.494168000	-0.668846000	-3.024098000
H	3.455120000	-0.576926000	-2.731081000
C	5.368494000	-3.238946000	0.350406000
H	6.417238000	-2.963484000	0.360869000
C	4.997169000	-4.568825000	0.370207000
H	5.739673000	-5.357471000	0.405580000
C	3.628343000	-4.878600000	0.307336000
C	2.704810000	-3.829431000	0.272371000
H	1.651001000	-4.037480000	0.175874000
C	3.140846000	-2.494790000	0.311690000
C	-3.333162000	1.258252000	-0.310181000
C	2.279573000	-1.302007000	0.255217000
C	-4.076841000	0.121292000	0.008369000
C	3.014690000	-0.120485000	0.013116000
C	-3.412251000	-1.061959000	0.332249000
C	2.362356000	1.108410000	-0.227297000
C	-2.005502000	-1.122584000	0.455211000
C	0.949116000	1.135033000	-0.383105000
C	-1.250874000	0.026682000	0.015308000
C	0.187086000	-0.022872000	0.015675000
C	-1.924897000	1.224700000	-0.425767000
C	0.867630000	-1.229927000	0.415045000
C	-1.129524000	2.264074000	-1.002449000
C	0.078530000	-2.261404000	1.016992000
H	-1.610505000	3.079372000	-1.527478000
H	0.573290000	-3.078515000	1.527278000
C	0.233098000	2.221929000	-0.978826000
C	-1.284005000	-2.210809000	1.038436000
H	0.783804000	3.007611000	-1.480801000
H	-1.819964000	-2.987740000	1.568463000
O	3.309921000	-6.187556000	0.277437000
C	1.927693000	-6.579843000	0.199623000
C	1.838339000	-8.113015000	0.200887000
C	0.344444000	-8.479605000	0.106203000
C	2.592307000	-8.688708000	-1.012881000
C	2.429437000	-8.674923000	1.507795000
H	1.387578000	-6.163080000	1.059891000
H	1.490317000	-6.170348000	-0.720322000
H	0.222257000	-9.568560000	0.107763000

H	-0.105353000	-8.093459000	-0.816631000
H	-0.221798000	-8.077713000	0.955273000
H	2.182011000	-8.300660000	-1.953491000
H	2.503837000	-9.781127000	-1.033184000
H	3.656520000	-8.434879000	-0.976291000
H	1.893384000	-8.286033000	2.382552000
H	3.486409000	-8.409411000	1.611207000
H	2.349884000	-9.768044000	1.523715000
H	10.854688000	-0.440919000	-0.058163000
N	-4.330414000	-2.137123000	0.537321000
N	-5.674547000	-1.805990000	0.506267000
C	-6.347597000	-2.951161000	0.638565000
C	-5.463712000	-4.039313000	0.737134000
C	-4.198606000	-3.490270000	0.656775000
H	-7.428067000	-2.937983000	0.643431000
H	-5.711570000	-5.084627000	0.843481000
H	-3.235808000	-3.970227000	0.643496000
Ru	-6.058629000	0.184705000	-0.004320000
C	-5.992571000	1.362736000	4.244268000
C	-5.607254000	0.988250000	2.961282000
N	-6.489015000	0.744443000	1.972311000
C	-7.831319000	0.871664000	2.244330000
C	-8.274410000	1.245515000	3.515227000
C	-7.351638000	1.494351000	4.527368000
C	-8.745504000	0.588796000	1.118967000
N	-8.096687000	0.248633000	-0.018628000
C	-8.750216000	-0.051007000	-1.164773000
C	-10.146866000	-0.014682000	-1.199361000
C	-10.837916000	0.334006000	-0.036969000
C	-10.142037000	0.639571000	1.134689000
C	-7.840297000	-0.389989000	-2.277852000
N	-6.496595000	-0.347307000	-1.987282000
C	-5.618509000	-0.643619000	-2.965183000
C	-6.009037000	-0.991386000	-4.254084000
C	-7.369689000	-1.037900000	-4.555713000
C	-8.288708000	-0.733513000	-3.555430000
H	-4.562763000	0.875127000	2.695942000
H	-5.235235000	1.545876000	4.998534000
H	-7.689669000	1.785088000	5.516559000
H	-9.336051000	1.341172000	3.710746000
H	-10.683137000	0.908715000	2.034200000
H	-11.922142000	0.367605000	-0.044133000
H	-10.691610000	-0.250451000	-2.106048000
H	-9.351515000	-0.762322000	-3.765155000
H	-7.711704000	-1.305360000	-5.550088000
H	-5.254422000	-1.219604000	-4.998720000
H	-4.572597000	-0.595263000	-2.686179000
N	-4.177585000	2.391167000	-0.522341000
N	-5.540761000	2.147712000	-0.507376000
C	-6.136395000	3.334504000	-0.644433000
C	-5.182622000	4.363200000	-0.729940000

C	-3.956802000	3.733118000	-0.636562000
C	3.302552000	2.240248000	-0.289365000
N	4.637910000	1.866737000	-0.295253000
C	5.576981000	2.825585000	-0.339291000
C	5.306174000	4.187690000	-0.351908000
C	3.963961000	4.584801000	-0.280542000
C	2.971785000	3.595739000	-0.244099000
O	3.533074000	5.860722000	-0.233962000
C	4.497557000	6.929554000	-0.246837000
C	3.760925000	8.274134000	-0.159423000
C	4.834876000	9.379512000	-0.176186000
C	2.955673000	8.352097000	1.151526000
C	2.822556000	8.443215000	-1.369269000
H	5.083106000	6.872153000	-1.173658000
H	5.178265000	6.807927000	0.605723000
H	5.430044000	9.346425000	-1.096964000
H	5.520073000	9.286501000	0.675300000
H	4.362317000	10.366584000	-0.118729000
H	3.610675000	8.240969000	2.024610000
H	2.193903000	7.567198000	1.196688000
H	2.450590000	9.321592000	1.231726000
H	3.382131000	8.401955000	-2.312005000
H	2.312093000	9.412180000	-1.323655000
H	2.059923000	7.658207000	-1.392418000
H	6.125433000	4.893378000	-0.391353000
H	6.604776000	2.479496000	-0.354507000
H	1.944237000	3.915640000	-0.144818000
H	-2.964972000	4.149442000	-0.610584000
H	-5.360939000	5.422619000	-0.836128000
H	-7.215346000	3.391944000	-0.662754000

Cartesian coordinates of DFT-optimized structure of **10b** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Ru	5.459480000	0.853480000	-0.017192000
N	5.361377000	-1.225610000	0.301772000
N	5.794623000	1.281547000	2.009187000
N	7.467708000	1.211454000	0.014018000
N	5.985538000	0.567521000	-2.027467000
C	4.882827000	1.290275000	3.001659000
H	3.869182000	1.045284000	2.707465000
C	5.202645000	1.590174000	4.321421000
H	4.423723000	1.581890000	5.075940000
C	6.525334000	1.896040000	4.641268000
H	6.811811000	2.135375000	5.660070000
C	7.478765000	1.887877000	3.627349000
H	8.513584000	2.119611000	3.850866000
C	7.102199000	1.578908000	2.317977000
C	8.053187000	1.544753000	1.188675000
C	9.424317000	1.812033000	1.231992000

H	9.913756000	2.080425000	2.160986000
C	10.162733000	1.727853000	0.049471000
C	9.537768000	1.383609000	-1.151233000
H	10.114889000	1.321271000	-2.066436000
C	8.164341000	1.125884000	-1.144032000
C	7.321374000	0.754930000	-2.298372000
C	7.820357000	0.599091000	-3.594108000
H	8.875527000	0.752269000	-3.788198000
C	6.961651000	0.247370000	-4.631614000
H	7.342981000	0.124769000	-5.639982000
C	5.609010000	0.057377000	-4.348836000
H	4.900684000	-0.217500000	-5.122650000
C	5.165965000	0.226743000	-3.041614000
H	4.124256000	0.091117000	-2.775940000
C	6.423139000	-2.055664000	0.365493000
H	7.395406000	-1.576600000	0.397928000
C	6.323694000	-3.433064000	0.378158000
H	7.207764000	-4.057819000	0.429135000
C	5.046039000	-4.009272000	0.287246000
C	3.932765000	-3.164138000	0.235034000
H	2.944395000	-3.578593000	0.116939000
C	4.092412000	-1.770400000	0.280736000
C	-3.008643000	0.773636000	-0.208367000
C	3.008788000	-0.772283000	0.207332000
C	-3.509820000	-0.520812000	0.032232000
C	3.509985000	0.522135000	-0.033338000
C	-2.630872000	-1.582694000	0.270377000
C	2.631050000	1.584017000	-0.271505000
C	-1.239787000	-1.387993000	0.400884000
C	1.239953000	1.389337000	-0.401960000
C	-0.712142000	-0.100631000	0.011120000
C	0.712298000	0.101993000	-0.012152000
C	-1.604864000	0.970066000	-0.353781000
C	1.605015000	-0.968707000	0.352743000
C	-1.019643000	2.147266000	-0.920732000
C	1.019809000	-2.145938000	0.919636000
H	-1.657259000	2.876091000	-1.404771000
H	1.657445000	-2.874800000	1.403602000
C	0.328366000	2.351077000	-0.939648000
C	-0.328198000	-2.349759000	0.938528000
H	0.711244000	3.233606000	-1.436598000
H	-0.711073000	-3.232328000	1.435409000
O	4.994180000	-5.354533000	0.248552000
C	3.718136000	-6.013899000	0.152661000
C	3.936893000	-7.533639000	0.129106000
C	2.545454000	-8.188811000	0.027411000
C	4.787252000	-7.926371000	-1.093912000
C	4.631301000	-7.988146000	1.426829000
H	3.101776000	-5.727249000	1.014923000
H	3.212825000	-5.685402000	-0.764793000
H	2.642282000	-9.280137000	0.006100000

H	2.022679000	-7.880847000	-0.886405000
H	1.914953000	-7.925492000	0.885473000
H	4.301846000	-7.617836000	-2.028229000
H	4.924648000	-9.013248000	-1.129827000
H	5.776774000	-7.459761000	-1.055096000
H	4.032264000	-7.725309000	2.307540000
H	5.616123000	-7.522344000	1.534465000
H	4.768105000	-9.075715000	1.425933000
H	11.228064000	1.931839000	0.063465000
N	3.317077000	2.831183000	-0.388459000
C	2.919066000	4.136436000	-0.405069000
C	4.051082000	4.928893000	-0.428160000
C	5.132579000	4.031924000	-0.402430000
N	4.697622000	2.769820000	-0.366378000
N	-3.316871000	-2.829887000	0.387219000
N	-4.697418000	-2.768560000	0.365064000
C	-5.132341000	-4.030675000	0.401045000
C	-4.050824000	-4.927617000	0.426824000
C	-2.918825000	-4.135130000	0.403785000
C	-4.092314000	1.771730000	-0.281708000
C	-3.932754000	3.165473000	-0.235808000
C	-5.046065000	4.010556000	-0.287983000
C	-6.323686000	3.434300000	-0.379043000
C	-6.423062000	2.056898000	-0.366533000
N	-5.361260000	1.226888000	-0.302844000
O	-4.994272000	5.355813000	-0.249105000
C	-3.718259000	6.015212000	-0.153058000
C	-3.937072000	7.534941000	-0.129314000
C	-2.545661000	8.190150000	-0.027461000
C	-4.631429000	7.989592000	-1.427014000
C	-4.787508000	7.927480000	1.093712000
H	-6.194376000	-4.230394000	0.394465000
H	-4.087133000	-6.006349000	0.450066000
H	-1.879529000	-4.411370000	0.365480000
H	-2.944422000	3.579969000	-0.117566000
H	-7.207784000	4.059017000	-0.429990000
H	-7.395302000	1.577784000	-0.399061000
H	-3.101842000	5.728699000	-1.015325000
H	-3.212984000	5.686612000	0.764379000
H	-2.022921000	7.882080000	0.886339000
H	-2.642530000	9.281469000	-0.006006000
H	-1.915108000	7.926971000	-0.885527000
H	-4.032339000	7.726892000	-2.307728000
H	-4.768273000	9.077157000	-1.425983000
H	-5.616230000	7.523769000	-1.534760000
H	-4.302142000	7.618835000	2.028012000
H	-5.777013000	7.460845000	1.054780000
H	-4.924940000	9.014348000	1.129767000
Ru	-5.459303000	-0.852223000	0.015963000
C	-5.609081000	-0.056378000	4.347640000
C	-5.165967000	-0.225654000	3.040433000

N	-5.985478000	-0.566418000	2.026227000
C	-7.321318000	-0.753903000	2.297059000
C	-7.820367000	-0.598155000	3.592778000
C	-6.961728000	-0.246449000	4.630344000
C	-8.164212000	-1.124829000	1.142655000
N	-7.467523000	-1.210281000	-0.015370000
C	-8.052928000	-1.543535000	-1.190076000
C	-9.424039000	-1.810896000	-1.233471000
C	-10.162514000	-1.726840000	-0.050979000
C	-9.537622000	-1.382639000	1.149776000
C	-7.101888000	-1.577557000	-2.319339000
N	-5.794339000	-1.280161000	-2.010466000
C	-4.882495000	-1.288766000	-3.002897000
C	-5.202239000	-1.588568000	-4.322696000
C	-6.524901000	-1.894467000	-4.642631000
C	-7.478376000	-1.886432000	-3.628753000
H	-4.124251000	-0.089968000	2.774811000
H	-4.900806000	0.218491000	5.121501000
H	-7.343112000	-0.123920000	5.638699000
H	-8.875540000	-0.751391000	3.786805000
H	-10.114788000	-1.320399000	2.064958000
H	-11.227831000	-1.930893000	-0.065034000
H	-9.913417000	-2.079257000	-2.162506000
H	-8.513176000	-2.118193000	-3.852333000
H	-6.811321000	-2.133729000	-5.661465000
H	-4.423283000	-1.580185000	-5.077178000
H	-3.868875000	-1.043752000	-2.708632000
H	4.087413000	6.007624000	-0.451415000
H	1.879778000	4.412704000	-0.366744000
H	6.194620000	4.231609000	-0.395911000

Cartesian coordinates of DFT-optimized structure of **11b** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Ru	5.629169000	-0.949220000	0.031262000
N	5.169759000	1.081668000	-0.276262000
N	6.069882000	-1.291200000	-1.991022000
N	7.670384000	-0.950575000	0.034131000
N	6.063575000	-0.592019000	2.052036000
N	-5.077527000	0.799973000	-0.257374000
C	5.189952000	-1.449655000	-2.999590000
H	4.144424000	-1.392628000	-2.721008000
C	5.578793000	-1.673017000	-4.315942000
H	4.822873000	-1.793488000	-5.084154000
C	6.939702000	-1.737447000	-4.614716000
H	7.280131000	-1.910061000	-5.630372000
C	7.860369000	-1.575367000	-3.583586000
H	8.923290000	-1.620347000	-3.790485000
C	7.414009000	-1.352967000	-2.278393000
C	8.324971000	-1.168268000	-1.130944000

C	9.722047000	-1.200478000	-1.149362000
H	10.266258000	-1.374989000	-2.070145000
C	10.414130000	-1.004170000	0.047725000
C	9.718387000	-0.781221000	1.238083000
H	10.260073000	-0.631498000	2.164700000
C	8.321420000	-0.758627000	1.205823000
C	7.407004000	-0.545482000	2.345752000
C	7.849511000	-0.309711000	3.649828000
H	8.911856000	-0.275186000	3.861567000
C	6.925770000	-0.117512000	4.673096000
H	7.263316000	0.065877000	5.687827000
C	5.565728000	-0.164146000	4.367389000
H	4.807591000	-0.019017000	5.129126000
C	5.180655000	-0.401938000	3.052384000
H	4.135765000	-0.445093000	2.768791000
C	6.070974000	2.083808000	-0.337357000
H	7.111865000	1.780998000	-0.364499000
C	5.733090000	3.422674000	-0.355066000
H	6.494651000	4.192023000	-0.406164000
C	4.374079000	3.767216000	-0.270714000
C	3.424899000	2.741627000	-0.215331000
H	2.379251000	2.977553000	-0.099511000
C	3.824710000	1.396592000	-0.258580000
C	-2.695852000	-2.327771000	0.254468000
C	2.932340000	0.224840000	-0.192250000
C	-3.442790000	-1.163355000	0.032614000
C	3.651643000	-0.964420000	0.026547000
C	-2.791066000	0.063779000	-0.182936000
C	2.971452000	-2.167986000	0.253704000
C	-3.744220000	1.186888000	-0.241461000
C	-3.427918000	2.544881000	-0.190643000
H	-2.404681000	2.874909000	-0.083634000
C	-4.429131000	3.524967000	-0.233195000
C	-5.766590000	3.115241000	-0.315804000
H	-6.592313000	3.812964000	-0.360803000
C	-6.024659000	1.750484000	-0.306920000
H	-7.049097000	1.394977000	-0.329702000
C	-1.370665000	0.096377000	-0.314786000
C	1.571803000	-2.218600000	0.401647000
C	-0.614746000	-1.075268000	0.045385000
C	0.823303000	-1.034413000	0.044083000
C	-1.295265000	-2.299854000	0.401898000
C	1.511339000	0.177343000	-0.320337000
C	-0.511056000	-3.377780000	0.926875000
C	0.721052000	1.235592000	-0.866859000
H	-1.003825000	-4.220849000	1.394614000
H	1.211633000	2.066566000	-1.357990000
C	0.849859000	-3.338944000	0.927314000
C	-0.643966000	1.198317000	-0.862255000
H	1.389648000	-4.152691000	1.395144000
H	-1.183827000	2.002382000	-1.346448000

O	4.088870000	5.083342000	-0.242501000
O	-4.009571000	4.804002000	-0.181800000
C	-4.981830000	5.865716000	-0.213578000
C	-4.255976000	7.215965000	-0.123416000
C	-5.337270000	8.313558000	-0.164419000
C	-3.299435000	7.384348000	-1.319062000
C	-3.472168000	7.308206000	1.199583000
C	2.717076000	5.511823000	-0.162637000
C	2.666459000	7.046356000	-0.190476000
C	1.182540000	7.452083000	-0.094766000
C	3.441198000	7.624169000	1.009076000
C	3.264168000	7.570336000	-1.510019000
H	-5.673268000	5.743653000	0.630192000
H	-5.553864000	5.798512000	-1.148084000
H	-6.035429000	8.221090000	0.676523000
H	-5.917310000	8.270352000	-1.094369000
H	-4.872580000	9.304263000	-0.105767000
H	-3.842681000	7.330909000	-2.270685000
H	-2.529182000	6.606293000	-1.323457000
H	-2.798719000	8.358308000	-1.272240000
H	-4.139702000	7.196900000	2.063089000
H	-2.976391000	8.282318000	1.281789000
H	-2.704641000	6.529981000	1.261504000
H	2.161556000	5.094103000	-1.012418000
H	2.275712000	5.129632000	0.767007000
H	1.087551000	8.543592000	-0.114975000
H	0.728374000	7.093557000	0.837049000
H	0.601217000	7.049745000	-0.933534000
H	3.024915000	7.265181000	1.958522000
H	3.382486000	8.718768000	1.009060000
H	4.498009000	7.340986000	0.972814000
H	2.714197000	7.179245000	-2.375076000
H	4.313797000	7.277361000	-1.613827000
H	3.211082000	8.664614000	-1.544848000
H	11.498663000	-1.026024000	0.053227000
N	3.865443000	-3.277512000	0.351599000
C	3.702117000	-4.632156000	0.327560000
C	4.955044000	-5.214795000	0.346097000
C	5.862761000	-4.141931000	0.358819000
N	5.213969000	-2.974821000	0.349461000
N	-3.526328000	-3.486007000	0.346880000
C	-3.287261000	-4.829386000	0.324646000
C	-4.505641000	-5.481190000	0.337407000
C	-5.472180000	-4.460941000	0.344827000
N	-4.889746000	-3.259242000	0.337724000
H	6.943317000	-4.152881000	0.361254000
H	5.179679000	-6.270745000	0.341579000
H	2.727679000	-5.084554000	0.265439000
H	-2.288806000	-5.226875000	0.268546000
H	-4.670751000	-6.548068000	0.332597000
H	-6.550361000	-4.533511000	0.342866000

Ru	-5.418906000	-1.258946000	0.029334000
C	-5.292620000	-1.927396000	-4.325922000
C	-4.927047000	-1.697121000	-3.004088000
N	-5.821844000	-1.604015000	-2.000549000
C	-7.157881000	-1.742033000	-2.299099000
C	-7.581050000	-1.974589000	-3.610198000
C	-6.645134000	-2.069395000	-4.635970000
C	-8.086783000	-1.625802000	-1.157097000
C	-9.479105000	-1.743275000	-1.187370000
C	-10.190865000	-1.603757000	0.006124000
C	-9.519078000	-1.352047000	1.204503000
C	-8.126035000	-1.242860000	1.183871000
N	-7.455546000	-1.381457000	0.015584000
C	-7.234945000	-0.986155000	2.333312000
N	-5.889126000	-0.947461000	2.049767000
C	-5.026658000	-0.713825000	3.058656000
C	-5.435022000	-0.512586000	4.372717000
C	-6.797615000	-0.551992000	4.668075000
C	-7.700533000	-0.790337000	3.635950000
H	-4.525500000	-1.993154000	-5.089664000
H	-3.888942000	-1.580439000	-2.716534000
H	-8.637981000	-2.079930000	-3.825502000
H	-6.967481000	-2.249781000	-5.656170000
H	-10.004609000	-1.939780000	-2.114641000
H	-11.272007000	-1.692196000	0.002513000
H	-10.076109000	-1.246347000	2.128143000
H	-3.979021000	-0.691027000	2.782810000
H	-4.692753000	-0.329030000	5.141747000
H	-7.153059000	-0.399375000	5.681793000
H	-8.764479000	-0.822978000	3.839560000

Cartesian coordinates of DFT-optimized structure of **7a<sub>ox</sub>** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Os	-5.504546000	-0.051799000	0.032316000
Os	5.495434000	0.096412000	0.001501000
N	-5.064135000	-2.104594000	0.293274000
N	5.055101000	2.149257000	-0.259401000
N	-5.975501000	0.236266000	2.059907000
N	5.965917000	-0.191717000	-2.026200000
N	-7.584088000	-0.081493000	0.045856000
N	7.575056000	0.126023000	-0.012600000
N	-5.992539000	-0.354628000	-1.989984000
N	5.984061000	0.399271000	2.023647000
N	-5.125921000	2.012358000	-0.236210000
N	5.116833000	-1.967743000	0.270192000
C	-5.084230000	0.398286000	3.064436000
C	5.074354000	-0.353725000	-3.030470000
H	4.031084000	-0.324210000	-2.743370000
C	-5.466786000	0.590312000	4.385176000

C	5.456543000	-0.545813000	-4.351310000
H	4.694118000	-0.669709000	-5.112088000
C	-6.825452000	0.619379000	4.700484000
C	6.815117000	-0.574958000	-4.666985000
C	-7.753159000	0.454052000	3.677239000
C	7.743115000	-0.409640000	-3.644001000
H	-8.814328000	0.473367000	3.894878000
C	-7.320130000	0.263043000	2.363810000
C	7.310455000	-0.218563000	-2.330465000
C	-8.235351000	0.079283000	1.225048000
C	8.225988000	-0.034802000	-1.191953000
C	-9.631258000	0.055668000	1.258326000
C	9.621886000	-0.011229000	-1.225613000
H	-10.169806000	0.180929000	2.190045000
H	10.160180000	-0.136521000	-2.157475000
C	-10.330189000	-0.134122000	0.064686000
C	10.321141000	0.178565000	-0.032165000
C	-9.641272000	-0.297920000	-1.138459000
C	9.632554000	0.342411000	1.171160000
C	-8.245081000	-0.268501000	-1.123850000
C	8.236359000	0.313038000	1.156916000
C	-7.339836000	-0.422846000	-2.274759000
C	7.331427000	0.467450000	2.308064000
C	-7.785946000	-0.625962000	-3.581917000
C	7.777888000	0.670593000	3.615092000
H	-8.849176000	-0.676898000	-3.783792000
C	-6.868701000	-0.762930000	-4.618629000
C	6.860916000	0.807620000	4.652040000
C	-5.507215000	-0.692262000	-4.322771000
C	5.499353000	0.736985000	4.356543000
H	4.744960000	0.837262000	5.128753000
C	-5.111545000	-0.488696000	-3.007523000
C	5.103328000	0.533394000	3.041403000
H	4.057360000	0.471446000	2.769986000
C	-5.961169000	-3.114714000	0.321701000
C	5.952151000	3.159353000	-0.287933000
H	-7.004575000	-2.822897000	0.338505000
H	6.995548000	2.867518000	-0.304898000
C	-5.611173000	-4.449412000	0.319084000
C	5.602176000	4.494060000	-0.285236000
H	-6.368738000	-5.223767000	0.342961000
H	6.359751000	5.268401000	-0.309207000
C	-4.249368000	-4.785514000	0.248431000
C	4.240388000	4.830185000	-0.214398000
C	-3.306392000	-3.750118000	0.224702000
C	3.297392000	3.794800000	-0.190559000
H	-2.257593000	-3.976082000	0.117616000
H	2.248607000	4.020773000	-0.083349000
C	-3.716965000	-2.412757000	0.288147000
C	3.707944000	2.457446000	-0.254062000
C	-2.826991000	-1.236763000	0.244284000

C	2.817937000	1.281467000	-0.210057000
C	-3.539863000	-0.025792000	0.023963000
C	3.530776000	0.070476000	0.010245000
C	-2.860796000	1.203321000	-0.201292000
C	2.851723000	-1.158624000	0.235592000
C	-3.780413000	2.356808000	-0.244721000
C	3.771317000	-2.312143000	0.278946000
C	-3.417524000	3.700245000	-0.197182000
C	3.408365000	-3.655562000	0.231574000
H	-2.382288000	3.995507000	-0.106116000
H	2.373099000	-3.950791000	0.140727000
C	-4.387538000	4.715227000	-0.223014000
C	4.378354000	-4.670579000	0.257303000
C	-5.738374000	4.347558000	-0.278154000
C	5.729211000	-4.302955000	0.312180000
H	-6.542056000	5.070910000	-0.305206000
H	6.532871000	-5.026333000	0.339146000
C	-6.044032000	2.994343000	-0.265871000
C	6.034916000	-2.949750000	0.299756000
H	-7.079778000	2.675672000	-0.270569000
H	7.070674000	-2.631116000	0.304256000
C	-1.458743000	1.197493000	-0.363158000
C	1.449680000	-1.152764000	0.397528000
C	-0.717988000	0.012241000	0.017878000
C	0.708930000	0.032497000	0.016491000
C	-1.424543000	-1.193221000	0.401010000
C	1.415483000	1.237953000	-0.366685000
C	-0.651658000	-2.251997000	0.982728000
C	0.642595000	2.296746000	-0.948364000
H	-1.160132000	-3.058473000	1.496195000
H	1.151067000	3.103230000	-1.461823000
C	0.708777000	-2.233165000	0.980282000
C	-0.717838000	2.277902000	-0.945905000
H	1.242091000	-3.025894000	1.489546000
H	-1.251152000	3.070630000	-1.455167000
O	-3.954861000	-6.094793000	0.199273000
O	3.918199000	-5.931626000	0.217705000
O	3.945902000	6.139457000	-0.165191000
O	-3.927434000	5.976296000	-0.183239000
C	-4.869004000	7.069529000	-0.193139000
C	-4.101997000	8.398202000	-0.142567000
C	-5.154642000	9.524226000	-0.146182000
C	-3.194168000	8.532214000	-1.379831000
C	-3.261662000	8.477637000	1.145962000
C	2.570090000	6.560596000	-0.076097000
C	2.514238000	8.095057000	-0.062909000
C	1.029064000	8.490487000	0.051562000
C	3.292726000	8.643263000	1.148101000
C	3.103157000	8.655923000	-1.371222000
C	-2.579037000	-6.515911000	0.110350000
C	-2.523158000	-8.050373000	0.097293000

C	-3.112141000	-8.611133000	1.405623000
C	-3.301573000	-8.598697000	-1.113709000
C	-1.037974000	-8.445795000	-0.017062000
C	4.859731000	-7.024898000	0.227513000
C	4.092664000	-8.353544000	0.177180000
C	3.252090000	-8.433039000	-1.111189000
C	3.185060000	-8.487434000	1.414622000
C	5.145269000	-9.479606000	0.180682000
H	-5.532913000	6.973128000	0.675234000
H	-5.472742000	7.009201000	-1.107400000
H	-5.817579000	9.455680000	0.724814000
H	-5.774726000	9.490744000	-1.050181000
H	-4.661004000	10.501949000	-0.115038000
H	-3.780492000	8.490174000	-2.306169000
H	-2.447308000	7.732184000	-1.414366000
H	-2.663706000	9.491170000	-1.361216000
H	-3.896152000	8.394818000	2.037101000
H	-2.733971000	9.436901000	1.197440000
H	-2.515476000	7.677378000	1.184991000
H	2.019043000	6.162717000	-0.937867000
H	2.131740000	6.151121000	0.842989000
H	0.929185000	9.581602000	0.063173000
H	0.580753000	8.103387000	0.974752000
H	0.445833000	8.110269000	-0.795917000
H	2.882352000	8.257488000	2.089532000
H	3.229465000	9.737107000	1.177199000
H	4.350491000	8.365550000	1.099387000
H	2.549692000	8.287064000	-2.243740000
H	4.153183000	8.369228000	-1.488703000
H	3.047407000	9.750478000	-1.376288000
H	-2.028078000	-6.117957000	0.972142000
H	-2.140603000	-6.106498000	-0.808724000
H	-2.558726000	-8.242193000	2.278139000
H	-3.056381000	-9.705686000	1.410786000
H	-4.162176000	-8.324435000	1.523022000
H	-4.359342000	-8.320986000	-1.065081000
H	-3.238302000	-9.692544000	-1.142702000
H	-2.891148000	-8.213007000	-2.055154000
H	-0.454788000	-8.065483000	0.830406000
H	-0.589621000	-8.058788000	-0.940270000
H	-0.938079000	-9.536911000	-0.028554000
H	5.463639000	-6.964520000	1.141659000
H	5.523481000	-6.928582000	-0.640990000
H	2.724341000	-9.392280000	-1.162496000
H	3.886422000	-8.350321000	-2.002450000
H	2.505936000	-7.632745000	-1.150145000
H	2.438221000	-7.687387000	1.449226000
H	3.771554000	-8.445327000	2.340849000
H	2.654576000	-9.446381000	1.396183000
H	5.808054000	-9.411141000	-0.690437000
H	4.651589000	-10.457313000	0.149688000

H	5.765514000	-9.446089000	1.084568000
H	-4.704578000	0.714222000	5.146170000
H	-7.157836000	0.767634000	5.722273000
H	-4.040881000	0.368834000	2.777613000
H	-10.186483000	-0.444773000	-2.063163000
H	-11.414438000	-0.154586000	0.072322000
H	-7.211052000	-0.920971000	-5.635651000
H	-4.752617000	-0.792496000	-5.094788000
H	-4.065652000	-0.426722000	-2.735820000
H	7.147216000	-0.723266000	-5.688860000
H	8.804223000	-0.429021000	-3.861930000
H	11.405388000	0.198996000	-0.040093000
H	10.178012000	0.489266000	2.095717000
H	8.841172000	0.721501000	3.816686000
H	7.203537000	0.965681000	5.668967000

Cartesian coordinates of DFT-optimized structure of **8a<sub>ox</sub>** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Os	5.421125000	0.949889000	0.030352000
N	5.317845000	-1.116797000	0.369302000
N	5.828650000	1.385108000	2.050678000
N	7.474476000	1.286099000	0.036246000
N	5.957453000	0.669181000	-1.987265000
C	4.924125000	1.419245000	3.053796000
H	3.901765000	1.197356000	2.775843000
C	5.268184000	1.716888000	4.366247000
H	4.496735000	1.729094000	5.127834000
C	6.600462000	1.992686000	4.671191000
H	6.903076000	2.228684000	5.685682000
C	7.542231000	1.959602000	3.647176000
H	8.584105000	2.169081000	3.857667000
C	7.147099000	1.655932000	2.343713000
C	8.081231000	1.600296000	1.205019000
C	9.458364000	1.830720000	1.233769000
H	9.963476000	2.082636000	2.158404000
C	10.181161000	1.729459000	0.043976000
C	9.535071000	1.403981000	-1.149729000
H	10.099290000	1.327232000	-2.071312000
C	8.156253000	1.182978000	-1.128850000
C	7.295034000	0.833311000	-2.272685000
C	7.773663000	0.672712000	-3.573638000
H	8.829094000	0.806678000	-3.778114000
C	6.897374000	0.341894000	-4.602866000
H	7.265118000	0.215666000	-5.615433000
C	5.545037000	0.178057000	-4.305619000
H	4.822043000	-0.078887000	-5.071489000
C	5.116685000	0.349216000	-2.995382000
H	4.075415000	0.233159000	-2.723351000
N	4.021824000	-1.616320000	0.385821000

C	-2.990920000	0.782690000	-0.232863000
C	2.973308000	-0.660351000	0.262346000
C	-3.498072000	-0.509906000	0.004774000
C	3.480462000	0.632247000	0.024747000
C	-2.606643000	-1.573603000	0.246374000
C	2.589036000	1.695942000	-0.216895000
C	-1.227555000	-1.360334000	0.381680000
C	1.209952000	1.482660000	-0.352231000
C	-0.712074000	-0.053940000	0.012711000
C	0.694467000	0.176265000	0.016737000
C	-1.615066000	1.020299000	-0.360316000
C	1.597455000	-0.897974000	0.389766000
C	-1.048959000	2.227560000	-0.885773000
C	1.031356000	-2.105254000	0.915188000
H	-1.690437000	2.955949000	-1.363583000
H	1.672846000	-2.833656000	1.392965000
C	0.291457000	2.446941000	-0.881937000
C	-0.309060000	-2.324635000	0.911352000
H	0.669915000	3.342260000	-1.356828000
H	-0.687525000	-3.219969000	1.386211000
H	11.251393000	1.904761000	0.047032000
N	-3.296370000	-2.814065000	0.364867000
N	-4.683902000	-2.753749000	0.340669000
C	-5.117790000	-4.015623000	0.383756000
C	-4.035210000	-4.910784000	0.415184000
C	-2.903648000	-4.122074000	0.387895000
H	-6.179232000	-4.216541000	0.377548000
H	-4.073265000	-5.989014000	0.443288000
H	-1.865805000	-4.403470000	0.349621000
Os	-5.438742000	-0.827508000	-0.000730000
C	-5.562465000	-0.055741000	4.335250000
C	-5.134161000	-0.226970000	3.025009000
N	-5.975003000	-0.546762000	2.016895000
C	-7.312610000	-0.710645000	2.302329000
C	-7.791193000	-0.549978000	3.603292000
C	-6.914831000	-0.219330000	4.632512000
C	-8.173905000	-1.060129000	1.158495000
N	-7.492139000	-1.163435000	-0.006591000
C	-8.098965000	-1.477452000	-1.175375000
C	-9.476157000	-1.707516000	-1.204142000
C	-10.198941000	-1.606081000	-0.014355000
C	-9.552781000	-1.280771000	1.179357000
C	-7.164847000	-1.533280000	-2.314072000
N	-5.846345000	-1.262698000	-2.021050000
C	-4.941835000	-1.297017000	-3.024173000
C	-5.285963000	-1.594600000	-4.336621000
C	-6.618293000	-1.870153000	-4.641552000
C	-7.560047000	-1.836890000	-3.617527000
H	-4.092873000	-0.111108000	2.752963000
H	-4.839415000	0.201062000	5.101116000
H	-7.282541000	-0.093046000	5.645084000

H	-8.846644000	-0.683761000	3.807780000
H	-10.116993000	-1.203871000	2.100933000
H	-11.269218000	-1.781108000	-0.017425000
H	-9.981325000	-1.959285000	-2.128786000
H	-8.601960000	-2.046188000	-3.828006000
H	-6.920959000	-2.106100000	-5.656039000
H	-4.514523000	-1.606953000	-5.098215000
H	-3.919429000	-1.075321000	-2.746236000
N	-4.039433000	1.738665000	-0.356310000
N	-5.335463000	1.239150000	-0.339718000
C	-6.148734000	2.296902000	-0.386507000
C	-5.407844000	3.490497000	-0.412842000
C	-4.084058000	3.103641000	-0.378549000
N	4.666294000	2.876102000	-0.311098000
H	-3.190304000	3.701182000	-0.334814000
H	-5.787483000	4.500362000	-0.442224000
H	-7.218864000	2.148964000	-0.386345000
N	3.278758000	2.936407000	-0.335370000
C	5.100178000	4.137972000	-0.354321000
C	4.017596000	5.033125000	-0.385878000
C	2.886035000	4.244412000	-0.358609000
C	4.066449000	-2.981300000	0.407862000
C	5.390235000	-3.368153000	0.442175000
C	6.131121000	-2.174553000	0.415961000
H	4.055650000	6.111352000	-0.414067000
H	1.848193000	4.525814000	-0.320402000
H	6.161618000	4.338900000	-0.348059000
H	7.201251000	-2.026605000	0.415852000
H	5.769876000	-4.378020000	0.471477000
H	3.172692000	-3.578833000	0.364065000

Cartesian coordinates of DFT-optimized structure of **9a<sub>ox</sub>** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Os	5.500286000	0.877132000	-0.243143000
N	5.418244000	-1.197673000	0.179266000
N	5.953177000	1.387030000	1.746754000
N	7.571201000	1.198635000	-0.273936000
N	6.029123000	0.509351000	-2.245272000
C	5.054219000	1.468297000	2.753542000
H	4.028015000	1.245803000	2.491621000
C	5.411296000	1.814397000	4.050111000
H	4.645483000	1.863061000	4.815807000
C	6.748178000	2.090272000	4.334820000
H	7.059946000	2.362484000	5.337334000
C	7.682147000	2.010714000	3.306582000
H	8.726825000	2.221541000	3.501089000
C	7.275327000	1.659329000	2.018870000
C	8.196219000	1.552828000	0.874338000
C	9.575249000	1.773105000	0.878125000

H	10.093135000	2.056768000	1.786252000
C	10.282753000	1.621193000	-0.315530000
C	9.619802000	1.255239000	-1.488038000
H	10.171855000	1.137200000	-2.412573000
C	8.239826000	1.045512000	-1.441740000
C	7.362290000	0.654160000	-2.557794000
C	7.819890000	0.433747000	-3.857532000
H	8.872572000	0.553536000	-4.083516000
C	6.926420000	0.061280000	-4.856909000
H	7.277419000	-0.110581000	-5.868640000
C	5.578543000	-0.085734000	-4.531131000
H	4.842986000	-0.375170000	-5.272978000
C	5.170235000	0.145058000	-3.224084000
H	4.133640000	0.042862000	-2.930621000
C	6.471014000	-2.038746000	0.264658000
H	7.450703000	-1.576342000	0.243122000
C	6.347215000	-3.409549000	0.365285000
H	7.222566000	-4.044477000	0.432159000
C	5.059739000	-3.969626000	0.344261000
C	3.956285000	-3.108328000	0.264543000
H	2.958247000	-3.511048000	0.196654000
C	4.141411000	-1.722298000	0.221626000
C	-2.904073000	0.741640000	-0.522856000
C	3.067098000	-0.714597000	0.107608000
C	-3.425006000	-0.500976000	-0.119978000
C	3.560319000	0.576600000	-0.218814000
C	-2.542621000	-1.526976000	0.262836000
C	2.691903000	1.656381000	-0.527427000
C	-1.158211000	-1.312633000	0.368112000
C	1.310109000	1.403473000	-0.671849000
C	-0.631239000	-0.070321000	-0.159839000
C	0.779877000	0.146805000	-0.180420000
C	-1.522658000	0.953751000	-0.666946000
C	1.677533000	-0.889403000	0.291291000
C	-0.940152000	2.080269000	-1.332190000
C	1.099378000	-2.008454000	0.974642000
H	-1.569572000	2.747501000	-1.906093000
H	1.741256000	-2.677696000	1.533270000
C	0.402912000	2.296062000	-1.330070000
C	-0.245791000	-2.207194000	1.014679000
H	0.797927000	3.128311000	-1.898341000
H	-0.629476000	-3.027698000	1.606706000
O	4.985686000	-5.307854000	0.394820000
C	3.698100000	-5.957514000	0.364290000
C	3.901073000	-7.476667000	0.453974000
C	2.501846000	-8.121403000	0.408409000
C	4.740129000	-7.970744000	-0.739805000
C	4.597745000	-7.839151000	1.779272000
H	3.098250000	-5.597598000	1.209867000
H	3.188165000	-5.691029000	-0.570074000
H	2.587603000	-9.211766000	0.473684000

H	1.980096000	-7.881830000	-0.526109000
H	1.876958000	-7.783793000	1.244152000
H	4.257060000	-7.721964000	-1.692848000
H	4.857655000	-9.059626000	-0.696887000
H	5.738487000	-7.521685000	-0.737328000
H	4.005607000	-7.505989000	2.640674000
H	5.587456000	-7.376244000	1.847244000
H	4.724176000	-8.924965000	1.858254000
H	11.354119000	1.788241000	-0.331917000
N	-3.244048000	-2.733808000	0.546552000
N	-4.631797000	-2.663241000	0.512938000
C	-5.078244000	-3.902914000	0.730296000
C	-4.004825000	-4.796127000	0.886067000
C	-2.865054000	-4.030403000	0.751343000
H	-6.141786000	-4.091193000	0.749815000
H	-4.053741000	-5.859861000	1.062304000
H	-1.830557000	-4.325781000	0.752853000
Os	-5.378351000	-0.804201000	-0.095036000
C	-5.518667000	0.593183000	4.085837000
C	-5.079948000	0.228353000	2.819592000
N	-5.911767000	-0.230880000	1.858245000
C	-7.255035000	-0.339910000	2.151295000
C	-7.744558000	0.014914000	3.409725000
C	-6.875847000	0.485560000	4.389348000
C	-8.110736000	-0.845641000	1.063581000
N	-7.419931000	-1.121141000	-0.070187000
C	-8.022138000	-1.597141000	-1.187785000
C	-9.401095000	-1.818386000	-1.193533000
C	-10.131997000	-1.541669000	-0.036595000
C	-9.491390000	-1.052198000	1.103339000
C	-7.079952000	-1.822934000	-2.297780000
N	-5.760213000	-1.519008000	-2.037216000
C	-4.852138000	-1.705205000	-3.020986000
C	-5.190360000	-2.187686000	-4.278648000
C	-6.523175000	-2.497601000	-4.549152000
C	-7.469460000	-2.311310000	-3.546346000
H	-4.035436000	0.297726000	2.543157000
H	-4.800996000	0.954741000	4.813744000
H	-7.252457000	0.762155000	5.368313000
H	-8.803490000	-0.077604000	3.619596000
H	-10.062182000	-0.839682000	1.999360000
H	-11.203637000	-1.707967000	-0.023234000
H	-9.902247000	-2.197549000	-2.076135000
H	-8.511380000	-2.544429000	-3.730389000
H	-6.821941000	-2.876602000	-5.520647000
H	-4.414952000	-2.314926000	-5.025755000
H	-3.829483000	-1.453232000	-2.770212000
N	-3.945141000	1.678703000	-0.783611000
N	-5.245247000	1.191555000	-0.713864000
C	-6.051364000	2.236880000	-0.916579000
C	-5.302930000	3.412073000	-1.098322000

C	-3.981753000	3.027929000	-0.995365000
C	3.405621000	2.942888000	-0.665046000
N	4.789417000	2.832060000	-0.654901000
C	5.529328000	3.948541000	-0.761746000
C	4.999361000	5.227942000	-0.855576000
C	3.606320000	5.364773000	-0.801870000
C	2.820591000	4.203819000	-0.699257000
O	2.938428000	6.527183000	-0.831277000
C	3.674774000	7.765828000	-0.916359000
C	2.686154000	8.940028000	-0.903133000
C	3.522154000	10.231736000	-0.996705000
C	1.878287000	8.937424000	0.408523000
C	1.736460000	8.846573000	-2.112373000
H	4.261997000	7.765327000	-1.843258000
H	4.361367000	7.828599000	-0.062884000
H	4.113686000	10.260808000	-1.919868000
H	4.210413000	10.327065000	-0.148036000
H	2.863902000	11.107733000	-0.993420000
H	2.539993000	9.010030000	1.280507000
H	1.284529000	8.023020000	0.507746000
H	1.192816000	9.792187000	0.434803000
H	2.295758000	8.857054000	-3.056028000
H	1.046479000	9.698115000	-2.121158000
H	1.141546000	7.928126000	-2.080005000
H	5.668537000	6.073490000	-0.942310000
H	6.603764000	3.806676000	-0.762651000
H	1.750482000	4.326075000	-0.613494000
H	-3.085603000	3.622654000	-1.023319000
H	-5.675922000	4.410171000	-1.270592000
H	-7.122284000	2.094657000	-0.908651000

Cartesian coordinates of DFT-optimized structure of **10a<sub>ox</sub>** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Os	-2.286521000	-1.285446000	0.065875000
N	-3.054971000	0.671383000	0.284719000
N	-2.575741000	-1.761471000	2.096055000
N	-4.019239000	-2.437026000	0.040129000
N	-2.806462000	-1.323335000	-1.972550000
C	-1.792267000	-1.366035000	3.124270000
H	-0.945694000	-0.745379000	2.860202000
C	-2.044474000	-1.723333000	4.442441000
H	-1.378159000	-1.375396000	5.223707000
C	-3.151230000	-2.522290000	4.728297000
H	-3.376727000	-2.819487000	5.746813000
C	-3.968296000	-2.932923000	3.679702000
H	-4.836285000	-3.551224000	3.874555000
C	-3.673567000	-2.547994000	2.371001000
C	-4.490237000	-2.937061000	1.208255000
C	-5.638793000	-3.731653000	1.212517000

H	-6.031690000	-4.140152000	2.135846000
C	-6.278330000	-3.995165000	-0.000107000
C	-5.774939000	-3.472033000	-1.192489000
H	-6.272988000	-3.680492000	-2.131726000
C	-4.624105000	-2.682225000	-1.147539000
C	-3.939178000	-2.043678000	-2.284535000
C	-4.384914000	-2.140373000	-3.603720000
H	-5.277184000	-2.712304000	-3.828269000
C	-3.686165000	-1.503005000	-4.624253000
H	-4.028975000	-1.575491000	-5.650758000
C	-2.542747000	-0.773163000	-4.299906000
H	-1.963797000	-0.257842000	-5.057949000
C	-2.137780000	-0.707427000	-2.973229000
H	-1.255320000	-0.153366000	-2.680106000
C	-4.362192000	1.014805000	0.277423000
H	-5.067187000	0.192065000	0.288950000
C	-4.810931000	2.318894000	0.246603000
H	-5.870960000	2.543216000	0.241685000
C	-3.862217000	3.352891000	0.186592000
C	-2.503160000	3.014746000	0.204292000
H	-1.754945000	3.784618000	0.106786000
C	-2.103343000	1.675892000	0.293642000
C	5.429594000	2.119191000	0.142571000
C	-0.708676000	1.190186000	0.298808000
C	5.361638000	3.522216000	0.342092000
C	-0.640697000	-0.212857000	0.099473000
C	4.113020000	4.162863000	0.503448000
C	0.607926000	-0.853419000	-0.062228000
C	2.920556000	3.433600000	0.604892000
C	1.800315000	-0.124069000	-0.164014000
C	2.966759000	2.029055000	0.248384000
C	1.754118000	1.280488000	0.192461000
C	4.234666000	1.389215000	-0.048132000
C	0.486233000	1.920297000	0.489076000
C	4.191479000	0.063232000	-0.592422000
C	0.529363000	3.246383000	1.033104000
H	5.085089000	-0.356000000	-1.035824000
H	-0.364303000	3.665702000	1.476320000
C	3.039991000	-0.658394000	-0.642344000
C	1.680841000	3.968031000	1.082988000
H	3.055071000	-1.628832000	-1.121915000
H	1.665719000	4.938574000	1.562350000
O	-4.340369000	4.604889000	0.106928000
C	-3.425590000	5.718136000	0.050919000
C	-4.228586000	7.024602000	-0.021987000
C	-3.207662000	8.178161000	-0.076972000
C	-5.099572000	7.039568000	-1.292503000
C	-5.112864000	7.172585000	1.230639000
H	-2.792894000	5.703497000	0.947876000
H	-2.786290000	5.609874000	-0.834413000
H	-3.729000000	9.140410000	-0.130449000

H	-2.559261000	8.098820000	-0.958110000
H	-2.569883000	8.192120000	0.815312000
H	-4.483478000	6.944459000	-2.195282000
H	-5.654957000	7.981847000	-1.362490000
H	-5.823423000	6.218308000	-1.286945000
H	-4.505722000	7.173225000	2.144333000
H	-5.837529000	6.355388000	1.304660000
H	-5.668367000	8.116763000	1.195597000
H	-7.171012000	-4.610797000	-0.016081000
N	0.477973000	-2.267330000	-0.137895000
C	1.363031000	-3.306831000	-0.074971000
C	0.643562000	-4.483538000	-0.084849000
C	-0.707442000	-4.097304000	-0.131881000
N	-0.815652000	-2.766952000	-0.151271000
H	-1.599246000	-4.707204000	-0.138919000
H	1.040280000	-5.486703000	-0.051624000
H	2.423639000	-3.143285000	0.005291000
N	4.243038000	5.576739000	0.579443000
N	5.536677000	6.076272000	0.593879000
C	5.428546000	7.406634000	0.574446000
C	4.077602000	7.792945000	0.526313000
C	3.358081000	6.616274000	0.515808000
C	6.824234000	1.633362000	0.148304000
C	7.223920000	0.294450000	0.237321000
C	8.582945000	-0.043812000	0.255518000
C	9.531767000	0.990130000	0.196429000
C	9.083136000	2.294265000	0.165956000
N	7.775949000	2.637790000	0.158130000
O	9.060937000	-1.295886000	0.334856000
C	8.146005000	-2.409064000	0.389833000
C	8.948813000	-3.715660000	0.462424000
C	7.927723000	-4.869126000	0.516344000
C	9.833646000	-3.863097000	-0.789873000
C	9.819211000	-3.731395000	1.733332000
H	6.320360000	8.016507000	0.582286000
H	3.680971000	8.796134000	0.492802000
H	2.297534000	6.452747000	0.434656000
H	6.475625000	-0.475415000	0.334185000
H	10.591778000	0.765732000	0.201790000
H	9.788208000	3.116950000	0.155182000
H	7.513738000	-2.393864000	-0.507417000
H	7.506297000	-2.301199000	1.274919000
H	7.278936000	-4.790176000	1.397234000
H	8.448927000	-5.831462000	0.569554000
H	7.290339000	-4.882549000	-0.376232000
H	9.226924000	-3.863193000	-1.703846000
H	10.389027000	-4.807354000	-0.755065000
H	10.558431000	-3.045938000	-0.863135000
H	9.202712000	-3.636667000	2.635874000
H	10.543173000	-2.910228000	1.728533000
H	10.374442000	-4.673782000	1.803092000

Os	7.007534000	4.594592000	0.377341000
C	7.259651000	4.078910000	4.742902000
C	6.855912000	4.014303000	3.415794000
N	7.525583000	4.630994000	2.416259000
C	8.658073000	5.350971000	2.729886000
C	9.102558000	5.446572000	4.049566000
C	8.402803000	4.808416000	5.068919000
C	9.344178000	5.990268000	1.594024000
N	8.740477000	5.745937000	0.405594000
C	9.212688000	6.246692000	-0.761721000
C	10.361330000	7.041167000	-0.764319000
C	10.999671000	7.303809000	0.449121000
C	10.495042000	6.779935000	1.640652000
C	8.397137000	5.858480000	-1.925534000
N	7.298947000	5.071909000	-1.652208000
C	6.516473000	4.677207000	-2.681468000
C	6.770058000	5.035338000	-3.999151000
C	7.877187000	5.834362000	-4.283366000
C	8.693241000	6.244217000	-3.233681000
H	5.973678000	3.460553000	3.121400000
H	6.679961000	3.562997000	5.499975000
H	8.744653000	4.880034000	6.095804000
H	9.994663000	6.018245000	4.275417000
H	10.992182000	6.987730000	2.580521000
H	11.892396000	7.919343000	0.466399000
H	10.755182000	7.450233000	-1.686989000
H	9.561507000	6.862536000	-3.427243000
H	8.103750000	6.132192000	-5.301460000
H	6.104505000	4.687976000	-4.781321000
H	5.669585000	4.056438000	-2.418674000

Cartesian coordinates of DFT-optimized structure of **11a<sub>ox</sub>** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Os	2.853548000	0.446678000	0.038747000
N	1.726936000	-1.329058000	0.237479000
N	3.319315000	0.532313000	2.088749000
N	4.806674000	-0.253486000	0.105164000
N	3.270705000	0.016147000	-1.976842000
N	-7.789139000	2.401076000	0.035473000
C	2.493743000	0.943487000	3.077342000
H	1.504839000	1.254174000	2.765351000
C	2.874150000	0.972138000	4.412554000
H	2.166219000	1.313084000	5.159600000
C	4.160991000	0.560671000	4.759662000
H	4.489847000	0.569818000	5.793261000
C	5.021295000	0.135028000	3.752582000
H	6.025731000	-0.190706000	3.995221000
C	4.592875000	0.124556000	2.423943000
C	5.441282000	-0.312523000	1.301905000

C	6.765170000	-0.752405000	1.366522000
H	7.290299000	-0.805157000	2.312717000
C	7.408841000	-1.124530000	0.184858000
C	6.736999000	-1.056291000	-1.037040000
H	7.240489000	-1.344865000	-1.951883000
C	5.413605000	-0.610339000	-1.053620000
C	4.537613000	-0.465782000	-2.229216000
C	4.933981000	-0.790775000	-3.527749000
H	5.933587000	-1.169186000	-3.705182000
C	4.047654000	-0.631537000	-4.588243000
H	4.352013000	-0.882443000	-5.598669000
C	2.766554000	-0.147060000	-4.324365000
H	2.038349000	-0.007088000	-5.115317000
C	2.418286000	0.162222000	-3.016137000
H	1.434352000	0.539820000	-2.768818000
C	2.228583000	-2.583419000	0.277958000
H	3.307603000	-2.658578000	0.343256000
C	1.449775000	-3.721118000	0.229863000
H	1.899830000	-4.706143000	0.264891000
C	0.058954000	-3.576804000	0.097624000
C	-0.478707000	-2.284196000	0.064371000
H	-1.536565000	-2.142163000	-0.088133000
C	0.354230000	-1.163832000	0.175585000
C	-4.463327000	4.577171000	-0.337309000
C	-0.085082000	0.244678000	0.134772000
C	-5.570813000	3.716961000	-0.166630000
C	1.010263000	1.131958000	-0.020650000
C	-5.380818000	2.324585000	0.020460000
C	0.787945000	2.512999000	-0.216847000
C	-6.661257000	1.588059000	0.024943000
C	-6.813260000	0.208808000	-0.073348000
H	-5.956667000	-0.440557000	-0.181359000
C	-8.087308000	-0.382416000	-0.080710000
C	-9.211201000	0.450074000	-0.000761000
H	-10.223479000	0.068626000	0.006907000
C	-9.002294000	1.821525000	0.037226000
H	-9.849491000	2.497078000	0.059838000
C	-4.070542000	1.821077000	0.187028000
C	-0.499256000	3.031482000	-0.398598000
C	-2.946809000	2.681849000	-0.123542000
C	-1.619974000	2.160023000	-0.094190000
C	-3.161567000	4.077853000	-0.460988000
C	-1.394403000	0.769893000	0.243935000
C	-2.043830000	4.839130000	-0.938878000
C	-2.511497000	0.027433000	0.748203000
H	-2.210938000	5.804390000	-1.398967000
H	-2.339341000	-0.927258000	1.228497000
C	-0.780118000	4.342286000	-0.908856000
C	-3.778242000	0.523914000	0.719986000
H	0.018223000	4.929288000	-1.344441000
H	-4.572993000	-0.051804000	1.176539000

O	-0.656322000	-4.709584000	0.003394000
O	-8.115955000	-1.720667000	-0.174428000
C	-9.387707000	-2.402075000	-0.202361000
C	-9.145526000	-3.911943000	-0.337883000
C	-10.530249000	-4.588698000	-0.362356000
C	-8.335460000	-4.428933000	0.866026000
C	-8.396746000	-4.212755000	-1.650177000
C	-2.089284000	-4.641398000	-0.137494000
C	-2.656615000	-6.066901000	-0.194084000
C	-4.184770000	-5.937969000	-0.349227000
C	-2.073304000	-6.821760000	-1.403646000
C	-2.328089000	-6.818583000	1.109759000
H	-9.972799000	-2.026594000	-1.051286000
H	-9.929215000	-2.179554000	0.725729000
H	-11.132088000	-4.241444000	-1.211015000
H	-11.091534000	-4.387152000	0.558153000
H	-10.417525000	-5.674735000	-0.454457000
H	-8.859461000	-4.232004000	1.809458000
H	-7.351716000	-3.950978000	0.917277000
H	-8.183461000	-5.511390000	0.785609000
H	-8.962309000	-3.854891000	-2.519410000
H	-8.251032000	-5.292847000	-1.765883000
H	-7.412254000	-3.733973000	-1.664955000
H	-2.505275000	-4.094523000	0.718404000
H	-2.331235000	-4.094240000	-1.057554000
H	-4.644575000	-6.931672000	-0.391277000
H	-4.450830000	-5.406659000	-1.271176000
H	-4.630045000	-5.398362000	0.495614000
H	-2.302266000	-6.301919000	-2.342213000
H	-2.499961000	-7.829506000	-1.465038000
H	-0.985687000	-6.918345000	-1.325108000
H	-2.748497000	-6.300672000	1.980777000
H	-1.246702000	-6.906477000	1.255528000
H	-2.750977000	-7.829387000	1.083406000
H	8.437068000	-1.467935000	0.216208000
N	2.006622000	3.248982000	-0.245199000
C	2.315756000	4.578083000	-0.185741000
C	3.689894000	4.698076000	-0.141411000
C	4.181772000	3.381967000	-0.152567000
N	3.175916000	2.504569000	-0.201245000
N	-4.854499000	5.945056000	-0.401402000
C	-4.179150000	7.130593000	-0.343359000
C	-5.105427000	8.153562000	-0.347184000
C	-6.360159000	7.522786000	-0.385358000
N	-6.217990000	6.195060000	-0.404563000
H	5.200850000	3.025347000	-0.115588000
H	4.259642000	5.613636000	-0.096079000
H	1.552953000	5.335942000	-0.144259000
H	-3.106245000	7.169092000	-0.270889000
H	-4.901643000	9.212935000	-0.316083000
H	-7.349939000	7.955787000	-0.388157000

Os	-7.386524000	4.467233000	-0.174086000
C	-7.183360000	4.893401000	4.203238000
C	-6.885710000	4.603349000	2.878075000
N	-7.739932000	4.863639000	1.863370000
C	-8.956105000	5.439381000	2.157902000
C	-9.301253000	5.747972000	3.474408000
C	-8.412584000	5.476109000	4.509985000
C	-9.838861000	5.694102000	1.006390000
C	-11.105980000	6.280911000	1.029778000
C	-11.793289000	6.443076000	-0.174262000
C	-11.220839000	6.023996000	-1.376376000
C	-9.951791000	5.441667000	-1.349372000
N	-9.301105000	5.294533000	-0.170721000
C	-9.181098000	4.936187000	-2.498861000
N	-7.937887000	4.421017000	-2.204585000
C	-7.184777000	3.932189000	-3.214923000
C	-7.611043000	3.932356000	-4.536739000
C	-8.866892000	4.454962000	-4.843713000
C	-9.653389000	4.957919000	-3.811867000
H	-6.456377000	4.661938000	4.973449000
H	-5.943611000	4.150650000	2.597254000
H	-10.263282000	6.199161000	3.685383000
H	-8.676704000	5.714272000	5.534667000
H	-11.553101000	6.607441000	1.960990000
H	-12.777975000	6.897442000	-0.175756000
H	-11.757349000	6.151739000	-2.308783000
H	-6.217016000	3.536580000	-2.934811000
H	-6.961131000	3.527311000	-5.304068000
H	-9.229674000	4.470495000	-5.865763000
H	-10.634334000	5.366202000	-4.023059000

Cartesian coordinates of DFT-optimized structure of **7box** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Ru	-5.468994000	-0.050317000	0.032798000
Ru	5.481207000	0.097058000	0.020057000
N	-5.060009000	-2.103965000	0.306338000
N	5.049038000	2.141015000	-0.258108000
N	-5.914155000	0.250776000	2.066988000
N	5.973222000	-0.196041000	-2.000480000
N	-7.561349000	-0.072076000	0.080284000
N	7.542736000	0.130500000	0.051233000
N	-5.997816000	-0.364460000	-1.979480000
N	5.902622000	0.406597000	2.055778000
N	-5.117729000	2.011372000	-0.257422000
N	5.111690000	-1.961432000	0.286935000
C	-5.003819000	0.413117000	3.047007000
C	5.107107000	-0.359363000	-3.020039000
H	4.057285000	-0.332609000	-2.754801000
C	-5.360412000	0.617140000	4.376043000

C	5.516525000	-0.550327000	-4.335375000
H	4.772007000	-0.676174000	-5.113540000
C	-6.711627000	0.656118000	4.712969000
C	6.881196000	-0.574944000	-4.619576000
C	-7.660212000	0.488326000	3.707481000
C	7.786745000	-0.407199000	-3.575694000
H	-8.716920000	0.514795000	3.944620000
C	-7.247699000	0.285887000	2.390138000
C	7.320554000	-0.218940000	-2.272860000
C	-8.184971000	0.097316000	1.263948000
C	8.213790000	-0.032235000	-1.111051000
C	-9.581046000	0.078913000	1.325138000
C	9.611185000	-0.009225000	-1.117566000
H	-10.104830000	0.211010000	2.264144000
H	10.170620000	-0.137417000	-2.036613000
C	-10.297712000	-0.116154000	0.143142000
C	10.283340000	0.184190000	0.091025000
C	-9.630553000	-0.289908000	-1.070602000
C	9.569579000	0.351470000	1.279420000
C	-8.233206000	-0.264285000	-1.073127000
C	8.172996000	0.320654000	1.231965000
C	-7.343705000	-0.429509000	-2.240979000
C	7.239942000	0.476491000	2.366667000
C	-7.812173000	-0.639145000	-3.538300000
C	7.661798000	0.681813000	3.681845000
H	-8.877990000	-0.688459000	-3.726062000
C	-6.907622000	-0.784615000	-4.586851000
C	6.721674000	0.819137000	4.699248000
C	-5.543497000	-0.715622000	-4.312401000
C	5.367469000	0.746364000	4.376219000
H	4.597002000	0.846775000	5.132563000
C	-5.130349000	-0.504949000	-3.000792000
C	5.002732000	0.539945000	3.049978000
H	3.962599000	0.475962000	2.754781000
C	-5.962325000	-3.103469000	0.339677000
C	5.947499000	3.146064000	-0.279861000
H	-7.004007000	-2.805070000	0.367597000
H	6.990570000	2.850669000	-0.285829000
C	-5.620526000	-4.442309000	0.329769000
C	5.602181000	4.483638000	-0.282832000
H	-6.381501000	-5.213035000	0.360595000
H	6.361277000	5.256801000	-0.301937000
C	-4.261966000	-4.785053000	0.244173000
C	4.240837000	4.822543000	-0.223788000
C	-3.312152000	-3.753697000	0.210500000
C	3.295164000	3.790009000	-0.204253000
H	-2.265560000	-3.984234000	0.090948000
H	2.246028000	4.018798000	-0.104654000
C	-3.720350000	-2.417306000	0.282170000
C	3.706890000	2.451358000	-0.263257000
C	-2.828023000	-1.239950000	0.230726000

C	2.819484000	1.272946000	-0.227358000
C	-3.531132000	-0.028871000	0.006330000
C	3.532115000	0.066989000	-0.003942000
C	-2.860343000	1.198425000	-0.227312000
C	2.853343000	-1.158997000	0.216114000
C	-3.778369000	2.356345000	-0.266322000
C	3.772721000	-2.312037000	0.267888000
C	-3.412517000	3.697787000	-0.215491000
C	3.412954000	-3.656853000	0.202815000
H	-2.377418000	3.994690000	-0.127630000
H	2.380381000	-3.955678000	0.091497000
C	-4.386904000	4.711337000	-0.234172000
C	4.387592000	-4.666577000	0.235437000
C	-5.736618000	4.341677000	-0.287024000
C	5.735370000	-4.293110000	0.317319000
H	-6.541660000	5.063666000	-0.308894000
H	6.541968000	-5.013195000	0.350474000
C	-6.038083000	2.985518000	-0.279534000
C	6.032920000	-2.936322000	0.323332000
H	-7.073506000	2.664144000	-0.282696000
H	7.067332000	-2.612286000	0.348934000
C	-1.457360000	1.190446000	-0.393334000
C	1.448723000	-1.156614000	0.372458000
C	-0.719393000	0.005871000	-0.007320000
C	0.708673000	0.026080000	-0.008886000
C	-1.424009000	-1.198266000	0.382812000
C	1.415072000	1.229509000	-0.390292000
C	-0.651211000	-2.258887000	0.960084000
C	0.644195000	2.287180000	-0.975941000
H	-1.158740000	-3.066941000	1.471880000
H	1.154401000	3.094103000	-1.487133000
C	0.709531000	-2.238342000	0.954486000
C	-0.716849000	2.270246000	-0.976008000
H	1.245186000	-3.033172000	1.458187000
H	-1.249878000	3.063138000	-1.485257000
O	-3.973408000	-6.094291000	0.193033000
O	3.934119000	-5.930854000	0.175104000
O	3.948777000	6.134229000	-0.181745000
O	-3.928577000	5.971456000	-0.191012000
C	-4.871171000	7.064800000	-0.189666000
C	-4.104109000	8.392986000	-0.131063000
C	-5.156850000	9.518929000	-0.125376000
C	-3.197888000	8.535412000	-1.368592000
C	-3.262078000	8.463449000	1.156949000
C	2.573780000	6.557503000	-0.105302000
C	2.518476000	8.091996000	-0.120409000
C	1.033450000	8.490925000	-0.015584000
C	3.295889000	8.662726000	1.080788000
C	3.109562000	8.627602000	-1.438332000
C	-2.599696000	-6.523317000	0.094867000
C	-2.550782000	-8.057832000	0.107086000

C	-3.125056000	-8.593090000	1.432548000
C	-3.346933000	-8.623810000	-1.084029000
C	-1.068599000	-8.461434000	-0.019443000
C	4.880923000	-7.018287000	0.183508000
C	4.121977000	-8.349940000	0.097797000
C	3.305483000	-8.412308000	-1.206979000
C	3.191868000	-8.507735000	1.315602000
C	5.179256000	-9.471505000	0.102618000
H	-5.531730000	6.960572000	0.680182000
H	-5.477400000	7.010390000	-1.102544000
H	-5.819162000	9.443282000	0.745455000
H	-5.777363000	9.492447000	-1.029256000
H	-4.663091000	10.496289000	-0.086768000
H	-3.785168000	8.498395000	-2.294527000
H	-2.449916000	7.736678000	-1.408910000
H	-2.668593000	9.494881000	-1.344650000
H	-3.895813000	8.377992000	2.048372000
H	-2.731666000	9.420956000	1.212680000
H	-2.517824000	7.661114000	1.191302000
H	2.024844000	6.145467000	-0.961746000
H	2.131216000	6.164439000	0.819078000
H	0.933984000	9.582144000	-0.026769000
H	0.583810000	8.123451000	0.914998000
H	0.450449000	8.093798000	-0.855510000
H	2.881691000	8.298203000	2.028967000
H	3.236864000	9.757205000	1.086863000
H	4.352616000	8.379812000	1.040456000
H	2.557154000	8.242316000	-2.304445000
H	4.159519000	8.337867000	-1.548754000
H	3.054571000	9.721903000	-1.464401000
H	-2.037681000	-6.114288000	0.943921000
H	-2.171148000	-6.130291000	-0.835796000
H	-2.559750000	-8.210296000	2.291367000
H	-3.072569000	-9.687516000	1.456503000
H	-4.172734000	-8.301074000	1.557859000
H	-4.402058000	-8.337321000	-1.028926000
H	-3.292002000	-9.718454000	-1.092072000
H	-2.944282000	-8.259713000	-2.037301000
H	-0.472528000	-8.067884000	0.812922000
H	-0.631029000	-8.093808000	-0.955671000
H	-0.973147000	-9.552996000	-0.011621000
H	5.469239000	-6.970534000	1.108703000
H	5.559413000	-6.905057000	-0.671564000
H	2.780158000	-9.371368000	-1.281927000
H	3.956096000	-8.316060000	-2.085069000
H	2.558999000	-7.612437000	-1.248377000
H	2.439666000	-7.712618000	1.347818000
H	3.760320000	-8.476142000	2.253441000
H	2.667659000	-9.469381000	1.272816000
H	5.858537000	-9.384907000	-0.754050000
H	4.690875000	-10.450688000	0.045204000

H	5.781720000	-9.450716000	1.018792000
H	-4.584180000	0.741547000	5.122471000
H	-7.025597000	0.813560000	5.739291000
H	-3.965363000	0.374996000	2.743060000
H	-10.191436000	-0.440742000	-1.985036000
H	-11.381877000	-0.133236000	0.168265000
H	-7.264928000	-0.947851000	-5.597972000
H	-4.800109000	-0.821651000	-5.094279000
H	-4.080139000	-0.443364000	-2.744898000
H	7.236867000	-0.721342000	-5.634001000
H	8.852454000	-0.422003000	-3.770988000
H	11.367710000	0.204885000	0.106692000
H	10.096205000	0.501221000	2.214528000
H	8.720352000	0.734284000	3.907116000
H	7.042985000	0.979113000	5.723063000

Cartesian coordinates of DFT-optimized structure of **8box** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Ru	4.933161000	-0.356676000	-0.207831000
N	5.455098000	0.154196000	1.767323000
N	7.004172000	-0.456924000	-0.238097000
N	5.345524000	-0.912751000	-2.196645000
C	4.598454000	0.459028000	2.760449000
H	3.546418000	0.431623000	2.505307000
C	5.021639000	0.790699000	4.043648000
H	4.285523000	1.027852000	4.803377000
C	6.387284000	0.808751000	4.318352000
H	6.753441000	1.063068000	5.307309000
C	7.281995000	0.492916000	3.299034000
H	8.348603000	0.499053000	3.488969000
C	6.802415000	0.167975000	2.029460000
C	7.682322000	-0.179237000	0.893914000
C	9.078591000	-0.239325000	0.901490000
H	9.645395000	-0.021506000	1.798573000
C	9.737783000	-0.589296000	-0.278028000
C	9.013775000	-0.872286000	-1.437340000
H	9.530501000	-1.142581000	-2.350249000
C	7.619048000	-0.797219000	-1.388997000
C	6.676997000	-1.056201000	-2.497930000
C	7.085743000	-1.424099000	-3.780499000
H	8.140781000	-1.532929000	-4.001446000
C	6.135380000	-1.650582000	-4.772861000
H	6.446279000	-1.937638000	-5.771723000
C	4.786453000	-1.501131000	-4.458486000
H	4.009043000	-1.664989000	-5.196105000
C	4.434861000	-1.131997000	-3.163953000
H	3.398276000	-1.003484000	-2.878294000
C	-3.308983000	1.213845000	-0.417853000
C	2.234282000	-1.397335000	0.163484000

C	-4.065537000	0.079221000	-0.074886000
C	2.990819000	-0.262663000	-0.179368000
C	-3.412413000	-1.123748000	0.247087000
C	2.337673000	0.940264000	-0.501457000
C	-2.015589000	-1.193349000	0.360143000
C	0.940858000	1.009785000	-0.614679000
C	-1.249128000	-0.057307000	-0.116748000
C	0.174401000	-0.126277000	-0.137823000
C	-1.915944000	1.148197000	-0.572383000
C	0.841222000	-1.331763000	0.317849000
C	-1.123886000	2.166365000	-1.196883000
C	0.049156000	-2.349976000	0.942269000
H	-1.611359000	2.973664000	-1.727221000
H	0.536621000	-3.157310000	1.472561000
C	0.232820000	2.100633000	-1.216969000
C	-1.307551000	-2.284243000	0.962354000
H	0.780163000	2.857796000	-1.762625000
H	-1.854892000	-3.041441000	1.507963000
H	10.821044000	-0.641755000	-0.293852000
N	-4.338747000	-2.180965000	0.467242000
N	-5.677740000	-1.829793000	0.458424000
C	-6.365350000	-2.962957000	0.595805000
C	-5.495536000	-4.065773000	0.675919000
C	-4.224988000	-3.537914000	0.576688000
H	-7.445321000	-2.935326000	0.618469000
H	-5.759118000	-5.107067000	0.781447000
H	-3.269843000	-4.032654000	0.543901000
Ru	-6.007865000	0.173426000	-0.045776000
C	-5.859251000	1.317933000	4.204804000
C	-5.508238000	0.948743000	2.910130000
N	-6.419327000	0.729533000	1.943215000
C	-7.750661000	0.873078000	2.245066000
C	-8.158835000	1.241038000	3.527799000
C	-7.208035000	1.467482000	4.519752000
C	-8.693205000	0.614141000	1.136545000
N	-8.078845000	0.273844000	-0.014631000
C	-8.757502000	-0.003800000	-1.146350000
C	-10.153773000	0.056324000	-1.153305000
C	-10.812436000	0.406291000	0.026509000
C	-10.087909000	0.689242000	1.185507000
C	-7.878102000	-0.351014000	-2.282290000
N	-6.530672000	-0.337340000	-2.020725000
C	-5.674472000	-0.642174000	-3.014234000
C	-6.098226000	-0.973742000	-4.297272000
C	-7.463988000	-0.991684000	-4.571396000
C	-8.358245000	-0.675846000	-3.551682000
H	-4.471784000	0.820163000	2.624024000
H	-5.081516000	1.481759000	4.942086000
H	-7.518490000	1.754587000	5.518738000
H	-9.213771000	1.349952000	3.749186000
H	-10.604227000	0.959526000	2.098652000

H	-11.895688000	0.458773000	0.042813000
H	-10.720978000	-0.161473000	-2.050139000
H	-9.424934000	-0.681891000	-3.741170000
H	-7.830581000	-1.245915000	-5.560215000
H	-5.362450000	-1.210899000	-5.057329000
H	-4.622325000	-0.614846000	-2.759546000
N	-4.134853000	2.356023000	-0.611873000
N	-5.500677000	2.136018000	-0.562555000
C	-6.079242000	3.330565000	-0.681114000
C	-5.109611000	4.344174000	-0.788858000
C	-3.893690000	3.695751000	-0.726767000
H	-2.894621000	4.095742000	-0.723268000
H	-5.274261000	5.406223000	-0.888088000
H	-7.157015000	3.407566000	-0.671492000
N	3.060196000	-2.539448000	0.357686000
C	2.819105000	-3.879201000	0.472433000
C	4.035062000	-4.527529000	0.534832000
C	5.004642000	-3.513834000	0.427429000
N	4.426013000	-2.319325000	0.308779000
N	3.263975000	1.997549000	-0.721426000
N	4.602997000	1.646494000	-0.712195000
C	5.290551000	2.779703000	-0.849479000
C	4.420667000	3.882438000	-0.929934000
C	3.150137000	3.354481000	-0.831017000
H	1.820066000	-4.279264000	0.468618000
H	4.199771000	-5.589570000	0.634043000
H	6.082424000	-3.590746000	0.418115000
H	2.194945000	3.849152000	-0.798545000
H	4.684191000	4.923745000	-1.035478000
H	6.370531000	2.752160000	-0.871831000

Cartesian coordinates of DFT-optimized structure of **9box** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Ru	4.930937000	-0.193225000	0.004791000
N	4.479142000	-2.232709000	0.314151000
N	5.443253000	0.111303000	2.023320000
N	7.030764000	-0.262614000	-0.001237000
N	5.408923000	-0.547795000	-2.013707000
C	4.559642000	0.298238000	3.022954000
H	3.513627000	0.283601000	2.744293000
C	4.953238000	0.499482000	4.341943000
H	4.198314000	0.644799000	5.106136000
C	6.312598000	0.508023000	4.645977000
H	6.654614000	0.661358000	5.663868000
C	7.233019000	0.315626000	3.618771000
H	8.295421000	0.319026000	3.830636000
C	6.784286000	0.118484000	2.312732000
C	7.688020000	-0.093850000	1.163522000
C	9.084789000	-0.132214000	1.188064000

H	9.634802000	0.000748000	2.111658000
C	9.766356000	-0.347213000	-0.010978000
C	9.064413000	-0.520229000	-1.204946000
H	9.598215000	-0.688101000	-2.132415000
C	7.668068000	-0.472408000	-1.170230000
C	6.745074000	-0.634663000	-2.312011000
C	7.172721000	-0.865758000	-3.619602000
H	8.231755000	-0.930992000	-3.838010000
C	6.235786000	-1.012338000	-4.639348000
H	6.561299000	-1.191676000	-5.658406000
C	4.881293000	-0.925083000	-4.325999000
H	4.113849000	-1.033258000	-5.083874000
C	4.509154000	-0.692736000	-3.005898000
H	3.467771000	-0.617231000	-2.720057000
C	5.359438000	-3.251147000	0.353320000
H	6.407662000	-2.975523000	0.367069000
C	4.986722000	-4.581426000	0.367773000
H	5.729846000	-5.369150000	0.401752000
C	3.619596000	-4.893714000	0.302783000
C	2.692142000	-3.841575000	0.267653000
H	1.638651000	-4.049573000	0.167993000
C	3.132412000	-2.514583000	0.312142000
C	-3.317521000	1.265241000	-0.316524000
C	2.267738000	-1.316980000	0.253138000
C	-4.064870000	0.123500000	0.003654000
C	2.992192000	-0.125838000	0.003777000
C	-3.399723000	-1.068010000	0.323967000
C	2.353170000	1.112323000	-0.246569000
C	-1.998995000	-1.125453000	0.451162000
C	0.948881000	1.132551000	-0.411515000
C	-1.241600000	0.023461000	0.003862000
C	0.187149000	-0.027492000	0.003384000
C	-1.916006000	1.223418000	-0.442891000
C	0.865314000	-1.238319000	0.418742000
C	-1.124084000	2.257928000	-1.035687000
C	0.077365000	-2.267698000	1.028059000
H	-1.609609000	3.065932000	-1.567011000
H	0.573085000	-3.078368000	1.546668000
C	0.236115000	2.217357000	-1.016655000
C	-1.282382000	-2.211956000	1.046845000
H	0.788769000	2.993724000	-1.529846000
H	-1.823973000	-2.980916000	1.582176000
O	3.301416000	-6.195887000	0.271602000
C	1.917487000	-6.596103000	0.192336000
C	1.838446000	-8.129306000	0.194250000
C	0.346186000	-8.503193000	0.099422000
C	2.595630000	-8.700789000	-1.019536000
C	2.432219000	-8.687153000	1.501694000
H	1.377676000	-6.180750000	1.052757000
H	1.482562000	-6.188444000	-0.728893000
H	0.230422000	-9.592729000	0.101339000

H	-0.105415000	-8.120006000	-0.823699000
H	-0.222225000	-8.104327000	0.948385000
H	2.183935000	-8.314713000	-1.960270000
H	2.511847000	-9.793443000	-1.039518000
H	3.658906000	-8.442979000	-0.982589000
H	1.894452000	-8.300364000	2.376244000
H	3.488234000	-8.417719000	1.605034000
H	2.357230000	-9.780460000	1.517677000
H	10.850411000	-0.380572000	-0.014806000
N	-4.316262000	-2.139331000	0.525992000
N	-5.660481000	-1.804730000	0.500519000
C	-6.334569000	-2.947656000	0.628089000
C	-5.452042000	-4.039556000	0.717359000
C	-4.186964000	-3.495067000	0.635857000
H	-7.414960000	-2.933259000	0.635672000
H	-5.703257000	-5.084613000	0.816857000
H	-3.225991000	-3.978715000	0.614688000
Ru	-6.026190000	0.191339000	0.000549000
C	-5.949459000	1.343432000	4.256522000
C	-5.570133000	0.976237000	2.969382000
N	-6.457481000	0.740446000	1.984034000
C	-7.797352000	0.868003000	2.262129000
C	-8.234393000	1.234509000	3.536564000
C	-7.306396000	1.475422000	4.546186000
C	-8.717646000	0.594970000	1.138566000
N	-8.077689000	0.262019000	-0.003491000
C	-8.735271000	-0.025940000	-1.147644000
C	-10.132010000	0.015187000	-1.176627000
C	-10.815715000	0.356455000	-0.008086000
C	-10.113981000	0.650198000	1.162716000
C	-7.831868000	-0.359975000	-2.268309000
N	-6.487527000	-0.325619000	-1.985021000
C	-5.614859000	-0.617748000	-2.968405000
C	-6.013762000	-0.953621000	-4.258167000
C	-7.375470000	-0.991763000	-4.552862000
C	-8.288422000	-0.691338000	-3.545501000
H	-4.526731000	0.863439000	2.700844000
H	-5.188202000	1.520373000	5.008118000
H	-7.639661000	1.760536000	5.538529000
H	-9.294826000	1.330966000	3.737310000
H	-10.649794000	0.913621000	2.066828000
H	-11.899791000	0.393630000	-0.009805000
H	-10.681773000	-0.211173000	-2.082455000
H	-9.352197000	-0.713916000	-3.750073000
H	-7.723802000	-1.249766000	-5.547443000
H	-5.263650000	-1.178992000	-5.008000000
H	-4.567112000	-0.576604000	-2.696365000
N	-4.157123000	2.397844000	-0.520774000
N	-5.521521000	2.157313000	-0.497764000
C	-6.114340000	3.344107000	-0.629094000
C	-5.157886000	4.371846000	-0.718580000

C	-3.933806000	3.741045000	-0.633163000
C	3.296426000	2.249155000	-0.305010000
N	4.628331000	1.876469000	-0.304455000
C	5.569190000	2.830202000	-0.341723000
C	5.296082000	4.192567000	-0.357125000
C	3.954792000	4.590113000	-0.294253000
C	2.959065000	3.597232000	-0.261397000
O	3.521758000	5.858110000	-0.253765000
C	4.481767000	6.936359000	-0.266978000
C	3.734719000	8.274937000	-0.187447000
C	4.802533000	9.386509000	-0.204978000
C	2.924710000	8.352675000	1.120592000
C	2.799917000	8.432757000	-1.401598000
H	5.068847000	6.875654000	-1.191930000
H	5.157554000	6.818641000	0.589295000
H	5.400673000	9.353793000	-1.123752000
H	5.485285000	9.301105000	0.649171000
H	4.323113000	10.370425000	-0.152768000
H	3.577088000	8.248409000	1.996382000
H	2.166372000	7.564395000	1.166016000
H	2.414405000	9.319744000	1.194998000
H	3.362874000	8.389799000	-2.342149000
H	2.284704000	9.399326000	-1.362104000
H	2.040758000	7.644270000	-1.423509000
H	6.115380000	4.898056000	-0.392839000
H	6.597035000	2.485545000	-0.351225000
H	1.931035000	3.916696000	-0.168016000
H	-2.941591000	4.156907000	-0.610931000
H	-5.335661000	5.431640000	-0.820582000
H	-7.193154000	3.405197000	-0.640121000

Cartesian coordinates of DFT-optimized structure of **10box** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Ru	5.410683000	0.838151000	-0.025072000
N	5.345468000	-1.242360000	0.297304000
N	5.776024000	1.259457000	2.004861000
N	7.451902000	1.211724000	0.010534000
N	5.972178000	0.565598000	-2.034235000
C	4.861387000	1.251379000	2.993613000
H	3.849449000	1.000969000	2.700591000
C	5.179815000	1.542529000	4.316195000
H	4.400443000	1.521071000	5.069546000
C	6.498880000	1.855121000	4.638216000
H	6.783458000	2.087604000	5.658935000
C	7.453655000	1.862609000	3.624763000
H	8.486537000	2.099067000	3.850542000
C	7.079201000	1.562197000	2.314433000
C	8.030190000	1.543342000	1.183600000
C	9.398306000	1.825499000	1.230511000

H	9.885230000	2.092815000	2.160671000
C	10.134740000	1.757749000	0.046472000
C	9.513462000	1.416401000	-1.156214000
H	10.089565000	1.367718000	-2.072375000
C	8.142884000	1.143444000	-1.146379000
C	7.303262000	0.768970000	-2.303289000
C	7.803442000	0.622569000	-3.598061000
H	8.856310000	0.788269000	-3.792422000
C	6.947271000	0.262771000	-4.635661000
H	7.329386000	0.147251000	-5.644347000
C	5.598631000	0.055427000	-4.353057000
H	4.892543000	-0.226341000	-5.125999000
C	5.153196000	0.216653000	-3.045113000
H	4.113212000	0.067360000	-2.782774000
C	6.409956000	-2.067021000	0.358753000
H	7.381415000	-1.586759000	0.386796000
C	6.310609000	-3.444556000	0.374959000
H	7.195535000	-4.067917000	0.424173000
C	5.034436000	-4.023905000	0.289505000
C	3.917510000	-3.178935000	0.237321000
H	2.929580000	-3.595385000	0.121997000
C	4.080377000	-1.788923000	0.279526000
C	-2.995636000	0.788548000	-0.205442000
C	2.995742000	-0.787298000	0.204425000
C	-3.496001000	-0.511953000	0.041805000
C	3.496109000	0.513209000	-0.042730000
C	-2.614888000	-1.587796000	0.280895000
C	2.614996000	1.589057000	-0.281779000
C	-1.232813000	-1.387869000	0.415463000
C	1.232931000	1.389120000	-0.416420000
C	-0.705613000	-0.100743000	0.011448000
C	0.705727000	0.101987000	-0.012439000
C	-1.603307000	0.974803000	-0.364410000
C	1.603419000	-0.973565000	0.363391000
C	-1.020556000	2.147809000	-0.947246000
C	1.020680000	-2.146585000	0.946205000
H	-1.661088000	2.866744000	-1.441051000
H	1.661223000	-2.865538000	1.439970000
C	0.324389000	2.348984000	-0.968035000
C	-0.324266000	-2.347749000	0.967039000
H	0.712592000	3.221827000	-1.477134000
H	-0.712468000	-3.220603000	1.476125000
O	4.983807000	-5.365203000	0.255380000
C	3.708848000	-6.031948000	0.160904000
C	3.936441000	-7.550132000	0.139253000
C	2.547965000	-8.212031000	0.039081000
C	4.788137000	-7.939792000	-1.083819000
C	4.633632000	-7.998989000	1.437455000
H	3.093515000	-5.746477000	1.023842000
H	3.203477000	-5.706089000	-0.757058000
H	2.650596000	-9.302779000	0.019763000

H	2.023453000	-7.908563000	-0.875209000
H	1.916518000	-7.950504000	0.896944000
H	4.300970000	-7.634584000	-2.018260000
H	4.930252000	-9.026011000	-1.118332000
H	5.775781000	-7.469133000	-1.045906000
H	4.033746000	-7.737867000	2.318040000
H	5.616477000	-7.528729000	1.543937000
H	4.775486000	-9.085817000	1.437731000
H	11.197679000	1.973279000	0.060737000
N	3.297137000	2.829692000	-0.394305000
C	2.897607000	4.137395000	-0.401384000
C	4.027881000	4.926873000	-0.422840000
C	5.111537000	4.028248000	-0.403314000
N	4.678209000	2.769066000	-0.373432000
N	-3.297034000	-2.828414000	0.393573000
N	-4.678107000	-2.767779000	0.372775000
C	-5.111437000	-4.026957000	0.402792000
C	-4.027785000	-4.925587000	0.422359000
C	-2.897507000	-4.136118000	0.400785000
C	-4.080284000	1.790164000	-0.280606000
C	-3.917432000	3.180183000	-0.238512000
C	-5.034366000	4.025138000	-0.290777000
C	-6.310533000	3.445771000	-0.376189000
C	-6.409868000	2.068236000	-0.359860000
N	-5.345372000	1.243589000	-0.298341000
O	-4.983746000	5.366437000	-0.256773000
C	-3.708791000	6.033196000	-0.162346000
C	-3.936389000	7.551382000	-0.140843000
C	-2.547918000	8.213295000	-0.040708000
C	-4.633557000	8.000112000	-1.439101000
C	-4.788109000	7.941156000	1.082175000
H	-6.173044000	-4.228796000	0.396870000
H	-4.066149000	-6.004091000	0.438919000
H	-1.858335000	-4.412878000	0.357632000
H	-2.929508000	3.596653000	-0.123217000
H	-7.195464000	4.069119000	-0.425458000
H	-7.381323000	1.587963000	-0.387854000
H	-3.093446000	5.747645000	-1.025249000
H	-3.203430000	5.707426000	0.755653000
H	-2.023422000	7.909918000	0.873622000
H	-2.650552000	9.304044000	-0.021499000
H	-1.916452000	7.951685000	-0.898533000
H	-4.033656000	7.738905000	-2.319650000
H	-4.775411000	9.086940000	-1.439485000
H	-5.616400000	7.529841000	-1.545555000
H	-4.300957000	7.636040000	2.016655000
H	-5.775750000	7.470487000	1.044290000
H	-4.930230000	9.027377000	1.116580000
Ru	-5.410571000	-0.836888000	0.024250000
C	-5.598343000	-0.053692000	4.352153000
C	-5.152966000	-0.215063000	3.044207000

N	-5.971995000	-0.564124000	2.033406000
C	-7.303067000	-0.767466000	2.302540000
C	-7.803188000	-0.620923000	3.597318000
C	-6.946970000	-0.261006000	4.634840000
C	-8.142737000	-1.142062000	1.145707000
N	-7.451808000	-1.210461000	-0.011228000
C	-8.030147000	-1.542196000	-1.184232000
C	-9.398266000	-1.824358000	-1.231054000
C	-10.134647000	-1.756484000	-0.046990000
C	-9.513315000	-1.415015000	1.155634000
C	-7.079211000	-1.561171000	-2.315106000
N	-5.776021000	-1.258402000	-2.005622000
C	-4.861424000	-1.250430000	-2.994412000
C	-5.179910000	-1.541721000	-4.316950000
C	-6.498989000	-1.854344000	-4.638880000
C	-7.453722000	-1.861720000	-3.625386000
H	-4.112994000	-0.065796000	2.781803000
H	-4.892220000	0.228166000	5.125031000
H	-7.329040000	-0.145372000	5.643530000
H	-8.856046000	-0.786601000	3.791746000
H	-10.089377000	-1.366235000	2.071815000
H	-11.197588000	-1.972014000	-0.061186000
H	-9.885231000	-2.091769000	-2.161165000
H	-8.486614000	-2.098200000	-3.851096000
H	-6.783611000	-2.086935000	-5.659563000
H	-4.400569000	-1.520346000	-5.070336000
H	-3.849472000	-0.999993000	-2.701459000
H	4.066240000	6.005379000	-0.439289000
H	1.858436000	4.414151000	-0.358233000
H	6.173142000	4.230093000	-0.397330000

Cartesian coordinates of DFT-optimized structure of **11box** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Ru	5.585845000	-0.946404000	0.034714000
N	5.145442000	1.089885000	-0.269824000
N	6.041458000	-1.276529000	-1.991963000
N	7.652075000	-0.948604000	0.029920000
N	6.050131000	-0.592822000	2.054799000
N	-5.055348000	0.810868000	-0.265451000
C	5.156032000	-1.427222000	-2.995953000
H	4.111207000	-1.370709000	-2.716382000
C	5.540854000	-1.643615000	-4.315112000
H	4.781761000	-1.758090000	-5.080777000
C	6.899621000	-1.708136000	-4.618291000
H	7.236492000	-1.874984000	-5.635939000
C	7.824756000	-1.553676000	-3.589349000
H	8.886641000	-1.598687000	-3.800078000
C	7.382821000	-1.338687000	-2.282648000
C	8.298310000	-1.163602000	-1.135976000

C	9.695186000	-1.204082000	-1.160651000
H	10.235687000	-1.376499000	-2.083672000
C	10.390365000	-1.019273000	0.035912000
C	9.700334000	-0.799944000	1.229670000
H	10.245227000	-0.659521000	2.155492000
C	8.303346000	-0.768942000	1.199093000
C	7.392926000	-0.555716000	2.343525000
C	7.840631000	-0.326702000	3.645846000
H	8.903428000	-0.299001000	3.854943000
C	6.920094000	-0.131804000	4.672098000
H	7.261599000	0.046301000	5.686289000
C	5.560017000	-0.168525000	4.370402000
H	4.804393000	-0.020993000	5.133837000
C	5.169229000	-0.400059000	3.055535000
H	4.123034000	-0.435498000	2.777524000
C	6.045667000	2.091616000	-0.326973000
H	7.087083000	1.791691000	-0.354377000
C	5.702835000	3.429716000	-0.340551000
H	6.462716000	4.200776000	-0.388185000
C	4.344072000	3.772697000	-0.255475000
C	3.395799000	2.742792000	-0.201897000
H	2.349638000	2.975597000	-0.083302000
C	3.803087000	1.403438000	-0.250383000
C	-2.684306000	-2.346291000	0.265519000
C	2.913320000	0.225551000	-0.184847000
C	-3.424907000	-1.168131000	0.038745000
C	3.637885000	-0.968943000	0.038596000
C	-2.773067000	0.067516000	-0.186767000
C	2.959919000	-2.183528000	0.263698000
C	-3.725297000	1.196482000	-0.248268000
C	-3.401314000	2.548175000	-0.198425000
H	-2.377820000	2.876408000	-0.089038000
C	-4.403838000	3.532159000	-0.246690000
C	-5.740549000	3.122561000	-0.328993000
H	-6.565298000	3.821018000	-0.376154000
C	-6.002958000	1.758134000	-0.316458000
H	-7.027792000	1.404921000	-0.338643000
C	-1.366933000	0.089062000	-0.331718000
C	1.567130000	-2.231801000	0.412629000
C	-0.609971000	-1.088664000	0.041895000
C	0.815956000	-1.047586000	0.042598000
C	-1.291318000	-2.313885000	0.414941000
C	1.505830000	0.169325000	-0.328210000
C	-0.509957000	-3.390398000	0.950251000
C	0.719025000	1.225130000	-0.894183000
H	-1.005629000	-4.225093000	1.429051000
H	1.216396000	2.045534000	-1.395536000
C	0.848167000	-3.350556000	0.949283000
C	-0.641317000	1.188865000	-0.894067000
H	1.391326000	-4.156566000	1.425825000
H	-1.184242000	1.981104000	-1.393183000

O	4.055903000	5.084518000	-0.223982000
O	-3.981947000	4.804659000	-0.200905000
C	-4.950064000	5.874450000	-0.238849000
C	-4.214905000	7.219837000	-0.161105000
C	-5.290808000	8.322804000	-0.205499000
C	-3.262942000	7.373698000	-1.362371000
C	-3.425180000	7.316943000	1.158030000
C	2.682491000	5.513367000	-0.139568000
C	2.633218000	7.047767000	-0.161183000
C	1.149252000	7.452776000	-0.062419000
C	3.409168000	7.620098000	1.040232000
C	3.229699000	7.576900000	-1.479222000
H	-5.638286000	5.759903000	0.608015000
H	-5.522617000	5.800669000	-1.171969000
H	-5.985364000	8.240685000	0.639403000
H	-5.875170000	8.276010000	-1.132495000
H	-4.819836000	9.310950000	-0.156428000
H	-3.810736000	7.316743000	-2.311108000
H	-2.496848000	6.591447000	-1.364672000
H	-2.756535000	8.344973000	-1.324445000
H	-4.089157000	7.213522000	2.025164000
H	-2.925868000	8.289821000	1.231525000
H	-2.659543000	6.536909000	1.221531000
H	2.126844000	5.098307000	-0.990261000
H	2.244898000	5.127300000	0.789937000
H	1.054580000	8.544311000	-0.077747000
H	0.695761000	7.090358000	0.868215000
H	0.567441000	7.054333000	-0.902641000
H	2.994264000	7.256586000	1.988528000
H	3.349677000	8.714555000	1.045088000
H	4.466238000	7.338172000	1.001389000
H	2.679177000	7.189230000	-2.345424000
H	4.279493000	7.285214000	-1.585074000
H	3.176021000	8.671201000	-1.509276000
H	11.474678000	-1.047594000	0.038378000
N	3.854418000	-3.286481000	0.358567000
C	3.695767000	-4.643162000	0.332627000
C	4.949733000	-5.219013000	0.348039000
C	5.854395000	-4.141670000	0.359166000
N	5.202281000	-2.978865000	0.352680000
N	-3.514745000	-3.497349000	0.356747000
C	-3.279413000	-4.842554000	0.327443000
C	-4.498715000	-5.488341000	0.337983000
C	-5.462874000	-4.464232000	0.349016000
N	-4.876714000	-3.266964000	0.347676000
H	6.934945000	-4.149930000	0.358374000
H	5.179674000	-6.273609000	0.341175000
H	2.723384000	-5.100409000	0.271506000
H	-2.282326000	-5.243687000	0.269768000
H	-4.668911000	-6.554069000	0.329056000
H	-6.541113000	-4.535214000	0.347659000

Ru	-5.363058000	-1.252899000	0.030146000
C	-5.287482000	-1.888637000	-4.323209000
C	-4.918924000	-1.662871000	-3.000823000
N	-5.816082000	-1.586309000	-1.999179000
C	-7.148630000	-1.734459000	-2.291949000
C	-7.573489000	-1.961709000	-3.601306000
C	-6.637899000	-2.041015000	-4.629676000
C	-8.073274000	-1.635158000	-1.143966000
C	-9.463670000	-1.774163000	-1.170957000
C	-10.168927000	-1.652139000	0.027375000
C	-9.496058000	-1.396686000	1.223393000
C	-8.105054000	-1.265519000	1.191823000
N	-7.444782000	-1.386513000	0.022593000
C	-7.211994000	-0.996572000	2.337821000
N	-5.871885000	-0.937010000	2.047859000
C	-5.001691000	-0.687248000	3.045038000
C	-5.405529000	-0.489822000	4.361641000
C	-6.763632000	-0.550471000	4.665869000
C	-7.671602000	-0.805239000	3.641162000
H	-4.521143000	-1.941647000	-5.088145000
H	-3.880826000	-1.538928000	-2.719441000
H	-8.629576000	-2.075117000	-3.814409000
H	-6.961217000	-2.217476000	-5.649990000
H	-9.990460000	-1.973739000	-2.096286000
H	-11.248401000	-1.757458000	0.029387000
H	-10.048785000	-1.304966000	2.150533000
H	-3.956176000	-0.648836000	2.766263000
H	-4.660041000	-0.293287000	5.123735000
H	-7.114160000	-0.401353000	5.681549000
H	-8.733023000	-0.853378000	3.852284000

Cartesian coordinates of DFT-optimized structure of **12** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Ru	-5.533455000	-0.048539000	0.032201000
Os	5.539396000	0.094213000	0.001424000
N	-5.080682000	-2.087615000	0.301356000
N	5.069060000	2.134228000	-0.256314000
N	-5.986330000	0.247223000	2.056049000
N	6.001073000	-0.195696000	-2.021306000
N	-7.574028000	-0.077861000	0.021893000
N	7.583709000	0.122360000	0.011582000
N	-5.957314000	-0.356465000	-1.997991000
N	5.972453000	0.395549000	2.030387000
N	-5.139508000	2.003216000	-0.232282000
N	5.127573000	-1.958657000	0.255013000
C	-5.110341000	0.409945000	3.068163000
C	5.124932000	-0.355633000	-3.041150000
H	4.078585000	-0.324433000	-2.763439000
C	-5.504672000	0.604165000	4.387156000

C	5.522175000	-0.547367000	-4.356529000
H	4.769860000	-0.669740000	-5.128006000
C	-6.867177000	0.633556000	4.686110000
C	6.886459000	-0.579246000	-4.655836000
C	-7.783583000	0.467037000	3.652175000
C	7.800541000	-0.416944000	-3.621136000
H	-8.847384000	0.486066000	3.858554000
C	-7.332159000	0.274730000	2.343670000
C	7.352676000	-0.225943000	-2.310681000
C	-8.237007000	0.088261000	1.192380000
C	8.254189000	-0.043828000	-1.163593000
C	-9.634151000	0.066885000	1.210940000
C	9.650186000	-0.023422000	-1.176770000
H	-10.184299000	0.197334000	2.135610000
H	10.199705000	-0.153462000	-2.101953000
C	-10.319751000	-0.127843000	0.009600000
C	10.337219000	0.169139000	0.024293000
C	-9.616973000	-0.297809000	-1.185461000
C	9.633144000	0.338413000	1.218906000
C	-8.220062000	-0.268883000	-1.154046000
C	8.237334000	0.311867000	1.192505000
C	-7.299159000	-0.426423000	-2.296796000
C	7.320061000	0.466764000	2.330995000
C	-7.733689000	-0.632397000	-3.608847000
C	7.751307000	0.671051000	3.644912000
H	-8.794693000	-0.685078000	-3.823507000
C	-6.804309000	-0.769884000	-4.635410000
C	6.824525000	0.805575000	4.672251000
C	-5.446002000	-0.696604000	-4.325393000
C	5.464454000	0.730956000	4.361934000
H	4.702438000	0.829451000	5.127314000
C	-5.068685000	-0.490047000	-3.003181000
C	5.083867000	0.527063000	3.043332000
H	4.041321000	0.462151000	2.757525000
C	-5.978960000	-3.093900000	0.332298000
C	5.966616000	3.146835000	-0.288417000
H	-7.021812000	-2.797101000	0.347004000
H	7.009686000	2.852650000	-0.297098000
C	-5.636464000	-4.431797000	0.334523000
C	5.619436000	4.481178000	-0.298532000
H	-6.396159000	-5.204262000	0.362077000
H	6.377773000	5.254877000	-0.325902000
C	-4.274971000	-4.770592000	0.265160000
C	4.256003000	4.817910000	-0.237133000
C	-3.329777000	-3.740770000	0.236591000
C	3.313997000	3.786783000	-0.208920000
H	-2.281675000	-3.970761000	0.130701000
H	2.265181000	4.015231000	-0.108269000
C	-3.735929000	-2.397550000	0.295841000
C	3.718108000	2.442383000	-0.260276000
C	-2.847814000	-1.223629000	0.252803000

C	2.830303000	1.272430000	-0.217049000
C	-3.558703000	-0.022528000	0.036307000
C	3.544244000	0.068468000	-0.002143000
C	-2.880642000	1.195394000	-0.187962000
C	2.862885000	-1.152328000	0.220820000
C	-3.796475000	2.348076000	-0.229138000
C	3.778428000	-2.301532000	0.261904000
C	-3.436076000	3.695822000	-0.170214000
C	3.419680000	-3.650236000	0.211275000
H	-2.401274000	3.991660000	-0.073304000
H	2.383937000	-3.944089000	0.120420000
C	-4.406655000	4.706650000	-0.191208000
C	4.386727000	-4.662880000	0.231977000
C	-5.757385000	4.338569000	-0.257561000
C	5.739443000	-4.296977000	0.289801000
H	-6.562068000	5.061188000	-0.282826000
H	6.542644000	-5.021157000	0.314884000
C	-6.057536000	2.982821000	-0.259128000
C	6.044834000	-2.944814000	0.283158000
H	-7.093120000	2.661057000	-0.272362000
H	7.080749000	-2.625914000	0.290426000
C	-1.466800000	1.194536000	-0.346448000
C	1.450079000	-1.149673000	0.380104000
C	-0.728136000	0.013315000	0.021196000
C	0.711964000	0.032861000	0.013553000
C	-1.431930000	-1.186433000	0.397257000
C	1.415099000	1.233593000	-0.361791000
C	-0.655969000	-2.247352000	0.963854000
C	0.638183000	2.293684000	-0.929027000
H	-1.159280000	-3.062292000	1.469720000
H	1.140735000	3.108443000	-1.435749000
C	0.708438000	-2.230532000	0.954564000
C	-0.726284000	2.276100000	-0.920133000
H	1.239615000	-3.033396000	1.450849000
H	-1.258218000	3.079216000	-1.415377000
O	-3.984120000	-6.085663000	0.223156000
O	3.927019000	-5.928760000	0.184172000
O	3.963335000	6.132629000	-0.200928000
O	-3.949177000	5.973133000	-0.135964000
C	-4.894376000	7.059464000	-0.134739000
C	-4.135115000	8.391701000	-0.055836000
C	-5.192181000	9.513372000	-0.051631000
C	-3.215437000	8.549834000	-1.281464000
C	-3.307218000	8.454393000	1.241672000
C	2.588310000	6.550830000	-0.127070000
C	2.525398000	8.085117000	-0.150815000
C	1.038746000	8.478027000	-0.047890000
C	3.300617000	8.666577000	1.046616000
C	3.113697000	8.615927000	-1.471926000
C	-2.610157000	-6.506079000	0.142823000
C	-2.550311000	-8.040614000	0.159673000

C	-3.136307000	-8.576196000	1.479869000
C	-3.329768000	-8.615109000	-1.038371000
C	-1.064764000	-8.436140000	0.051161000
C	4.870343000	-7.016852000	0.183611000
C	4.108279000	-8.348062000	0.115178000
C	3.274065000	-8.415893000	-1.178005000
C	3.194331000	-8.498201000	1.346077000
C	5.163378000	-9.471593000	0.111639000
H	-5.565847000	6.947992000	0.726449000
H	-5.492716000	7.013926000	-1.053920000
H	-5.863973000	9.426983000	0.811003000
H	-5.802851000	9.492257000	-0.962432000
H	-4.703709000	10.492846000	0.001151000
H	-3.791800000	8.517188000	-2.214467000
H	-2.462980000	7.755260000	-1.319574000
H	-2.691660000	9.512016000	-1.243816000
H	-3.950088000	8.356828000	2.125355000
H	-2.782114000	9.413930000	1.312803000
H	-2.559934000	7.654975000	1.275910000
H	2.039873000	6.132274000	-0.980976000
H	2.145521000	6.161319000	0.798996000
H	0.933869000	9.568684000	-0.066801000
H	0.591463000	8.114903000	0.885531000
H	0.457032000	8.071788000	-0.884405000
H	2.889324000	8.304537000	1.997041000
H	3.235603000	9.760813000	1.047346000
H	4.358797000	8.389059000	1.006756000
H	2.562012000	8.223934000	-2.335515000
H	4.164473000	8.328827000	-1.581422000
H	3.054994000	9.709948000	-1.504181000
H	-2.057888000	-6.092333000	0.996617000
H	-2.169550000	-6.113719000	-0.783072000
H	-2.581783000	-8.189034000	2.343817000
H	-3.079532000	-9.670458000	1.507183000
H	-4.186276000	-8.287677000	1.593247000
H	-4.387240000	-8.335491000	-0.994637000
H	-3.267108000	-9.709472000	-1.044151000
H	-2.920065000	-8.249724000	-1.988211000
H	-0.480358000	-8.035680000	0.888571000
H	-0.618888000	-8.068811000	-0.881285000
H	-0.962164000	-9.527104000	0.063862000
H	5.473249000	-6.967862000	1.099603000
H	5.537636000	-6.910883000	-0.681501000
H	2.747028000	-9.374888000	-1.241738000
H	3.912870000	-8.323904000	-2.065224000
H	2.527946000	-7.615409000	-1.212764000
H	2.444015000	-7.701611000	1.384173000
H	3.775431000	-8.462528000	2.276025000
H	2.668071000	-9.459278000	1.315589000
H	5.831081000	-9.390932000	-0.754716000
H	4.672910000	-10.450441000	0.066355000

H	5.778506000	-9.446831000	1.019343000
H	-4.752024000	0.729455000	5.157832000
H	-7.211558000	0.782999000	5.704118000
H	-4.063775000	0.379899000	2.789165000
H	-10.153120000	-0.448349000	-2.115325000
H	-11.404314000	-0.147272000	0.004843000
H	-7.135566000	-0.930361000	-5.656095000
H	-4.683446000	-0.797354000	-5.089934000
H	-4.025968000	-0.425693000	-2.715910000
H	7.230925000	-0.727393000	-5.673850000
H	8.864687000	-0.437821000	-3.825591000
H	11.421645000	0.187274000	0.029205000
H	10.168792000	0.486996000	2.149451000
H	8.812671000	0.724448000	3.857635000
H	7.156087000	0.964616000	5.692907000

Cartesian coordinates of DFT-optimized structure of **13** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Ru	4.994221000	-0.359596000	-0.209237000
N	5.481123000	0.159256000	1.766317000
N	7.030483000	-0.457727000	-0.236939000
N	5.375215000	-0.920043000	-2.196643000
C	4.627950000	0.467990000	2.762087000
H	3.575977000	0.437333000	2.504040000
C	5.050203000	0.805586000	4.043657000
H	4.314840000	1.045403000	4.803749000
C	6.417215000	0.826803000	4.318169000
H	6.783649000	1.085734000	5.306047000
C	7.310658000	0.508100000	3.299302000
H	8.377732000	0.516593000	3.488541000
C	6.830949000	0.176758000	2.029834000
C	7.712024000	-0.174099000	0.897039000
C	9.108254000	-0.234439000	0.903187000
H	9.674895000	-0.012079000	1.799746000
C	9.769830000	-0.590107000	-0.274080000
C	9.045445000	-0.878786000	-1.432556000
H	9.563541000	-1.153612000	-2.343809000
C	7.650580000	-0.804228000	-1.388574000
C	6.709448000	-1.066951000	-2.496677000
C	7.120450000	-1.440874000	-3.778369000
H	8.176228000	-1.551687000	-3.996521000
C	6.173187000	-1.670441000	-4.772295000
H	6.486076000	-1.961820000	-5.769502000
C	4.822514000	-1.518170000	-4.460816000
H	4.047152000	-1.684836000	-5.200443000
C	4.469609000	-1.143593000	-3.168594000
H	3.432852000	-1.012194000	-2.882163000
C	-3.313390000	1.205481000	-0.411569000
C	2.259211000	-1.389270000	0.150934000

C	-4.071288000	0.078909000	-0.076463000
C	3.014276000	-0.264261000	-0.181801000
C	-3.416280000	-1.116317000	0.237013000
C	2.361804000	0.928702000	-0.494211000
C	-2.011021000	-1.195211000	0.341044000
C	0.955477000	1.008191000	-0.600362000
C	-1.245984000	-0.058280000	-0.119326000
C	0.189846000	-0.127820000	-0.140672000
C	-1.910890000	1.148008000	-0.558204000
C	0.855452000	-1.333046000	0.297978000
C	-1.114553000	2.171332000	-1.163435000
C	0.060718000	-2.357155000	0.902920000
H	-1.595982000	2.990883000	-1.680836000
H	0.543538000	-3.177104000	1.418688000
C	0.245815000	2.104986000	-1.183262000
C	-1.299683000	-2.291731000	0.923535000
H	0.790087000	2.875074000	-1.714465000
H	-1.842487000	-3.061795000	1.455994000
H	10.853233000	-0.642483000	-0.288765000
N	-4.349661000	-2.174927000	0.459070000
N	-5.693723000	-1.825537000	0.442006000
C	-6.382368000	-2.962693000	0.592071000
C	-5.511364000	-4.059189000	0.686794000
C	-4.239344000	-3.529130000	0.586442000
H	-7.462117000	-2.933272000	0.611082000
H	-5.771970000	-5.100238000	0.803580000
H	-3.284257000	-4.023677000	0.562898000
Os	-6.069743000	0.176238000	-0.044847000
C	-5.903101000	1.316927000	4.214066000
C	-5.549331000	0.948199000	2.923229000
N	-6.456414000	0.727605000	1.944657000
C	-7.795562000	0.875426000	2.249666000
C	-8.201069000	1.244717000	3.534709000
C	-7.254580000	1.469549000	4.528783000
C	-8.736582000	0.618996000	1.146591000
N	-8.113260000	0.275704000	-0.012035000
C	-8.803787000	-0.003732000	-1.149522000
C	-10.198839000	0.058152000	-1.147746000
C	-10.858627000	0.409066000	0.032153000
C	-10.130399000	0.692568000	1.189710000
C	-7.927917000	-0.348341000	-2.281851000
N	-6.571666000	-0.331669000	-2.020119000
C	-5.722068000	-0.637401000	-3.026988000
C	-6.151106000	-0.967701000	-4.305347000
C	-7.520399000	-0.987964000	-4.576373000
C	-8.408290000	-0.674218000	-3.552760000
H	-4.513185000	0.817187000	2.636269000
H	-5.126806000	1.479919000	4.953555000
H	-7.566056000	1.757132000	5.527373000
H	-9.256807000	1.355322000	3.753147000
H	-10.645891000	0.963759000	2.103578000

H	-11.941833000	0.461669000	0.049592000
H	-10.767250000	-0.160420000	-2.044159000
H	-9.476229000	-0.681479000	-3.737124000
H	-7.890122000	-1.242142000	-5.564098000
H	-5.418370000	-1.203844000	-5.069139000
H	-4.669437000	-0.608004000	-2.773583000
N	-4.146085000	2.349986000	-0.606265000
N	-5.516525000	2.132692000	-0.546543000
C	-6.095916000	3.331490000	-0.677158000
C	-5.126006000	4.338371000	-0.801163000
C	-3.908919000	3.687236000	-0.739629000
H	-2.910099000	4.086753000	-0.746963000
H	-5.287872000	5.399931000	-0.911731000
H	-7.173486000	3.407034000	-0.662341000
N	3.089010000	-2.536467000	0.344562000
C	2.848073000	-3.874673000	0.457883000
C	4.064977000	-4.525715000	0.523460000
C	5.033663000	-3.512825000	0.421328000
N	4.454871000	-2.315694000	0.301068000
N	3.292305000	1.991012000	-0.712855000
N	4.631296000	1.639871000	-0.707180000
C	5.318931000	2.775897000	-0.845680000
C	4.449663000	3.877345000	-0.922478000
C	3.178108000	3.346297000	-0.821772000
H	1.848829000	-4.273728000	0.450961000
H	4.227582000	-5.588337000	0.622643000
H	6.111642000	-3.588004000	0.415945000
H	2.222485000	3.839639000	-0.787651000
H	4.710855000	4.919497000	-1.028033000
H	6.398870000	2.747046000	-0.870546000

Cartesian coordinates of DFT-optimized structure of **14** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Ru	4.788695000	-0.232542000	-0.207043000
N	5.321905000	0.678685000	1.607143000
N	6.824542000	-0.329496000	-0.269043000
N	5.122953000	-1.184768000	-2.047839000
C	4.492425000	1.183362000	2.541089000
H	3.434460000	1.099691000	2.322320000
C	4.944999000	1.777537000	3.714505000
H	4.227592000	2.166216000	4.428841000
C	6.318461000	1.858678000	3.941526000
H	6.708356000	2.315580000	4.845136000
C	7.187718000	1.341281000	2.985200000
H	8.259267000	1.392523000	3.138883000
C	6.677981000	0.754600000	1.824483000
C	7.532567000	0.181793000	0.764419000
C	8.928933000	0.127398000	0.745464000
H	9.516784000	0.529636000	1.562155000

C	9.562816000	-0.460066000	-0.351565000
C	8.811265000	-0.981413000	-1.406866000
H	9.308075000	-1.435801000	-2.256059000
C	7.417442000	-0.902836000	-1.341541000
C	6.450011000	-1.388150000	-2.346702000
C	6.831010000	-2.015408000	-3.535263000
H	7.881659000	-2.167407000	-3.752990000
C	5.860604000	-2.443587000	-4.436814000
H	6.150166000	-2.931343000	-5.361766000
C	4.517280000	-2.232971000	-4.127578000
H	3.724514000	-2.547940000	-4.797155000
C	4.194650000	-1.603737000	-2.929784000
H	3.164489000	-1.420077000	-2.648464000
C	-3.546478000	1.277339000	-0.463874000
C	2.071693000	-1.178208000	0.421484000
C	-4.280915000	0.174069000	0.033623000
C	2.808807000	-0.139373000	-0.147492000
C	-3.622100000	-0.990478000	0.497736000
C	2.138647000	0.964042000	-0.677060000
C	-2.204666000	-0.995623000	0.613267000
C	0.728519000	1.016686000	-0.758316000
C	-1.452628000	0.050655000	-0.035125000
C	-0.015614000	-0.012150000	-0.071329000
C	-2.141968000	1.160929000	-0.646829000
C	0.668953000	-1.103984000	0.579141000
C	-1.368854000	2.045675000	-1.464646000
C	-0.108928000	-1.992970000	1.384682000
H	-1.877207000	2.752905000	-2.107921000
H	0.387080000	-2.685672000	2.052503000
C	-0.008340000	1.976511000	-1.520459000
C	-1.471517000	-1.941457000	1.398781000
H	0.512436000	2.628927000	-2.209565000
H	-2.005742000	-2.596968000	2.075245000
H	10.645862000	-0.511848000	-0.384089000
Os	-6.273210000	0.257306000	0.071909000
C	-6.099900000	1.850616000	4.175959000
C	-5.750297000	1.351844000	2.929374000
N	-6.662088000	1.011995000	1.987911000
C	-8.001876000	1.172862000	2.288649000
C	-8.402214000	1.672142000	3.531527000
C	-7.451990000	2.014944000	4.486522000
C	-8.944367000	0.786628000	1.228214000
N	-8.317301000	0.332163000	0.106689000
C	-9.013243000	-0.077882000	-0.990958000
C	-10.409018000	-0.039604000	-0.984236000
C	-11.069140000	0.422941000	0.156722000
C	-10.338921000	0.840060000	1.272255000
C	-8.137879000	-0.524310000	-2.084547000
N	-6.780347000	-0.459638000	-1.831114000
C	-5.928590000	-0.857230000	-2.805584000
C	-6.356216000	-1.323055000	-4.040535000

C	-7.726655000	-1.390320000	-4.303379000
C	-8.616002000	-0.986728000	-3.314131000
H	-4.714851000	1.208812000	2.646036000
H	-5.320482000	2.104564000	4.886001000
H	-7.759616000	2.402372000	5.452038000
H	-9.457927000	1.791076000	3.746040000
H	-10.854167000	1.198250000	2.155986000
H	-12.152975000	0.458492000	0.176527000
H	-10.978174000	-0.362381000	-1.848364000
H	-9.684381000	-1.028693000	-3.491511000
H	-8.094640000	-1.749497000	-5.258645000
H	-5.622146000	-1.627025000	-4.778718000
H	-4.876408000	-0.788519000	-2.558627000
N	2.916161000	-2.257763000	0.824334000
C	2.691040000	-3.545015000	1.217964000
C	3.915188000	-4.162744000	1.386080000
C	4.871575000	-3.188143000	1.053570000
N	4.278961000	-2.044385000	0.703534000
N	3.054876000	1.962589000	-1.129598000
N	4.396815000	1.622910000	-1.089315000
C	5.071354000	2.708321000	-1.475161000
C	4.191661000	3.768999000	-1.751473000
C	2.927469000	3.266948000	-1.510460000
H	1.696176000	-3.942009000	1.318766000
H	4.090400000	-5.181340000	1.697822000
H	5.949758000	-3.257869000	1.036852000
H	1.969504000	3.755082000	-1.552231000
H	4.442112000	4.768361000	-2.073942000
H	6.150478000	2.677798000	-1.523462000
C	-4.564252000	-2.072807000	0.812549000
C	-4.229330000	-3.416995000	1.046034000
C	-5.221501000	-4.363796000	1.312330000
C	-6.563496000	-3.945433000	1.330940000
C	-6.843256000	-2.627067000	1.040472000
N	-5.897290000	-1.698271000	0.767992000
O	-4.998035000	-5.671210000	1.548812000
C	-3.650049000	-6.174549000	1.532349000
C	-3.669681000	-7.677468000	1.847520000
C	-2.209099000	-8.167606000	1.807706000
C	-4.259343000	-7.914704000	3.250789000
C	-4.498957000	-8.429878000	0.789533000
C	-4.404170000	2.438929000	-0.738865000
N	-5.768173000	2.180437000	-0.636169000
C	-6.635768000	3.185705000	-0.862303000
C	-6.263443000	4.486739000	-1.164363000
C	-4.892897000	4.781582000	-1.205527000
C	-3.977317000	3.745195000	-0.985028000
O	-4.367906000	6.001319000	-1.433749000
C	-5.250771000	7.118785000	-1.646039000
C	-4.414130000	8.389870000	-1.852139000
C	-5.403494000	9.550701000	-2.073955000

C	-3.510388000	8.233916000	-3.089791000
C	-3.558285000	8.668502000	-0.601950000
H	-3.196421000	-3.719183000	0.978128000
H	-7.358077000	-4.651536000	1.541720000
H	-7.868818000	-2.277818000	1.010399000
H	-3.056016000	-5.632884000	2.280149000
H	-3.213065000	-5.995495000	0.541265000
H	-1.761210000	-8.012996000	0.818496000
H	-2.164516000	-9.239391000	2.031371000
H	-1.590276000	-7.644987000	2.547290000
H	-3.671043000	-7.397010000	4.018691000
H	-4.256728000	-8.984395000	3.490029000
H	-5.291329000	-7.554880000	3.313226000
H	-4.090970000	-8.273784000	-0.216863000
H	-5.540957000	-8.094391000	0.789352000
H	-4.488658000	-9.506988000	0.992840000
H	-7.685705000	2.927409000	-0.784496000
H	-7.029154000	5.232228000	-1.333421000
H	-2.926082000	3.995304000	-0.975957000
H	-5.906714000	7.227699000	-0.772642000
H	-5.872509000	6.920976000	-2.528896000
H	-6.032353000	9.378635000	-2.956037000
H	-4.857566000	10.487981000	-2.230106000
H	-6.062466000	9.687623000	-1.207829000
H	-4.105295000	8.046045000	-3.992204000
H	-2.808844000	7.402665000	-2.966363000
H	-2.928767000	9.148211000	-3.255071000
H	-4.187568000	8.789688000	0.288529000
H	-2.980570000	9.590719000	-0.733106000
H	-2.855262000	7.851139000	-0.412029000

Cartesian coordinates of DFT-optimized structure of **15** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Os	4.796470000	-0.234276000	-0.206483000
N	5.342060000	0.680094000	1.603206000
N	6.839380000	-0.332534000	-0.270652000
N	5.138489000	-1.191346000	-2.043950000
C	4.515227000	1.191314000	2.543550000
H	3.456993000	1.108217000	2.328303000
C	4.973010000	1.786866000	3.711120000
H	4.257411000	2.178145000	4.425875000
C	6.348385000	1.868414000	3.935873000
H	6.740412000	2.327674000	4.837187000
C	7.213213000	1.347942000	2.978937000
H	8.285316000	1.398635000	3.128858000
C	6.704276000	0.757317000	1.819576000
C	7.555097000	0.183592000	0.763816000
C	8.950160000	0.127105000	0.739115000
H	9.538770000	0.532091000	1.553964000

C	9.583656000	-0.463728000	-0.356568000
C	8.829679000	-0.988218000	-1.408797000
H	9.324976000	-1.445324000	-2.257469000
C	7.436757000	-0.911531000	-1.346001000
C	6.470829000	-1.397826000	-2.344844000
C	6.847826000	-2.029892000	-3.532437000
H	7.898758000	-2.182396000	-3.748453000
C	5.879334000	-2.461331000	-4.432639000
H	6.168662000	-2.952416000	-5.355727000
C	4.534797000	-2.248866000	-4.122919000
H	3.741947000	-2.566340000	-4.791240000
C	4.209677000	-1.616778000	-2.930381000
H	3.179694000	-1.432561000	-2.650648000
C	-3.559943000	1.275603000	-0.464807000
C	2.058014000	-1.176480000	0.430978000
C	-4.291258000	0.175938000	0.034234000
C	2.797906000	-0.139039000	-0.145256000
C	-3.635740000	-0.984918000	0.500399000
C	2.125306000	0.963779000	-0.681528000
C	-2.217715000	-0.991502000	0.617013000
C	0.716220000	1.016283000	-0.760533000
C	-1.464559000	0.052227000	-0.033526000
C	-0.027584000	-0.010912000	-0.069296000
C	-2.154430000	1.160025000	-0.647965000
C	0.656238000	-1.101417000	0.585764000
C	-1.382463000	2.043786000	-1.467315000
C	-0.123820000	-1.988310000	1.392397000
H	-1.891604000	2.751069000	-2.110055000
H	0.370251000	-2.679364000	2.063000000
C	-0.022069000	1.974230000	-1.524431000
C	-1.486314000	-1.936761000	1.404325000
H	0.497308000	2.624841000	-2.216033000
H	-2.022038000	-2.592223000	2.079790000
H	10.666515000	-0.515573000	-0.390375000
Ru	-6.263356000	0.258545000	0.071914000
C	-6.077959000	1.855398000	4.172958000
C	-5.731526000	1.354976000	2.922882000
N	-6.643014000	1.016795000	1.988551000
C	-7.977168000	1.175470000	2.287722000
C	-8.381014000	1.674550000	3.528992000
C	-7.428339000	2.018548000	4.483227000
C	-8.923296000	0.786614000	1.223373000
N	-8.303617000	0.333945000	0.106375000
C	-8.991991000	-0.075202000	-0.986820000
C	-10.389068000	-0.038740000	-0.984926000
C	-11.047794000	0.424365000	0.156400000
C	-10.318848000	0.841963000	1.272364000
C	-8.113399000	-0.525500000	-2.084107000
N	-6.761733000	-0.463608000	-1.831646000
C	-5.909899000	-0.860958000	-2.798386000
C	-6.334590000	-1.329054000	-4.036797000

C	-7.703187000	-1.394083000	-4.299884000
C	-8.594923000	-0.987730000	-3.311876000
H	-4.695890000	1.211856000	2.638361000
H	-5.298127000	2.109882000	4.882349000
H	-7.735799000	2.406261000	5.448845000
H	-9.436361000	1.793146000	3.745452000
H	-10.834637000	1.200304000	2.155631000
H	-12.131788000	0.459916000	0.176241000
H	-10.958823000	-0.361967000	-1.848403000
H	-9.662953000	-1.028484000	-3.491596000
H	-8.071020000	-1.753759000	-5.255189000
H	-5.600144000	-1.634763000	-4.773881000
H	-4.857501000	-0.792914000	-2.549886000
N	2.905861000	-2.250295000	0.841311000
C	2.685934000	-3.530291000	1.261381000
C	3.910657000	-4.146128000	1.432408000
C	4.867278000	-3.182687000	1.076303000
N	4.273012000	-2.042537000	0.707347000
N	3.044510000	1.955951000	-1.141285000
N	4.391776000	1.620164000	-1.089616000
C	5.067095000	2.702021000	-1.493203000
C	4.185418000	3.753057000	-1.790399000
C	2.920755000	3.253598000	-1.546236000
H	1.692217000	-3.925664000	1.376227000
H	4.086001000	-5.159111000	1.761701000
H	5.944988000	-3.253231000	1.053618000
H	1.963275000	3.741026000	-1.599938000
H	4.435057000	4.747293000	-2.128782000
H	6.146120000	2.671391000	-1.536557000
C	-4.578582000	-2.070955000	0.815511000
C	-4.241701000	-3.415632000	1.042013000
C	-5.237014000	-4.361128000	1.307200000
C	-6.576965000	-3.939748000	1.330214000
C	-6.851658000	-2.616664000	1.045834000
N	-5.905151000	-1.693299000	0.777824000
O	-5.015346000	-5.669793000	1.539320000
C	-3.668441000	-6.175776000	1.519348000
C	-3.690525000	-7.679226000	1.831922000
C	-2.230961000	-8.172132000	1.789100000
C	-4.278529000	-7.917844000	3.235665000
C	-4.522849000	-8.428173000	0.773881000
C	-4.417175000	2.440915000	-0.740636000
N	-5.775567000	2.179085000	-0.645535000
C	-6.643618000	3.179090000	-0.868224000
C	-6.275382000	4.485027000	-1.164543000
C	-4.906281000	4.782703000	-1.200316000
C	-3.987707000	3.747432000	-0.980158000
O	-4.382788000	6.004110000	-1.423696000
C	-5.267291000	7.119909000	-1.637022000
C	-4.432815000	8.393068000	-1.839131000
C	-5.423940000	9.552154000	-2.062141000

C	-3.525363000	8.240662000	-3.074496000
C	-3.580945000	8.671815000	-0.586245000
H	-3.209481000	-3.719993000	0.971099000
H	-7.372934000	-4.644892000	1.539352000
H	-7.876764000	-2.264149000	1.018803000
H	-3.071749000	-5.636823000	2.266974000
H	-3.232847000	-5.996001000	0.527783000
H	-1.784210000	-8.016580000	0.799518000
H	-2.188063000	-9.244409000	2.010766000
H	-1.610050000	-7.652007000	2.528702000
H	-3.687931000	-7.402805000	4.003589000
H	-4.277797000	-8.987971000	3.472970000
H	-5.309630000	-7.555911000	3.300365000
H	-4.115904000	-8.271320000	-0.232827000
H	-5.564119000	-8.090435000	0.775641000
H	-4.514614000	-9.505644000	0.975395000
H	-7.693717000	2.918091000	-0.793719000
H	-7.042222000	5.229600000	-1.332847000
H	-2.936896000	3.999823000	-0.967281000
H	-5.926067000	7.226306000	-0.765419000
H	-5.886188000	6.921963000	-2.521856000
H	-6.050092000	9.379878000	-2.946116000
H	-4.879558000	10.490760000	-2.215701000
H	-6.085553000	9.686645000	-1.197649000
H	-4.117427000	8.053158000	-3.978863000
H	-2.822729000	7.410434000	-2.950408000
H	-2.944882000	9.156229000	-3.236746000
H	-4.212899000	8.790716000	0.302655000
H	-3.004651000	9.595318000	-0.714621000
H	-2.876905000	7.855557000	-0.395356000

Cartesian coordinates of DFT-optimized structure of **16** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Os	5.643674000	-0.955395000	0.034536000
N	5.170269000	1.076201000	-0.271282000
N	6.094360000	-1.301404000	-1.985134000
N	7.690504000	-0.952141000	0.036693000
N	6.087409000	-0.596651000	2.052949000
N	-5.084343000	0.803343000	-0.251643000
C	5.214800000	-1.468035000	-2.999954000
H	4.169309000	-1.414849000	-2.722416000
C	5.607050000	-1.693061000	-4.312062000
H	4.851681000	-1.819295000	-5.079903000
C	6.969686000	-1.752856000	-4.611823000
H	7.310674000	-1.927201000	-5.626839000
C	7.887648000	-1.583964000	-3.581156000
H	8.950991000	-1.625562000	-3.786613000
C	7.444253000	-1.359103000	-2.274981000
C	8.352178000	-1.167388000	-1.133191000

C	9.748312000	-1.187942000	-1.148356000
H	10.292414000	-1.359825000	-2.069752000
C	10.441485000	-0.983757000	0.047014000
C	9.744287000	-0.763384000	1.237171000
H	10.285331000	-0.606897000	2.163104000
C	8.348209000	-0.750918000	1.211402000
C	7.436593000	-0.542046000	2.347359000
C	7.875871000	-0.301692000	3.652087000
H	8.938587000	-0.262090000	3.861108000
C	6.954648000	-0.112034000	4.676308000
H	7.292524000	0.074631000	5.690173000
C	5.592951000	-0.165477000	4.371293000
H	4.835245000	-0.022022000	5.133790000
C	5.204652000	-0.406969000	3.060865000
H	4.159870000	-0.454766000	2.779576000
C	6.070941000	2.084026000	-0.341593000
H	7.112024000	1.783577000	-0.366137000
C	5.729292000	3.419386000	-0.370865000
H	6.489952000	4.189110000	-0.427891000
C	4.368818000	3.763009000	-0.289789000
C	3.422385000	2.736980000	-0.228042000
H	2.376625000	2.972593000	-0.114333000
C	3.818889000	1.390226000	-0.260474000
C	-2.704824000	-2.326740000	0.255901000
C	2.925526000	0.223867000	-0.189048000
C	-3.451261000	-1.161685000	0.035249000
C	3.646539000	-0.968560000	0.030683000
C	-2.798596000	0.065105000	-0.177371000
C	2.961737000	-2.172871000	0.262133000
C	-3.750704000	1.189014000	-0.233850000
C	-3.432882000	2.546545000	-0.178799000
H	-2.409183000	2.874818000	-0.070621000
C	-4.433039000	3.527799000	-0.218030000
C	-5.770904000	3.119577000	-0.301936000
H	-6.595948000	3.818208000	-0.344463000
C	-6.030419000	1.755097000	-0.297973000
H	-7.055291000	1.401010000	-0.322130000
C	-1.377927000	0.096963000	-0.308457000
C	1.563390000	-2.220954000	0.408788000
C	-0.622326000	-1.075083000	0.051086000
C	0.815778000	-1.035030000	0.050559000
C	-1.304573000	-2.299358000	0.405669000
C	1.504591000	0.176136000	-0.314943000
C	-0.521926000	-3.377853000	0.931671000
C	0.714124000	1.233866000	-0.862198000
H	-1.016002000	-4.220340000	1.399168000
H	1.204068000	2.063371000	-1.356207000
C	0.838835000	-3.340151000	0.934357000
C	-0.651011000	1.198101000	-0.856050000
H	1.376139000	-4.153712000	1.405092000
H	-1.190387000	2.002685000	-1.340056000

O	4.082644000	5.079130000	-0.270238000
O	-4.012324000	4.806311000	-0.162185000
C	-4.983830000	5.868880000	-0.187425000
C	-4.257211000	7.218153000	-0.089111000
C	-5.338033000	8.316471000	-0.121411000
C	-3.302236000	7.394174000	-1.284902000
C	-3.471734000	7.301304000	1.233492000
C	2.710389000	5.505789000	-0.190624000
C	2.656676000	7.040088000	-0.227243000
C	1.172400000	7.443622000	-0.129249000
C	3.434010000	7.626479000	0.966444000
C	3.249283000	7.557345000	-1.551749000
H	-5.675251000	5.742229000	0.655681000
H	-5.556032000	5.807815000	-1.122272000
H	-6.034939000	8.218861000	0.719980000
H	-5.919476000	8.279571000	-1.050746000
H	-4.872787000	9.306560000	-0.057052000
H	-3.846864000	7.347237000	-2.236078000
H	-2.532136000	6.616017000	-1.295754000
H	-2.801197000	8.367676000	-1.232322000
H	-4.138381000	7.185399000	2.097087000
H	-2.974809000	8.274364000	1.321121000
H	-2.705008000	6.521859000	1.289751000
H	2.154234000	5.082148000	-1.037087000
H	2.271388000	5.127768000	0.741892000
H	1.075552000	8.534820000	-0.155717000
H	0.721848000	7.089948000	0.806159000
H	0.589231000	7.035282000	-0.963790000
H	3.021772000	7.271733000	1.919240000
H	3.372364000	8.720912000	0.960489000
H	4.491406000	7.345778000	0.928225000
H	2.696748000	7.160866000	-2.412723000
H	4.298890000	7.264929000	-1.657505000
H	3.194878000	8.651359000	-1.592536000
H	11.526005000	-0.997204000	0.051241000
N	3.857303000	-3.280306000	0.364943000
C	3.697253000	-4.635731000	0.361797000
C	4.950231000	-5.218263000	0.380848000
C	5.859982000	-4.149310000	0.372900000
N	5.210711000	-2.979613000	0.350141000
N	-3.535720000	-3.484924000	0.343712000
C	-3.296611000	-4.828297000	0.319981000
C	-4.515030000	-5.480027000	0.327142000
C	-5.481600000	-4.459762000	0.332839000
N	-4.899206000	-3.258045000	0.329979000
H	6.940227000	-4.159702000	0.369228000
H	5.173734000	-6.274370000	0.389573000
H	2.723191000	-5.089779000	0.311149000
H	-2.297922000	-5.225706000	0.267015000
H	-4.680196000	-6.546885000	0.319791000
H	-6.559763000	-4.532422000	0.326867000

Ru	-5.427463000	-1.256557000	0.026537000
C	-5.286314000	-1.906534000	-4.331130000
C	-4.925140000	-1.682204000	-3.007067000
N	-5.823310000	-1.593214000	-2.006191000
C	-7.158422000	-1.728966000	-2.309927000
C	-7.577207000	-1.955601000	-3.623453000
C	-6.637834000	-2.046577000	-4.646412000
C	-8.091241000	-1.616552000	-1.170740000
C	-9.483580000	-1.732370000	-1.206435000
C	-10.199476000	-1.596628000	-0.014978000
C	-9.531722000	-1.350284000	1.186770000
C	-8.138505000	-1.242615000	1.171601000
N	-7.463942000	-1.377438000	0.005163000
C	-7.251231000	-0.991422000	2.325220000
N	-5.904411000	-0.952649000	2.046471000
C	-5.045144000	-0.723967000	3.059212000
C	-5.457819000	-0.527761000	4.372671000
C	-6.821473000	-0.567216000	4.663210000
C	-7.721098000	-0.800605000	3.627076000
H	-4.516620000	-1.969239000	-5.092540000
H	-3.888021000	-1.566966000	-2.715403000
H	-8.633455000	-2.059377000	-3.842776000
H	-6.956779000	-2.222405000	-5.668476000
H	-10.005993000	-1.924622000	-2.136355000
H	-11.280695000	-1.683802000	-0.022811000
H	-10.091950000	-1.247502000	2.108807000
H	-3.996588000	-0.701011000	2.786883000
H	-4.718044000	-0.348011000	5.144993000
H	-7.180220000	-0.418470000	5.676339000
H	-8.785749000	-0.833341000	3.826957000

Cartesian coordinates of DFT-optimized structure of **17** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 2, multiplicity = 1

Os	5.473418000	0.860289000	-0.025549000
N	5.362290000	-1.223937000	0.276579000
N	5.806119000	1.278220000	2.003647000
N	7.487105000	1.217775000	0.019797000
N	6.020411000	0.590834000	-2.032951000
C	4.888526000	1.283222000	2.998176000
H	3.876500000	1.040542000	2.698354000
C	5.204196000	1.575833000	4.317633000
H	4.421294000	1.564254000	5.067991000
C	6.526716000	1.879797000	4.647261000
H	6.807750000	2.113752000	5.668666000
C	7.483529000	1.875814000	3.638320000
H	8.517577000	2.105643000	3.867307000
C	7.117622000	1.574326000	2.323790000
C	8.072431000	1.544368000	1.204670000
C	9.443325000	1.805626000	1.253610000

H	9.927034000	2.067378000	2.187542000
C	10.190624000	1.724935000	0.076207000
C	9.571467000	1.388213000	-1.129801000
H	10.154027000	1.327953000	-2.041737000
C	8.198433000	1.134829000	-1.137894000
C	7.364599000	0.774781000	-2.295396000
C	7.869027000	0.623195000	-3.589907000
H	8.926482000	0.773068000	-3.773896000
C	7.018701000	0.281626000	-4.635886000
H	7.406977000	0.163194000	-5.641941000
C	5.661617000	0.095943000	-4.363323000
H	4.958069000	-0.171369000	-5.144119000
C	5.207187000	0.258310000	-3.062073000
H	4.163307000	0.125207000	-2.805912000
C	6.424603000	-2.059937000	0.343914000
H	7.397384000	-1.582959000	0.372984000
C	6.320749000	-3.434705000	0.364132000
H	7.204041000	-4.060262000	0.417356000
C	5.041202000	-4.009871000	0.278764000
C	3.930616000	-3.163457000	0.223886000
H	2.941903000	-3.577244000	0.108244000
C	4.086938000	-1.768841000	0.262225000
C	-3.016168000	0.770669000	-0.215250000
C	3.003096000	-0.775938000	0.187466000
C	-3.517258000	-0.524120000	0.023964000
C	3.505299000	0.522654000	-0.049697000
C	-2.637843000	-1.586479000	0.256447000
C	2.621418000	1.585210000	-0.287553000
C	-1.246043000	-1.392344000	0.383001000
C	1.232128000	1.388593000	-0.417369000
C	-0.718703000	-0.104272000	-0.004936000
C	0.705770000	0.098648000	-0.030390000
C	-1.612952000	0.967053000	-0.364650000
C	1.599383000	-0.972548000	0.331445000
C	-1.029506000	2.145538000	-0.930684000
C	1.014293000	-2.150473000	0.897012000
H	-1.668386000	2.874793000	-1.412468000
H	1.651578000	-2.879633000	1.380785000
C	0.318112000	2.350375000	-0.951820000
C	-0.333688000	-2.354949000	0.916694000
H	0.698439000	3.233526000	-1.449422000
H	-0.715316000	-3.238723000	1.412459000
O	4.987775000	-5.355222000	0.246858000
C	3.709944000	-6.012863000	0.164543000
C	3.925640000	-7.533132000	0.151416000
C	2.532270000	-8.186441000	0.065344000
C	4.766022000	-7.936990000	-1.074865000
C	4.629034000	-7.978713000	1.447399000
H	3.099938000	-5.718001000	1.028649000
H	3.199099000	-5.690506000	-0.752052000
H	2.627163000	-9.278046000	0.051737000

H	2.003203000	-7.884617000	-0.846898000
H	1.908667000	-7.915376000	0.926048000
H	4.273833000	-7.635388000	-2.007887000
H	4.901814000	-9.024292000	-1.103007000
H	5.756388000	-7.471326000	-1.047423000
H	4.037485000	-7.707264000	2.330548000
H	5.615735000	-7.514418000	1.543654000
H	4.763281000	-9.066568000	1.454293000
H	11.256364000	1.925182000	0.098397000
N	3.308856000	2.831254000	-0.402873000
C	2.913505000	4.137140000	-0.435826000
C	4.045171000	4.930307000	-0.452734000
C	5.128115000	4.038597000	-0.407385000
N	4.693632000	2.773652000	-0.364555000
N	-3.323646000	-2.833804000	0.372600000
N	-4.704296000	-2.772137000	0.355064000
C	-5.139341000	-4.034288000	0.389470000
C	-4.057892000	-4.931474000	0.409277000
C	-2.925807000	-4.139140000	0.384822000
C	-4.099659000	1.769481000	-0.282106000
C	-3.939022000	3.163004000	-0.233897000
C	-5.051897000	4.008958000	-0.280437000
C	-6.330269000	3.433723000	-0.367288000
C	-6.430488000	2.056351000	-0.357056000
N	-5.369005000	1.225449000	-0.299462000
O	-4.998762000	5.354110000	-0.239886000
C	-3.721542000	6.012262000	-0.151740000
C	-3.938752000	7.532219000	-0.128509000
C	-2.546179000	8.186354000	-0.036244000
C	-4.640881000	7.985905000	-1.422383000
C	-4.781156000	7.926979000	1.099345000
H	-6.201447000	-4.233899000	0.385836000
H	-4.094300000	-6.010260000	0.429864000
H	-1.886685000	-4.415528000	0.342764000
H	-2.950034000	3.576623000	-0.118449000
H	-7.214171000	4.059090000	-0.413576000
H	-7.403237000	1.578066000	-0.386574000
H	-3.110249000	5.724209000	-1.017161000
H	-3.211372000	5.684082000	0.763145000
H	-2.018016000	7.878979000	0.874657000
H	-2.642177000	9.277753000	-0.015532000
H	-1.921202000	7.921627000	-0.897922000
H	-4.047810000	7.721157000	-2.306555000
H	-4.776274000	9.073648000	-1.422020000
H	-5.626971000	7.521273000	-1.523203000
H	-4.289831000	7.619696000	2.030970000
H	-5.770971000	7.460439000	1.067506000
H	-4.918142000	9.013929000	1.134540000
Ru	-5.467051000	-0.854580000	0.014345000
C	-5.597545000	-0.067003000	4.348098000
C	-5.160288000	-0.233915000	3.038626000

N	-5.984276000	-0.573134000	2.027529000
C	-7.318811000	-0.761471000	2.304031000
C	-7.812075000	-0.608086000	3.602242000
C	-6.948872000	-0.257936000	4.636527000
C	-8.166704000	-1.130359000	1.152705000
N	-7.475265000	-1.212508000	-0.008750000
C	-8.065836000	-1.543878000	-1.181429000
C	-9.436847000	-1.812597000	-1.219040000
C	-10.169903000	-1.731912000	-0.032952000
C	-9.539773000	-1.389688000	1.165626000
C	-7.119991000	-1.574895000	-2.315109000
N	-5.811169000	-1.277465000	-2.011649000
C	-4.903989000	-1.283497000	-3.008365000
C	-5.229701000	-1.580794000	-4.327275000
C	-6.553691000	-1.886715000	-4.641711000
C	-7.502445000	-1.881173000	-3.623407000
H	-4.119836000	-0.097420000	2.768462000
H	-4.885892000	0.206750000	5.119247000
H	-7.325757000	-0.137210000	5.646793000
H	-8.866343000	-0.761787000	3.800746000
H	-10.112722000	-1.330299000	2.083652000
H	-11.235037000	-1.937168000	-0.042477000
H	-9.930193000	-2.079530000	-2.146389000
H	-8.538182000	-2.112940000	-3.842607000
H	-6.844730000	-2.124059000	-5.659682000
H	-4.454246000	-1.570535000	-5.085331000
H	-3.889127000	-1.038623000	-2.718294000
H	4.079945000	6.008818000	-0.484444000
H	1.874246000	4.414097000	-0.410998000
H	6.189636000	4.238771000	-0.390981000

Cartesian coordinates of DFT-optimized structure of **12ox** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Ru	-5.501257000	-0.053157000	0.014894000
Os	5.486605000	0.095074000	-0.006564000
N	-5.060105000	-2.093406000	0.295771000
N	5.060350000	2.156334000	-0.261995000
N	-5.993814000	0.242838000	2.033441000
N	5.927031000	-0.190287000	-2.043773000
N	-7.553737000	-0.089140000	-0.024379000
N	7.586978000	0.115015000	-0.074786000
N	-5.906076000	-0.365439000	-2.022223000
N	6.050262000	0.398174000	1.996698000
N	-5.124748000	2.002579000	-0.251933000
N	5.117624000	-1.973671000	0.275513000
C	-5.133056000	0.409180000	3.057255000
C	5.004077000	-0.345361000	-3.019739000
H	3.969208000	-0.307088000	-2.705595000
C	-5.548066000	0.601390000	4.370514000

C	5.348948000	-0.541011000	-4.350694000
H	4.564402000	-0.659028000	-5.089315000
C	-6.914296000	0.624348000	4.649012000
C	6.697224000	-0.580288000	-4.703285000
C	-7.814869000	0.453880000	3.601473000
C	7.655422000	-0.420780000	-3.706986000
H	-8.881508000	0.467604000	3.792202000
C	-7.342911000	0.264256000	2.300514000
C	7.260499000	-0.225909000	-2.383280000
C	-8.231017000	0.074655000	1.135581000
C	8.205364000	-0.047132000	-1.268077000
C	-9.628366000	0.049830000	1.135701000
C	9.599895000	-0.029533000	-1.339066000
H	-10.191722000	0.178812000	2.052337000
H	10.113003000	-0.155017000	-2.284744000
C	-10.295730000	-0.146228000	-0.075278000
C	10.329363000	0.155706000	-0.163577000
C	-9.576525000	-0.314164000	-1.260458000
C	9.672691000	0.321646000	1.056683000
C	-8.180203000	-0.281482000	-1.208154000
C	8.276576000	0.298791000	1.075552000
C	-7.242645000	-0.437371000	-2.338686000
C	7.401914000	0.459248000	2.249139000
C	-7.659043000	-0.644553000	-3.655730000
C	7.878655000	0.662687000	3.544292000
H	-8.716726000	-0.698623000	-3.885062000
C	-6.715051000	-0.781784000	-4.669364000
C	6.984465000	0.806482000	4.600573000
C	-5.361867000	-0.707170000	-4.340967000
C	5.617048000	0.742497000	4.335953000
H	4.880222000	0.847694000	5.124027000
C	-5.002859000	-0.499025000	-3.013597000
C	5.189877000	0.538423000	3.030303000
H	4.137696000	0.480948000	2.783973000
C	-5.957375000	-3.100200000	0.317529000
C	5.958246000	3.163858000	-0.295477000
H	-7.000852000	-2.805993000	0.321776000
H	7.001064000	2.871402000	-0.326881000
C	-5.611111000	-4.437279000	0.322067000
C	5.608911000	4.499191000	-0.282384000
H	-6.369633000	-5.211098000	0.340082000
H	6.366581000	5.273063000	-0.312431000
C	-4.249186000	-4.775032000	0.265463000
C	4.248611000	4.835550000	-0.195229000
C	-3.304749000	-3.742223000	0.248117000
C	3.304191000	3.799085000	-0.164784000
H	-2.255184000	-3.970393000	0.151848000
H	2.256520000	4.024394000	-0.046126000
C	-3.717093000	-2.402792000	0.304651000
C	3.714575000	2.464484000	-0.237801000
C	-2.830869000	-1.224358000	0.269771000

C	2.820343000	1.288234000	-0.185993000
C	-3.544410000	-0.021190000	0.044609000
C	3.521775000	0.075183000	0.036403000
C	-2.865519000	1.202861000	-0.174478000
C	2.852542000	-1.153065000	0.271502000
C	-3.785478000	2.354412000	-0.230707000
C	3.771532000	-2.311439000	0.303394000
C	-3.427742000	3.700737000	-0.169153000
C	3.401662000	-3.651099000	0.262957000
H	-2.395737000	4.000864000	-0.055995000
H	2.364127000	-3.942539000	0.189611000
C	-4.402379000	4.709246000	-0.208571000
C	4.369646000	-4.671161000	0.274238000
C	-5.749840000	4.334503000	-0.292583000
C	5.722143000	-4.309373000	0.309177000
H	-6.556858000	5.053910000	-0.330534000
H	6.523234000	-5.035698000	0.325694000
C	-6.046231000	2.977666000	-0.294250000
C	6.032716000	-2.956995000	0.291781000
H	-7.080340000	2.652760000	-0.320910000
H	7.069713000	-2.642685000	0.282085000
C	-1.458189000	1.202201000	-0.327081000
C	1.448672000	-1.143693000	0.440558000
C	-0.718239000	0.021369000	0.054536000
C	0.712568000	0.041826000	0.054080000
C	-1.424355000	-1.180683000	0.434099000
C	1.415097000	1.246547000	-0.336564000
C	-0.654708000	-2.236790000	1.022196000
C	0.641841000	2.305855000	-0.913502000
H	-1.165509000	-3.043732000	1.532865000
H	1.148138000	3.114724000	-1.425172000
C	0.707047000	-2.221370000	1.023762000
C	-0.719525000	2.283349000	-0.908841000
H	1.237951000	-3.014252000	1.535131000
H	-1.254775000	3.078538000	-1.412441000
O	-3.956583000	-6.087426000	0.223122000
O	3.903565000	-5.927597000	0.242485000
O	3.953879000	6.142158000	-0.139215000
O	-3.950298000	5.975193000	-0.152406000
C	-4.898712000	7.060472000	-0.171452000
C	-4.142920000	8.394572000	-0.094977000
C	-5.202765000	9.513633000	-0.108646000
C	-3.212646000	8.545707000	-1.313470000
C	-3.327212000	8.468630000	1.209643000
C	2.577829000	6.564917000	-0.038162000
C	2.523536000	8.099226000	-0.028845000
C	1.039346000	8.495138000	0.098285000
C	3.313346000	8.650590000	1.173343000
C	3.100446000	8.655805000	-1.344310000
C	-2.581721000	-6.509264000	0.146831000
C	-2.525903000	-8.043971000	0.146123000

C	-3.122496000	-8.593916000	1.455612000
C	-3.298182000	-8.601780000	-1.064462000
C	-1.040560000	-8.441695000	0.043185000
C	4.839550000	-7.027508000	0.239550000
C	4.063708000	-8.351118000	0.198916000
C	3.208987000	-8.426480000	-1.080369000
C	3.168947000	-8.478486000	1.446365000
C	5.109969000	-9.483138000	0.191972000
H	-5.579204000	6.953244000	0.682911000
H	-5.485181000	7.004718000	-1.097442000
H	-5.881871000	9.432517000	0.748726000
H	-5.805271000	9.484089000	-1.024576000
H	-4.716730000	10.494440000	-0.059240000
H	-3.780935000	8.507596000	-2.251170000
H	-2.459783000	7.751024000	-1.340495000
H	-2.689331000	9.508103000	-1.276731000
H	-3.977699000	8.374872000	2.088102000
H	-2.806195000	9.430486000	1.278858000
H	-2.577247000	7.672329000	1.256200000
H	2.019729000	6.165034000	-0.894105000
H	2.149102000	6.157695000	0.886174000
H	0.939922000	9.586299000	0.107578000
H	0.599612000	8.110857000	1.026756000
H	0.448185000	8.112668000	-0.742657000
H	2.910104000	8.269481000	2.119700000
H	3.252426000	9.744636000	1.198393000
H	4.370197000	8.370788000	1.116826000
H	2.539471000	8.283765000	-2.210633000
H	4.149630000	8.369525000	-1.470248000
H	3.044044000	9.750262000	-1.352375000
H	-2.035202000	-6.105512000	1.008955000
H	-2.135725000	-6.107229000	-0.772119000
H	-2.573501000	-8.218413000	2.328162000
H	-3.067883000	-9.688480000	1.469972000
H	-4.172783000	-8.305018000	1.564907000
H	-4.355516000	-8.321131000	-1.024487000
H	-3.237173000	-9.696016000	-1.083409000
H	-2.881409000	-8.225319000	-2.006864000
H	-0.461441000	-8.054413000	0.890331000
H	-0.586880000	-8.063146000	-0.880969000
H	-0.941090000	-9.532961000	0.041849000
H	5.455128000	-6.969529000	1.145793000
H	5.491442000	-6.933495000	-0.637889000
H	2.673390000	-9.381691000	-1.124076000
H	3.834526000	-8.350442000	-1.978394000
H	2.468450000	-7.620664000	-1.113179000
H	2.426325000	-7.674853000	1.487975000
H	3.765572000	-8.438125000	2.366149000
H	2.633582000	-9.434787000	1.434867000
H	5.763937000	-9.418693000	-0.686047000
H	4.610155000	-10.457835000	0.166370000

H	5.739647000	-9.453029000	1.089407000
H	-4.807228000	0.729677000	5.151886000
H	-7.274518000	0.771721000	5.661734000
H	-4.082120000	0.383959000	2.795749000
H	-10.099236000	-0.465947000	-2.197542000
H	-11.380022000	-0.168364000	-0.095344000
H	-7.032158000	-0.943194000	-5.694308000
H	-4.588496000	-0.807713000	-5.094422000
H	-3.964033000	-0.433753000	-2.713586000
H	6.999671000	-0.731584000	-5.733788000
H	8.709679000	-0.448108000	-3.954541000
H	11.413077000	0.171440000	-0.198900000
H	10.240952000	0.465355000	1.967606000
H	8.946279000	0.708496000	3.722060000
H	7.350065000	0.964710000	5.609315000

Cartesian coordinates of DFT-optimized structure of **13ox** complex by B3LYP/Def2-TZVP; 6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Ru	4.965342000	-0.358095000	-0.208565000
N	5.465851000	0.165107000	1.766057000
N	7.014801000	-0.457134000	-0.238225000
N	5.355851000	-0.924279000	-2.196095000
C	4.613474000	0.476207000	2.761157000
H	3.560951000	0.447424000	2.506293000
C	5.038033000	0.814717000	4.041975000
H	4.303644000	1.056477000	4.802188000
C	6.404758000	0.833962000	4.314663000
H	6.772770000	1.093290000	5.301750000
C	7.296905000	0.512811000	3.295081000
H	8.364074000	0.519784000	3.482875000
C	6.815064000	0.181024000	2.027280000
C	7.695056000	-0.171966000	0.893485000
C	9.091379000	-0.231779000	0.899553000
H	9.658822000	-0.008052000	1.795068000
C	9.751053000	-0.589457000	-0.277811000
C	9.026246000	-0.880173000	-1.435146000
H	9.543368000	-1.156365000	-2.346350000
C	7.631426000	-0.804997000	-1.388703000
C	6.689136000	-1.069825000	-2.496149000
C	7.099948000	-1.444619000	-3.776908000
H	8.155607000	-1.554153000	-3.995435000
C	6.151933000	-1.676723000	-4.769887000
H	6.464574000	-1.968840000	-5.766857000
C	4.801876000	-1.526197000	-4.457871000
H	4.025963000	-1.694875000	-5.196251000
C	4.449080000	-1.150251000	-3.165766000
H	3.412032000	-1.020481000	-2.880672000
C	-3.300169000	1.215969000	-0.424194000
C	2.248799000	-1.392031000	0.161887000

C	-4.051979000	0.078263000	-0.075183000
C	3.006387000	-0.263447000	-0.180067000
C	-3.403588000	-1.127302000	0.252834000
C	2.351489000	0.933437000	-0.501250000
C	-2.005932000	-1.194871000	0.364496000
C	0.951069000	1.006186000	-0.612958000
C	-1.243143000	-0.057847000	-0.117201000
C	0.184158000	-0.126946000	-0.138416000
C	-1.906492000	1.148256000	-0.577636000
C	0.851790000	-1.329494000	0.314875000
C	-1.112753000	2.164405000	-1.200805000
C	0.061675000	-2.346157000	0.941762000
H	-1.597018000	2.971232000	-1.734394000
H	0.550284000	-3.153869000	1.470412000
C	0.244596000	2.095218000	-1.217756000
C	-1.295916000	-2.283904000	0.965164000
H	0.793040000	2.852648000	-1.761921000
H	-1.839801000	-3.041030000	1.513936000
H	10.834390000	-0.641855000	-0.293482000
N	-4.332835000	-2.182923000	0.473122000
N	-5.677688000	-1.839297000	0.448387000
C	-6.361697000	-2.976663000	0.589641000
C	-5.486553000	-4.071322000	0.687848000
C	-4.217703000	-3.538054000	0.596513000
H	-7.441775000	-2.953663000	0.603305000
H	-5.745730000	-5.112787000	0.800639000
H	-3.260629000	-4.029505000	0.578523000
Os	-6.014495000	0.173469000	-0.045467000
C	-5.894503000	1.273472000	4.210584000
C	-5.542690000	0.919115000	2.914202000
N	-6.458985000	0.709818000	1.944003000
C	-7.792218000	0.850713000	2.250579000
C	-8.195003000	1.204330000	3.538159000
C	-7.243023000	1.419646000	4.530521000
C	-8.730938000	0.604595000	1.141909000
N	-8.111521000	0.275522000	-0.013601000
C	-8.794674000	0.010042000	-1.149376000
C	-10.189775000	0.071337000	-1.154324000
C	-10.849604000	0.409164000	0.027888000
C	-10.124588000	0.679405000	1.189117000
C	-7.918326000	-0.324651000	-2.285562000
N	-6.569046000	-0.314541000	-2.019684000
C	-5.707243000	-0.610764000	-3.016802000
C	-6.130937000	-0.927470000	-4.301374000
C	-7.496340000	-0.941262000	-4.580153000
C	-8.392387000	-0.635663000	-3.559802000
H	-4.506992000	0.793748000	2.626780000
H	-5.114932000	1.428842000	4.947478000
H	-7.551188000	1.695431000	5.533124000
H	-9.249591000	1.310480000	3.761537000
H	-10.639509000	0.940473000	2.105510000

H	-11.932612000	0.462020000	0.044299000
H	-10.755122000	-0.137014000	-2.054350000
H	-9.458575000	-0.638402000	-3.751004000
H	-7.860067000	-1.184397000	-5.572536000
H	-5.392844000	-1.156999000	-5.061255000
H	-4.656037000	-0.587143000	-2.761051000
N	-4.129151000	2.356846000	-0.618025000
N	-5.499575000	2.144904000	-0.552265000
C	-6.074304000	3.343284000	-0.674722000
C	-5.100734000	4.348276000	-0.800998000
C	-3.887247000	3.694645000	-0.747021000
H	-2.887024000	4.091197000	-0.758639000
H	-5.261228000	5.410075000	-0.907621000
H	-7.151458000	3.424892000	-0.655819000
N	3.075719000	-2.535280000	0.360811000
C	2.834683000	-3.874141000	0.484002000
C	4.050883000	-4.522602000	0.551235000
C	5.020324000	-3.509608000	0.438952000
N	4.442390000	-2.314837000	0.311665000
N	3.278633000	1.991895000	-0.725885000
N	4.618534000	1.640644000	-0.716185000
C	5.305022000	2.774275000	-0.862120000
C	4.434913000	3.876163000	-0.947741000
C	3.164333000	3.347913000	-0.844120000
H	1.835963000	-4.274927000	0.481753000
H	4.214866000	-5.584311000	0.656481000
H	6.098106000	-3.586356000	0.430633000
H	2.209412000	3.843146000	-0.813446000
H	4.697365000	4.917244000	-1.059386000
H	6.384965000	2.746733000	-0.885280000

Cartesian coordinates of DFT-optimized structure of **14ox** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Ru	4.757149000	-0.222118000	-0.203062000
N	5.288475000	0.688820000	1.615488000
N	6.803758000	-0.311786000	-0.257082000
N	5.111463000	-1.170654000	-2.045571000
C	4.453592000	1.189833000	2.546091000
H	3.396494000	1.104554000	2.324854000
C	4.900360000	1.783682000	3.722132000
H	4.179000000	2.169409000	4.433916000
C	6.272205000	1.867864000	3.954353000
H	6.657582000	2.324552000	4.859925000
C	7.146656000	1.353862000	3.000649000
H	8.217347000	1.407767000	3.158441000
C	6.642710000	0.767630000	1.837774000
C	7.503610000	0.199137000	0.779786000
C	8.900326000	0.150207000	0.767599000
H	9.483148000	0.552256000	1.587764000

C	9.540435000	-0.431850000	-0.328365000
C	8.795822000	-0.952944000	-1.388361000
H	9.297893000	-1.402955000	-2.236592000
C	7.401438000	-0.879424000	-1.327704000
C	6.440073000	-1.366457000	-2.338628000
C	6.829539000	-1.988210000	-3.526733000
H	7.881701000	-2.134504000	-3.740287000
C	5.864977000	-2.418417000	-4.433879000
H	6.161120000	-2.901979000	-5.358865000
C	4.519798000	-2.215337000	-4.130285000
H	3.731342000	-2.531912000	-4.804002000
C	4.188630000	-1.591113000	-2.931963000
H	3.156041000	-1.414002000	-2.656269000
C	-3.543740000	1.273289000	-0.486071000
C	2.055643000	-1.181136000	0.419240000
C	-4.262524000	0.164459000	0.025318000
C	2.793191000	-0.136719000	-0.151750000
C	-3.616778000	-1.004451000	0.500854000
C	2.119544000	0.967855000	-0.687817000
C	-2.206961000	-1.001847000	0.621873000
C	0.714101000	1.009750000	-0.777897000
C	-1.459024000	0.043194000	-0.046329000
C	-0.029506000	-0.017063000	-0.081654000
C	-2.147840000	1.150157000	-0.677870000
C	0.658005000	-1.104133000	0.579551000
C	-1.378787000	2.028352000	-1.506932000
C	-0.113915000	-1.986762000	1.399391000
H	-1.890012000	2.723210000	-2.160626000
H	0.388561000	-2.669385000	2.072263000
C	-0.020261000	1.958283000	-1.557902000
C	-1.474487000	-1.941018000	1.416672000
H	0.504198000	2.600398000	-2.253323000
H	-2.008580000	-2.587760000	2.101011000
H	10.623747000	-0.479563000	-0.356442000
Os	-6.226671000	0.250654000	0.077216000
C	-6.063731000	1.788882000	4.186855000
C	-5.728006000	1.297970000	2.931866000
N	-6.657275000	0.986284000	2.000739000
C	-7.987162000	1.161226000	2.307959000
C	-8.373020000	1.650340000	3.556125000
C	-7.408561000	1.968421000	4.507499000
C	-8.938324000	0.799781000	1.243084000
N	-8.328078000	0.348798000	0.122255000
C	-9.024224000	-0.037948000	-0.972008000
C	-10.419439000	0.023261000	-0.969360000
C	-11.067878000	0.486653000	0.176284000
C	-10.331539000	0.879091000	1.295156000
C	-8.157526000	-0.498777000	-2.069745000
N	-6.805841000	-0.462616000	-1.814955000
C	-5.951785000	-0.881344000	-2.775759000
C	-6.385785000	-1.342398000	-4.011762000

C	-7.753375000	-1.379108000	-4.280243000
C	-8.641038000	-0.953480000	-3.296800000
H	-4.696239000	1.142950000	2.644656000
H	-5.274926000	2.021831000	4.892876000
H	-7.703677000	2.348575000	5.479417000
H	-9.424711000	1.781470000	3.780263000
H	-10.837983000	1.237058000	2.183162000
H	-12.150691000	0.541363000	0.197636000
H	-10.993614000	-0.282453000	-1.835466000
H	-9.708643000	-0.974000000	-3.479023000
H	-8.124380000	-1.732719000	-5.236046000
H	-5.653916000	-1.664272000	-4.743704000
H	-4.899222000	-0.835899000	-2.528817000
N	2.899346000	-2.255666000	0.823404000
C	2.676839000	-3.545579000	1.214787000
C	3.901653000	-4.157473000	1.386052000
C	4.856796000	-3.178609000	1.056953000
N	4.262711000	-2.037826000	0.706031000
N	3.031044000	1.966700000	-1.137202000
N	4.374959000	1.631974000	-1.088763000
C	5.046256000	2.717622000	-1.473885000
C	4.163259000	3.775295000	-1.757641000
C	2.900681000	3.271147000	-1.521843000
H	1.683483000	-3.947839000	1.310949000
H	4.080230000	-5.175864000	1.696199000
H	5.935118000	-3.246065000	1.043063000
H	1.941975000	3.757545000	-1.568943000
H	4.412708000	4.774750000	-2.080262000
H	6.125724000	2.692152000	-1.516296000
C	-4.563959000	-2.093910000	0.818805000
C	-4.218998000	-3.430233000	1.043771000
C	-5.212249000	-4.384604000	1.308389000
C	-6.553240000	-3.968831000	1.327791000
C	-6.837829000	-2.648378000	1.044813000
N	-5.892994000	-1.721129000	0.780788000
O	-4.982689000	-5.684572000	1.540765000
C	-3.631392000	-6.190638000	1.523782000
C	-3.655408000	-7.693383000	1.836952000
C	-2.195079000	-8.184767000	1.796992000
C	-4.245966000	-7.931188000	3.239762000
C	-4.485138000	-8.442644000	0.777046000
C	-4.405356000	2.444234000	-0.757576000
N	-5.765862000	2.191829000	-0.648055000
C	-6.631153000	3.196586000	-0.862666000
C	-6.253636000	4.497566000	-1.165391000
C	-4.883989000	4.785799000	-1.216994000
C	-3.968000000	3.740220000	-1.002569000
O	-4.352987000	5.993837000	-1.448918000
C	-5.226150000	7.124193000	-1.661880000
C	-4.374665000	8.383511000	-1.874205000
C	-5.352845000	9.553918000	-2.096819000

C	-3.476841000	8.213091000	-3.114287000
C	-3.512443000	8.656418000	-0.627129000
H	-3.185193000	-3.728810000	0.974121000
H	-7.346240000	-4.677359000	1.534896000
H	-7.864101000	-2.301838000	1.018179000
H	-3.040112000	-5.649356000	2.273172000
H	-3.197697000	-6.009828000	0.532249000
H	-1.746587000	-8.029621000	0.808204000
H	-2.152752000	-9.256840000	2.019119000
H	-1.576036000	-7.664355000	2.537839000
H	-3.657680000	-7.415024000	4.008602000
H	-4.243892000	-9.001161000	3.477120000
H	-5.278044000	-7.571551000	3.302454000
H	-4.076976000	-8.285045000	-0.228978000
H	-5.527250000	-8.107396000	0.777501000
H	-4.475126000	-9.519921000	0.978704000
H	-7.681696000	2.944112000	-0.778495000
H	-7.017044000	5.246582000	-1.327726000
H	-2.915707000	3.985147000	-1.001383000
H	-5.875400000	7.238984000	-0.785028000
H	-5.851084000	6.926715000	-2.541781000
H	-5.985476000	9.386253000	-2.976952000
H	-4.796717000	10.484373000	-2.256882000
H	-6.007883000	9.700480000	-1.229379000
H	-4.076401000	8.027290000	-4.013949000
H	-2.782261000	7.376082000	-2.989768000
H	-2.887297000	9.121149000	-3.284877000
H	-4.137528000	8.786710000	0.264921000
H	-2.926081000	9.572274000	-0.763244000
H	-2.816446000	7.832999000	-0.437099000

Cartesian coordinates of DFT-optimized structure of **15ox** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Os	4.738395000	-0.227765000	-0.204972000
N	5.323604000	0.662134000	1.613907000
N	6.831846000	-0.322156000	-0.261342000
N	5.143542000	-1.162344000	-2.050333000
C	4.481411000	1.158880000	2.546229000
H	3.425272000	1.078191000	2.324416000
C	4.929534000	1.741935000	3.724876000
H	4.205836000	2.123126000	4.436172000
C	6.300559000	1.821925000	3.962420000
H	6.683444000	2.271099000	4.872369000
C	7.177018000	1.313663000	3.008128000
H	8.247124000	1.364237000	3.168280000
C	6.678529000	0.736970000	1.840040000
C	7.535039000	0.177395000	0.779790000
C	8.930541000	0.126047000	0.766631000
H	9.512190000	0.519316000	1.591328000

C	9.569740000	-0.445676000	-0.334345000
C	8.824104000	-0.955114000	-1.398302000
H	9.323390000	-1.397908000	-2.251454000
C	7.430929000	-0.880939000	-1.336781000
C	6.472099000	-1.358266000	-2.348467000
C	6.853590000	-1.972023000	-3.541456000
H	7.904645000	-2.118038000	-3.758529000
C	5.885266000	-2.394262000	-4.447662000
H	6.176978000	-2.871595000	-5.376866000
C	4.541707000	-2.191337000	-4.137560000
H	3.749739000	-2.501357000	-4.809612000
C	4.211478000	-1.575942000	-2.936672000
H	3.180305000	-1.400245000	-2.659255000
C	-3.548914000	1.276335000	-0.472839000
C	2.040927000	-1.191450000	0.426609000
C	-4.281873000	0.171714000	0.029581000
C	2.776572000	-0.139167000	-0.152637000
C	-3.624410000	-0.995017000	0.496074000
C	2.107982000	0.975363000	-0.695881000
C	-2.215331000	-0.996928000	0.616179000
C	0.708023000	1.014691000	-0.782733000
C	-1.460770000	0.047319000	-0.042770000
C	-0.034475000	-0.015023000	-0.079431000
C	-2.153581000	1.155659000	-0.663804000
C	0.649559000	-1.107127000	0.587244000
C	-1.386409000	2.034738000	-1.497172000
C	-0.127049000	-1.990791000	1.404435000
H	-1.902061000	2.730812000	-2.146427000
H	0.371810000	-2.670609000	2.082626000
C	-0.029641000	1.967559000	-1.557361000
C	-1.485905000	-1.937980000	1.415239000
H	0.491008000	2.606353000	-2.258396000
H	-2.025467000	-2.582865000	2.097300000
H	10.652688000	-0.494549000	-0.363163000
Ru	-6.230893000	0.256040000	0.074319000
C	-6.040302000	1.852742000	4.175204000
C	-5.699118000	1.352393000	2.923218000
N	-6.615786000	1.016524000	1.993995000
C	-7.947293000	1.176746000	2.297606000
C	-8.345805000	1.675372000	3.539809000
C	-7.388355000	2.017371000	4.490549000
C	-8.899302000	0.790666000	1.235964000
N	-8.288713000	0.337552000	0.117750000
C	-8.979364000	-0.067744000	-0.971730000
C	-10.376456000	-0.026702000	-0.966216000
C	-11.028185000	0.437550000	0.178166000
C	-10.294513000	0.851389000	1.291946000
C	-8.106211000	-0.522241000	-2.073093000
N	-6.754565000	-0.466858000	-1.827001000
C	-5.907587000	-0.869571000	-2.794981000
C	-6.340067000	-1.337255000	-4.031294000

C	-7.709126000	-1.395282000	-4.288561000
C	-8.595281000	-0.983149000	-3.297399000
H	-4.664415000	1.208833000	2.636736000
H	-5.257012000	2.105375000	4.881180000
H	-7.691580000	2.404827000	5.457484000
H	-9.399871000	1.795608000	3.760601000
H	-10.805672000	1.210606000	2.177237000
H	-12.111901000	0.477008000	0.202141000
H	-10.950559000	-0.346958000	-1.827607000
H	-9.664003000	-1.018835000	-3.472814000
H	-8.082735000	-1.754102000	-5.241818000
H	-5.609816000	-1.647495000	-4.770397000
H	-4.853611000	-0.807714000	-2.553045000
N	2.885251000	-2.265370000	0.825936000
C	2.661457000	-3.554275000	1.218980000
C	3.883344000	-4.173212000	1.380849000
C	4.842902000	-3.203348000	1.044417000
N	4.252212000	-2.057970000	0.698515000
N	3.023431000	1.969802000	-1.143193000
N	4.371261000	1.640129000	-1.086562000
C	5.043451000	2.726844000	-1.471383000
C	4.158510000	3.778467000	-1.763495000
C	2.896143000	3.272651000	-1.533119000
H	1.666592000	-3.950364000	1.323937000
H	4.058358000	-5.191996000	1.690695000
H	5.920492000	-3.277037000	1.023524000
H	1.936955000	3.757044000	-1.588508000
H	4.407607000	4.776713000	-2.089108000
H	6.122990000	2.702985000	-1.508548000
C	-4.568831000	-2.081642000	0.817530000
C	-4.230509000	-3.423658000	1.042343000
C	-5.228033000	-4.367602000	1.314802000
C	-6.565880000	-3.941544000	1.341881000
C	-6.840135000	-2.618158000	1.056850000
N	-5.891786000	-1.698986000	0.784847000
O	-5.008607000	-5.673518000	1.548825000
C	-3.662666000	-6.186127000	1.526064000
C	-3.691600000	-7.687990000	1.844593000
C	-2.234275000	-8.187469000	1.799462000
C	-4.276599000	-7.918247000	3.250963000
C	-4.530361000	-8.436947000	0.791650000
C	-4.407202000	2.443741000	-0.749710000
N	-5.762818000	2.179852000	-0.651501000
C	-6.631962000	3.177883000	-0.874054000
C	-6.262998000	4.483207000	-1.173932000
C	-4.894885000	4.782558000	-1.212767000
C	-3.974804000	3.746529000	-0.990373000
O	-4.371868000	6.000474000	-1.439639000
C	-5.255560000	7.118399000	-1.656597000
C	-4.418556000	8.388877000	-1.863092000
C	-5.408342000	9.548550000	-2.089520000

C	-3.512025000	8.230740000	-3.098432000
C	-3.565863000	8.670415000	-0.611388000
H	-3.199556000	-3.731221000	0.965165000
H	-7.362740000	-4.644538000	1.554411000
H	-7.864479000	-2.263915000	1.033073000
H	-3.062157000	-5.646442000	2.269826000
H	-3.231184000	-6.011990000	0.531925000
H	-1.789676000	-8.037808000	0.808020000
H	-2.195899000	-9.259047000	2.025015000
H	-1.609043000	-7.667558000	2.535538000
H	-3.681702000	-7.402753000	4.015223000
H	-4.279549000	-8.987429000	3.492173000
H	-5.306129000	-7.552126000	3.317246000
H	-4.125770000	-8.285655000	-0.216833000
H	-5.570274000	-8.095050000	0.795338000
H	-4.526049000	-9.513581000	0.997309000
H	-7.681823000	2.917711000	-0.796874000
H	-7.030348000	5.227242000	-1.341950000
H	-2.924111000	3.999612000	-0.977498000
H	-5.912974000	7.227281000	-0.784570000
H	-5.874197000	6.917023000	-2.540548000
H	-6.035058000	9.374284000	-2.972649000
H	-4.862410000	10.485638000	-2.246433000
H	-6.069215000	9.686950000	-1.225125000
H	-4.104715000	8.040369000	-4.001738000
H	-2.809791000	7.400528000	-2.971638000
H	-2.930975000	9.145227000	-3.264311000
H	-4.197143000	8.792819000	0.277466000
H	-2.988814000	9.592897000	-0.743199000
H	-2.862251000	7.854242000	-0.418352000

Cartesian coordinates of DFT-optimized structure of **16ox** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Os	5.590435000	-0.947881000	0.037260000
N	5.152323000	1.098247000	-0.262039000
N	6.070032000	-1.244338000	-1.992007000
N	7.690794000	-0.976550000	0.018949000
N	6.112967000	-0.582314000	2.043291000
N	-5.067875000	0.802771000	-0.248977000
C	5.168446000	-1.358490000	-2.992096000
H	4.128014000	-1.277569000	-2.705674000
C	5.541133000	-1.570788000	-4.313229000
H	4.773141000	-1.656669000	-5.073330000
C	6.895648000	-1.666735000	-4.628216000
H	7.219754000	-1.830419000	-5.650192000
C	7.832387000	-1.546580000	-3.605863000
H	8.891088000	-1.614566000	-3.824687000
C	7.409251000	-1.336342000	-2.293550000
C	8.330599000	-1.193994000	-1.152854000

C	9.724999000	-1.262132000	-1.183682000
H	10.255655000	-1.435700000	-2.111904000
C	10.430135000	-1.102675000	0.010182000
C	9.750371000	-0.877006000	1.207910000
H	10.301095000	-0.751708000	2.132116000
C	8.355259000	-0.816452000	1.186190000
C	7.458512000	-0.583089000	2.331407000
C	7.909721000	-0.363419000	3.632864000
H	8.972813000	-0.365339000	3.840743000
C	6.995425000	-0.139831000	4.658055000
H	7.341472000	0.030217000	5.671761000
C	5.634691000	-0.136019000	4.355754000
H	4.883333000	0.035878000	5.117886000
C	5.233507000	-0.357599000	3.044553000
H	4.186912000	-0.362992000	2.769366000
C	6.051372000	2.103561000	-0.330303000
H	7.093056000	1.807125000	-0.361110000
C	5.703405000	3.438610000	-0.352565000
H	6.461742000	4.210242000	-0.409762000
C	4.344088000	3.779639000	-0.264884000
C	3.398099000	2.746722000	-0.200556000
H	2.351923000	2.977424000	-0.080731000
C	3.804913000	1.409344000	-0.240872000
C	-2.693138000	-2.335655000	0.283656000
C	2.909684000	0.234935000	-0.167319000
C	-3.440453000	-1.165453000	0.059048000
C	3.624880000	-0.965605000	0.061190000
C	-2.784525000	0.065026000	-0.157064000
C	2.953901000	-2.182267000	0.297762000
C	-3.737081000	1.190917000	-0.223637000
C	-3.416767000	2.545914000	-0.170621000
H	-2.394248000	2.875174000	-0.053792000
C	-4.417657000	3.528000000	-0.224051000
C	-5.753872000	3.117385000	-0.315223000
H	-6.578932000	3.815344000	-0.366378000
C	-6.014350000	1.752857000	-0.305922000
H	-7.038946000	1.398963000	-0.334753000
C	-1.372326000	0.092552000	-0.294268000
C	1.560651000	-2.226010000	0.449777000
C	-0.614818000	-1.080168000	0.074770000
C	0.814621000	-1.039739000	0.074493000
C	-1.298181000	-2.304326000	0.439349000
C	1.501441000	0.178306000	-0.305200000
C	-0.519088000	-3.378859000	0.980020000
C	0.711913000	1.232808000	-0.865549000
H	-1.016967000	-4.214360000	1.455339000
H	1.203971000	2.053880000	-1.370649000
C	0.839774000	-3.342839000	0.985600000
C	-0.649358000	1.191345000	-0.859088000
H	1.379143000	-4.148001000	1.467626000
H	-1.194566000	1.985053000	-1.353681000

O	4.052776000	5.087858000	-0.242470000
O	-3.997471000	4.804453000	-0.173615000
C	-4.967837000	5.869393000	-0.219415000
C	-4.238688000	7.218130000	-0.137127000
C	-5.317613000	8.317640000	-0.189270000
C	-3.278943000	7.375188000	-1.331748000
C	-3.458223000	7.318663000	1.187251000
C	2.677707000	5.516657000	-0.153870000
C	2.627393000	7.050546000	-0.191215000
C	1.143812000	7.454801000	-0.084072000
C	3.412777000	7.636331000	0.997507000
C	3.212039000	7.565861000	-1.520030000
H	-5.663219000	5.754844000	0.621933000
H	-5.534211000	5.794700000	-1.156550000
H	-6.017559000	8.233719000	0.651027000
H	-5.895776000	8.268222000	-1.120030000
H	-4.850511000	9.307554000	-0.137793000
H	-3.820230000	7.316749000	-2.284148000
H	-2.510813000	6.594967000	-1.329096000
H	-2.775538000	8.347945000	-1.290455000
H	-4.127951000	7.214141000	2.049864000
H	-2.961917000	8.292933000	1.263640000
H	-2.691240000	6.540494000	1.256717000
H	2.118709000	5.092065000	-0.997263000
H	2.248195000	5.138624000	0.782386000
H	1.048410000	8.546005000	-0.110477000
H	0.698873000	7.102269000	0.854390000
H	0.555239000	7.046909000	-0.914929000
H	3.006374000	7.282388000	1.953028000
H	3.351325000	8.730632000	0.991021000
H	4.470014000	7.355878000	0.952726000
H	2.653788000	7.169390000	-2.377228000
H	4.261017000	7.273486000	-1.632344000
H	3.157826000	8.659744000	-1.560676000
H	11.513362000	-1.153304000	0.006871000
N	3.849966000	-3.286967000	0.387721000
C	3.686528000	-4.641673000	0.369409000
C	4.937125000	-5.226522000	0.368157000
C	5.848584000	-4.158681000	0.361096000
N	5.202257000	-2.989414000	0.359987000
N	-3.522149000	-3.490237000	0.369559000
C	-3.283660000	-4.835180000	0.348857000
C	-4.501781000	-5.483993000	0.353604000
C	-5.468479000	-4.462004000	0.353301000
N	-4.886364000	-3.262086000	0.349356000
H	6.928798000	-4.173132000	0.346776000
H	5.159561000	-6.282462000	0.363858000
H	2.710857000	-5.093742000	0.326265000
H	-2.285634000	-5.234952000	0.299172000
H	-4.668802000	-6.550452000	0.347081000
H	-6.546537000	-4.535059000	0.342839000

Ru	-5.398204000	-1.258573000	0.036363000
C	-5.236898000	-1.917474000	-4.319897000
C	-4.884417000	-1.690545000	-2.993648000
N	-5.789903000	-1.600131000	-2.000178000
C	-7.121961000	-1.737125000	-2.311814000
C	-7.532161000	-1.965863000	-3.627009000
C	-6.585643000	-2.058228000	-4.643619000
C	-8.063078000	-1.624741000	-1.178518000
C	-9.454849000	-1.744739000	-1.224800000
C	-10.178458000	-1.610138000	-0.038235000
C	-9.520230000	-1.361335000	1.167881000
C	-8.127162000	-1.249600000	1.160817000
N	-7.446763000	-1.382631000	0.000106000
C	-7.248599000	-0.994025000	2.321076000
N	-5.900753000	-0.950837000	2.053097000
C	-5.049375000	-0.717450000	3.070801000
C	-5.473034000	-0.520317000	4.380897000
C	-6.838074000	-0.564231000	4.660855000
C	-7.729270000	-0.802731000	3.618261000
H	-4.461907000	-1.981211000	-5.075645000
H	-3.848973000	-1.574856000	-2.697147000
H	-8.586714000	-2.070397000	-3.853186000
H	-6.897880000	-2.235774000	-5.667373000
H	-9.970404000	-1.939384000	-2.157850000
H	-11.259298000	-1.700410000	-0.053303000
H	-10.086889000	-1.259766000	2.085883000
H	-3.998620000	-0.691059000	2.808459000
H	-4.739543000	-0.336681000	5.158097000
H	-7.205158000	-0.415052000	5.670839000
H	-8.795108000	-0.838971000	3.810194000

Cartesian coordinates of DFT-optimized structure of **17ox** complex by B3LYP/Def2-TZVP;  
6-31G(d,p)/CH<sub>3</sub>CN, charge = 3, multiplicity = 2

Os	5.429809000	0.849766000	-0.023629000
N	5.355301000	-1.241659000	0.285695000
N	5.898977000	1.236641000	1.992332000
N	7.496816000	1.223704000	-0.055327000
N	5.957914000	0.580011000	-2.044151000
C	5.014818000	1.206668000	3.013975000
H	3.995328000	0.953961000	2.753109000
C	5.379320000	1.480890000	4.326026000
H	4.625790000	1.443249000	5.104318000
C	6.707402000	1.796010000	4.608936000
H	7.024653000	2.014101000	5.622888000
C	7.627073000	1.823324000	3.564761000
H	8.666228000	2.060267000	3.758117000
C	7.212913000	1.542466000	2.262977000
C	8.119944000	1.542512000	1.102271000
C	9.487103000	1.826928000	1.102932000

H	10.003942000	2.083322000	2.019713000
C	10.182755000	1.775615000	-0.105938000
C	9.520577000	1.444452000	-1.288934000
H	10.063900000	1.404838000	-2.225207000
C	8.152767000	1.167667000	-1.237015000
C	7.279175000	0.795112000	-2.362666000
C	7.729932000	0.651431000	-3.674861000
H	8.773495000	0.826515000	-3.906401000
C	6.840807000	0.281741000	-4.679698000
H	7.186448000	0.168735000	-5.701480000
C	5.505547000	0.059621000	-4.346589000
H	4.774350000	-0.231689000	-5.091890000
C	5.103456000	0.217307000	-3.026548000
H	4.075486000	0.057572000	-2.728392000
C	6.414779000	-2.077893000	0.334164000
H	7.390579000	-1.607128000	0.341759000
C	6.302191000	-3.452779000	0.363433000
H	7.182903000	-4.082523000	0.402652000
C	5.019708000	-4.021844000	0.306708000
C	3.909595000	-3.166361000	0.266451000
H	2.916815000	-3.575186000	0.171705000
C	4.080931000	-1.778804000	0.295774000
C	-3.000321000	0.790801000	-0.190218000
C	2.995790000	-0.775486000	0.237417000
C	-3.500119000	-0.509472000	0.038507000
C	3.491799000	0.529571000	-0.008759000
C	-2.615362000	-1.576360000	0.281688000
C	2.617880000	1.610194000	-0.239565000
C	-1.234225000	-1.373458000	0.432304000
C	1.232959000	1.412041000	-0.370066000
C	-0.705682000	-0.082768000	0.044958000
C	0.709461000	0.121739000	0.028521000
C	-1.601597000	0.988496000	-0.328284000
C	1.604106000	-0.958092000	0.401293000
C	-1.020310000	2.167116000	-0.896886000
C	1.017447000	-2.132638000	0.978022000
H	-1.660475000	2.890819000	-1.384276000
H	1.653774000	-2.851983000	1.476508000
C	0.325230000	2.375043000	-0.911819000
C	-0.327619000	-2.332562000	0.989104000
H	0.711002000	3.254758000	-1.410817000
H	-0.718401000	-3.207807000	1.492371000
O	4.954799000	-5.360632000	0.287307000
C	3.670205000	-6.016512000	0.234889000
C	3.882824000	-7.536741000	0.232601000
C	2.485613000	-8.185669000	0.177107000
C	4.700067000	-7.954580000	-1.004546000
C	4.607262000	-7.971669000	1.520558000
H	3.080289000	-5.709943000	1.108169000
H	3.146564000	-5.699635000	-0.675720000
H	2.577553000	-9.277482000	0.173065000

H	1.941987000	-7.891838000	-0.729133000
H	1.877665000	-7.904162000	1.045582000
H	4.192839000	-7.659638000	-1.931526000
H	4.830845000	-9.042539000	-1.024591000
H	5.692917000	-7.493385000	-0.998734000
H	4.032505000	-7.689213000	2.411223000
H	5.597549000	-7.510911000	1.594692000
H	4.737173000	-9.059825000	1.535463000
H	11.244767000	1.994050000	-0.126113000
N	3.304200000	2.851440000	-0.349159000
C	2.904921000	4.157514000	-0.334162000
C	4.033188000	4.951350000	-0.347004000
C	5.118650000	4.058977000	-0.345377000
N	4.688015000	2.795229000	-0.334387000
N	-3.294985000	-2.822581000	0.382015000
N	-4.676650000	-2.767100000	0.341342000
C	-5.104982000	-4.029346000	0.365522000
C	-4.018510000	-4.922948000	0.400272000
C	-2.890705000	-4.127990000	0.395356000
C	-4.087791000	1.786846000	-0.273222000
C	-3.933178000	3.178994000	-0.217240000
C	-5.051283000	4.019204000	-0.281006000
C	-6.323600000	3.435349000	-0.391930000
C	-6.416879000	2.057400000	-0.387988000
N	-5.350926000	1.234170000	-0.314571000
O	-5.007502000	5.362397000	-0.235634000
C	-3.737027000	6.032080000	-0.121869000
C	-3.969530000	7.549629000	-0.096104000
C	-2.584838000	8.216327000	0.021666000
C	-4.654588000	8.001868000	-1.399631000
C	-4.835713000	7.931043000	1.119383000
H	-6.165649000	-4.234997000	0.343722000
H	-4.051783000	-6.001787000	0.415727000
H	-1.850062000	-4.400959000	0.367282000
H	-2.949271000	3.598996000	-0.081897000
H	-7.210311000	4.055518000	-0.451015000
H	-7.385890000	1.573484000	-0.435934000
H	-3.108791000	5.753124000	-0.977901000
H	-3.241284000	5.704084000	0.800769000
H	-2.068628000	7.909812000	0.939644000
H	-2.691736000	9.306590000	0.045681000
H	-1.943671000	7.961618000	-0.831053000
H	-4.045052000	7.745669000	-2.275050000
H	-4.799279000	9.088364000	-1.397291000
H	-5.635009000	7.529485000	-1.518178000
H	-4.356425000	7.625299000	2.057744000
H	-5.820292000	7.455088000	1.069826000
H	-4.984039000	9.016396000	1.156074000
Ru	-5.428468000	-0.847494000	-0.007686000
C	-5.669042000	-0.085596000	4.327076000
C	-5.201692000	-0.239858000	3.026134000

N	-6.000732000	-0.581998000	1.996758000
C	-7.337830000	-0.786119000	2.242933000
C	-7.860652000	-0.645900000	3.530311000
C	-7.023384000	-0.292752000	4.585056000
C	-8.158419000	-1.156875000	1.071588000
N	-7.445965000	-1.223770000	-0.075299000
C	-8.007151000	-1.553885000	-1.260036000
C	-9.374281000	-1.836633000	-1.327950000
C	-10.130850000	-1.770876000	-0.156145000
C	-9.528851000	-1.430353000	1.056925000
C	-7.038137000	-1.569600000	-2.375244000
N	-5.739121000	-1.264017000	-2.044368000
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C	-7.392006000	-1.869986000	-3.692266000
H	-4.157112000	-0.089990000	2.781420000
H	-4.976794000	0.191040000	5.114507000
H	-7.423292000	-0.182336000	5.587516000
H	-8.917033000	-0.812024000	3.705359000
H	-10.120229000	-1.383004000	1.963597000
H	-11.193344000	-1.986992000	-0.188160000
H	-9.846265000	-2.103054000	-2.266265000
H	-8.420998000	-2.108400000	-3.934086000
H	-6.691347000	-2.093113000	-5.716464000
H	-4.317852000	-1.524240000	-5.090574000
H	-3.804311000	-1.004750000	-2.711004000
H	4.068071000	6.029910000	-0.348247000
H	1.865062000	4.430521000	-0.283692000
H	6.179469000	4.263959000	-0.340360000