

Theoretical DFT Investigation of Structure and Electronic Properties of η^5 -Cyclopentadienyl Half-sandwich Organochalcogenide Complexes

Supplementary Information

G.T. Oyeniyi¹, Iu.A. Melchakova², S.P. Polyutov³, and P.V. Avramov^{1,*}

¹ *Department of Chemistry, Kyungpook National University, 80 Daehak-ro, Daegu 41566, Republic Korea*

² *School of Physics and Engineering, ITMO University, St Petersburg 197101, Russia*

³ *International Research Center of Spectroscopy and Quantum Chemistry at Siberian Federal University, Krasnoyarsk, Russia*

Table S1. Total energy (in *a.u.*) for Cp fragment (E_{F1}), EPh₃ fragments (E_{F2}) and E_P for [Cp][(EPh₃)].

Complexes	$E_{F1(Cp)}$	$E_{F2(EPh_3)}$	$E_P(Cp(EPh_3))$
[Cp][(TePh ₃)] (1)	-193.4990	-963.1264	-1156.5299
[Cp ^{Me4}][(TePh ₃)] (2)	-350.8071	-963.1264	-1313.8443
[Cp ^{Me5}][(TePh ₃)] (3)	-390.1351	-963.1264	-1353.1736
[Cp][(SePh ₃)] (4)	-193.4990	-1068.3049	-1261.7039
[Cp ^{Me5}][(SePh ₃)] (5)	-390.1351	-1068.3049	-1458.3473

Atomic coordinates of all η^5 -cyclopentadienyl half-sandwich organochalcogenides complexes optimized at *ab initio* TPSS/(cc-pVTZ-PP/6-31G*)

[Cp][(TePh₃)]

C	- 1.8 5 9 9 1 5 0 0 0	- 0.4 0 1 3 8 8 0 0 0	- 6.2 1 1 9 9 3 0 0 0
C	- 3.0 7 2 7 2 7 0 0 0	0.2 2 3 7 8 2 0 0 0	- 6.5 4 1 5 5 4 0 0 0

C	-1.327350000	-0.257012000	-4.923192000
H	-3.494131000	0.111768000	-7.540239000
H	-0.385120000	-0.738726000	-4.662687000
C	-3.747273000	0.998341000	-5.587194000
C	-2.004918000	0.504097000	-3.956298000
H	-4.683282000	1.489810000	-5.844774000
H	-1.593939000	0.600088000	-2.953353000
C	-3.215379000	1.130904000	-4.292436000
H	-1.333435000	-0.997380000	-6.956708000
C	-2.173869000	2.245327000	-0.660392000
C	-3.181868000	1.445629000	-1.230922000
C	-1.380150000	1.751339000	0.387728000
H	-0.599693000	2.376843000	0.821011000
C	-3.398226000	0.147879000	-0.733462000
C	-1.598845000	0.455607000	0.877037000
H	-4.180626000	-0.477564000	-1.160667000
H	-0.988263000	0.070266000	1.693193000
C	-2.609581000	-0.342949000	0.317919000
H	-2.783906000	-1.348761000	0.700804000
H	-2.002436000	3.258620000	-1.031291000
C	-6.844735000	-1.269161000	-3.011295000
C	-8.027378000	-0.842352000	-2.389179000
C	-5.763568000	-0.385263000	-3.158391000
H	-8.864027000	-1.531320000	-2.278534000
H	-4.846240000	-0.716663000	-3.641826000
C	-8.135039000	0.474344000	-1.915723000
C	-5.877046000	0.930921000	-2.680985000
H	-9.053429000	0.810320000	-1.435021000
C	-7.062366000	1.365387000	-2.066619000

H	-7.152345000	2.396057000	-1.723607000
H	-6.760182000	-2.289365000	-3.385324000
C	-5.829110000	3.603945000	-4.748287000
C	-6.374360000	4.340306000	-3.646208000
C	-5.453826000	5.355296000	-3.303463000
C	-4.344887000	5.272936000	-4.186869000
C	-4.575173000	4.209900000	-5.090878000
H	-6.348145000	2.828829000	-5.308597000
H	-7.342184000	4.160670000	-3.185190000
H	-5.568234000	6.069063000	-2.490767000
H	-3.462091000	5.907496000	-4.165376000
H	-3.916363000	3.891372000	-5.894921000
Te	-4.295896000	2.390018000	-2.891007000

[Cp^{Me4}][(TePh₃)]

C	0.829495000	-0.454103000	4.452869000
C	0.311929000	0.727612000	3.899942000
C	1.138946000	-1.540061000	3.620448000
H	0.076351000	1.576145000	4.542149000
H	1.546896000	-2.456796000	4.045868000
C	0.092238000	0.819677000	2.517881000
C	0.933339000	-1.449006000	2.234444000
H	-0.310619000	1.733948000	2.084950000
H	1.196570000	-2.284309000	1.585908000
C	0.411246000	-0.267219000	1.687848000
H	0.993396000	-0.526946000	5.527477000
C	1.628119000	-2.602367000	-1.024831000
C	1.758659000	-1.206546000	-0.888498000

C	2.746228000	-3.399771000	-1.317608000
H	2.634853000	-4.479971000	-1.413396000
C	3.017035000	-0.611737000	-1.081557000
C	4.001312000	-2.800620000	-1.497094000
H	3.131355000	0.468178000	-1.002585000
H	4.870955000	-3.414046000	-1.731237000
C	4.132714000	-1.407575000	-1.385652000
H	5.105533000	-0.938570000	-1.535759000
H	0.649583000	-3.075320000	-0.905381000
C	2.359534000	3.511127000	0.071221000
C	1.840492000	4.362346000	-0.917136000
C	1.837697000	2.218741000	0.234428000
H	2.245912000	5.366377000	-1.037955000
H	2.233400000	1.557802000	1.003740000
C	0.795495000	3.923503000	-1.743777000
C	0.793948000	1.780812000	-0.599304000
H	0.386870000	4.584412000	-2.507798000
C	0.268295000	2.632745000	-1.582678000
H	-0.560973000	2.291439000	-2.202959000
H	3.168073000	3.852152000	0.717683000
C	-2.589745000	0.996312000	-0.060590000
C	-2.690037000	0.781622000	-1.478563000
C	-2.944828000	-0.587081000	-1.719742000
C	-2.999546000	-1.247489000	-0.460356000
C	-2.808798000	-0.278349000	0.565945000
H	-2.635511000	1.559890000	-2.238086000
Te	-0.141790000	-0.168350000	-0.407412000
C	-3.116593000	-1.245580000	-3.064474000
H	-2.746810000	-0.597380000	-3.872146000

H	-2.572097000	-2.202059000	-3.119172000
H	-4.176217000	-1.470347000	-3.276260000
C	-3.258656000	-2.715476000	-0.240452000
H	-2.860117000	-3.319938000	-1.070232000
H	-2.795164000	-3.065671000	0.694565000
H	-4.338162000	-2.938364000	-0.169378000
C	-2.885593000	-0.557827000	2.043670000
H	-2.263261000	-1.422229000	2.325880000
H	-2.537333000	0.299272000	2.634571000
H	-3.920431000	-0.784093000	2.352588000
C	-2.532484000	2.340730000	0.623085000
H	-2.404341000	2.226494000	1.708926000
H	-1.703375000	2.959720000	0.244584000
H	-3.464889000	2.907896000	0.462048000

[Cp^{Me5}][(TePh₃)]

C	0.995354000	2.269705000	3.891112000
C	0.978675000	3.004912000	2.695713000
C	0.802638000	0.880245000	3.861165000
H	1.130117000	4.083975000	2.714463000
H	0.816548000	0.305836000	4.787270000
C	0.760724000	2.353989000	1.472910000
C	0.592170000	0.222010000	2.639173000
H	0.742284000	2.927292000	0.545590000
H	0.443813000	-0.856246000	2.615171000
C	0.577115000	0.960901000	1.445382000
H	1.156809000	2.777696000	4.841172000
C	0.037988000	-2.983151000	0.156790000

C	0.852247000	-1.843402000	0.210101000
C	0.550090000	-4.227711000	0.559111000
H	-0.082366000	-5.114208000	0.515387000
C	2.177883000	-1.935849000	0.664170000
C	1.871619000	-4.324376000	1.016900000
H	2.808094000	-1.048915000	0.696702000
H	2.270632000	-5.288359000	1.331224000
C	2.683976000	-3.179086000	1.069336000
H	3.712111000	-3.254577000	1.423422000
H	-0.988005000	-2.894389000	-0.192896000
C	4.126662000	1.510099000	-1.376002000
C	4.163196000	1.374528000	-2.772265000
C	2.972825000	1.150448000	-0.661748000
H	5.059282000	1.656021000	-3.324710000
H	2.948177000	1.267885000	0.421329000
C	3.041208000	0.883330000	-3.456345000
C	1.847701000	0.648833000	-1.340776000
H	3.062815000	0.781565000	-4.541452000
C	1.886455000	0.528228000	-2.742052000
H	1.013519000	0.155976000	-3.283690000
H	4.994926000	1.897119000	-0.841960000
C	-2.748176000	1.361432000	-0.818893000
C	-2.955292000	0.196638000	-1.611791000
C	-2.885446000	-0.939693000	-0.768130000
C	-2.600374000	-0.488579000	0.564895000
C	-2.553396000	0.950652000	0.529876000
Te	-0.064013000	0.041337000	-0.397699000
C	-3.187827000	-2.355221000	-1.194248000
H	-4.219887000	-2.439478000	-1.574276000

H	-2.523483000	-2.709820000	-2.000152000
H	-3.097339000	-3.052382000	-0.347582000
C	-2.604446000	-1.322616000	1.821423000
H	-2.205626000	-2.332342000	1.642482000
H	-1.987961000	-0.852700000	2.602293000
H	-3.623094000	-1.436781000	2.232443000
C	-2.462576000	1.852316000	1.730888000
H	-1.862464000	1.400926000	2.533898000
H	-2.002116000	2.817733000	1.475139000
H	-3.465326000	2.063652000	2.142933000
C	-2.780189000	2.784443000	-1.313452000
H	-2.194234000	3.447224000	-0.658936000
H	-2.371839000	2.863757000	-2.332897000
H	-3.808296000	3.186060000	-1.345744000
C	-3.224201000	0.169047000	-3.093866000
H	-2.745339000	1.019170000	-3.603789000
H	-2.848365000	-0.759666000	-3.549992000
H	-4.304335000	0.226018000	-3.318766000

[Cp][(SePh₃)]

C	-2.078651000	-0.535148000	-6.220824000
C	-3.013271000	0.491560000	-6.427168000
C	-1.768602000	-0.952672000	-4.917608000
H	-3.248981000	0.822717000	-7.438027000
H	-1.036213000	-1.743244000	-4.755797000
C	-3.639933000	1.102367000	-5.331430000
C	-2.396354000	-0.353190000	-3.813913000
H	-4.345261000	1.922057000	-5.470497000

H	-2.156907000	-0.671971000	-2.801074000
C	-3.333651000	0.666076000	-4.034726000
H	-1.586995000	-1.003124000	-7.072911000
C	-2.071645000	1.895039000	-0.812528000
C	-3.111549000	1.011456000	-1.137877000
C	-1.182340000	1.558232000	0.217540000
H	-0.369089000	2.237245000	0.471669000
C	-3.288170000	-0.190361000	-0.438563000
C	-1.345135000	0.355950000	0.923789000
H	-4.105117000	-0.862875000	-0.691450000
H	-0.657889000	0.100057000	1.729388000
C	-2.397635000	-0.512477000	0.598715000
H	-2.531157000	-1.442084000	1.151454000
H	-1.978303000	2.836436000	-1.353471000
C	-6.681044000	-1.931138000	-2.577307000
C	-7.845588000	-1.467073000	-1.945793000
C	-5.596451000	-1.064926000	-2.786152000
H	-8.684882000	-2.143786000	-1.789182000
H	-4.694497000	-1.418594000	-3.282218000
C	-7.934150000	-0.130910000	-1.526325000
C	-5.693943000	0.265506000	-2.352847000
H	-8.841052000	0.233067000	-1.044485000
C	-6.857801000	0.744053000	-1.735114000
H	-6.914734000	1.792718000	-1.440702000
H	-6.615631000	-2.966035000	-2.912471000
Se	-4.288021000	1.650969000	-2.599084000
C	-4.567919000	4.197806000	-3.950467000
C	-5.835859000	4.004788000	-3.347530000
C	-5.670423000	4.101385000	-1.936514000

C	-4.299327000	4.360236000	-1.671412000
C	-3.612048000	4.405503000	-2.914300000
H	-4.360877000	4.212625000	-5.018739000
H	-6.774051000	3.830487000	-3.870259000
H	-6.462924000	4.042139000	-1.192427000
H	-3.854422000	4.497363000	-0.688066000
H	-2.553607000	4.616913000	-3.055769000

[Cp^{Me5}][(SePh₃)]

C	3.039010000	-1.746605000	-3.330440000
C	2.053016000	-2.549140000	-2.739163000
C	3.174663000	-0.404375000	-2.946478000
H	1.942405000	-3.591257000	-3.036532000
H	3.938873000	0.221256000	-3.406984000
C	1.200107000	-2.008190000	-1.767168000
C	2.330278000	0.141498000	-1.968643000
H	0.421166000	-2.617242000	-1.308491000
H	2.433439000	1.185334000	-1.678090000
C	1.347014000	-0.668472000	-1.383638000
H	3.697353000	-2.163590000	-4.091385000
C	0.007553000	2.366840000	-1.506301000
C	0.245730000	1.829174000	-0.230901000
C	-0.080492000	3.756132000	-1.664040000
H	-0.253727000	4.174200000	-2.654922000
C	0.361440000	2.667484000	0.887796000
C	0.048419000	4.602653000	-0.552593000
H	0.522055000	2.244101000	1.877376000
H	-0.026672000	5.681834000	-0.677458000

C	0.265882000	4.056125000	0.719773000
H	0.359254000	4.708581000	1.587111000
H	-0.106622000	1.708297000	-2.365287000
C	3.483840000	0.124153000	2.602291000
C	3.081957000	-0.716797000	3.653087000
C	2.633163000	0.345689000	1.511670000
H	3.749292000	-0.886177000	4.497205000
H	2.942748000	0.995834000	0.695740000
C	1.826543000	-1.337543000	3.616696000
C	1.376742000	-0.276281000	1.487332000
H	1.512916000	-1.990612000	4.430292000
C	0.967624000	-1.115127000	2.529291000
H	-0.014235000	-1.584560000	2.482410000
H	4.461243000	0.605084000	2.631238000
Se	0.021667000	-0.111511000	0.013790000
C	-2.348192000	-1.566114000	-0.821057000
C	-2.268263000	-1.884711000	0.564922000
C	-2.477973000	-0.678670000	1.306637000
C	-2.689126000	0.383176000	0.374602000
C	-2.597145000	-0.162757000	-0.944013000
C	-2.291561000	-2.537623000	-1.973308000
H	-1.687005000	-2.153772000	-2.809493000
H	-1.862349000	-3.503907000	-1.671769000
H	-3.296514000	-2.747629000	-2.377843000
C	-2.877750000	0.566199000	-2.234229000
H	-2.684982000	1.644258000	-2.141980000
H	-2.259677000	0.185781000	-3.061860000
H	-3.930306000	0.453889000	-2.546948000
C	-3.025581000	1.809706000	0.725136000

H	-2.584656000	2.104607000	1.688320000
H	-2.652336000	2.514747000	-0.031552000
H	-4.114899000	1.966639000	0.807146000
C	-2.587025000	-0.544162000	2.806475000
H	-2.216100000	-1.438891000	3.326082000
H	-2.017297000	0.316077000	3.190788000
H	-3.632961000	-0.401566000	3.126210000
C	-2.080673000	-3.268675000	1.137739000
H	-1.368377000	-3.865159000	0.547681000
H	-1.698473000	-3.238642000	2.168455000
H	-3.025471000	-3.837685000	1.166835000