

The importance of strain (preorganization) in beryllium bonds.

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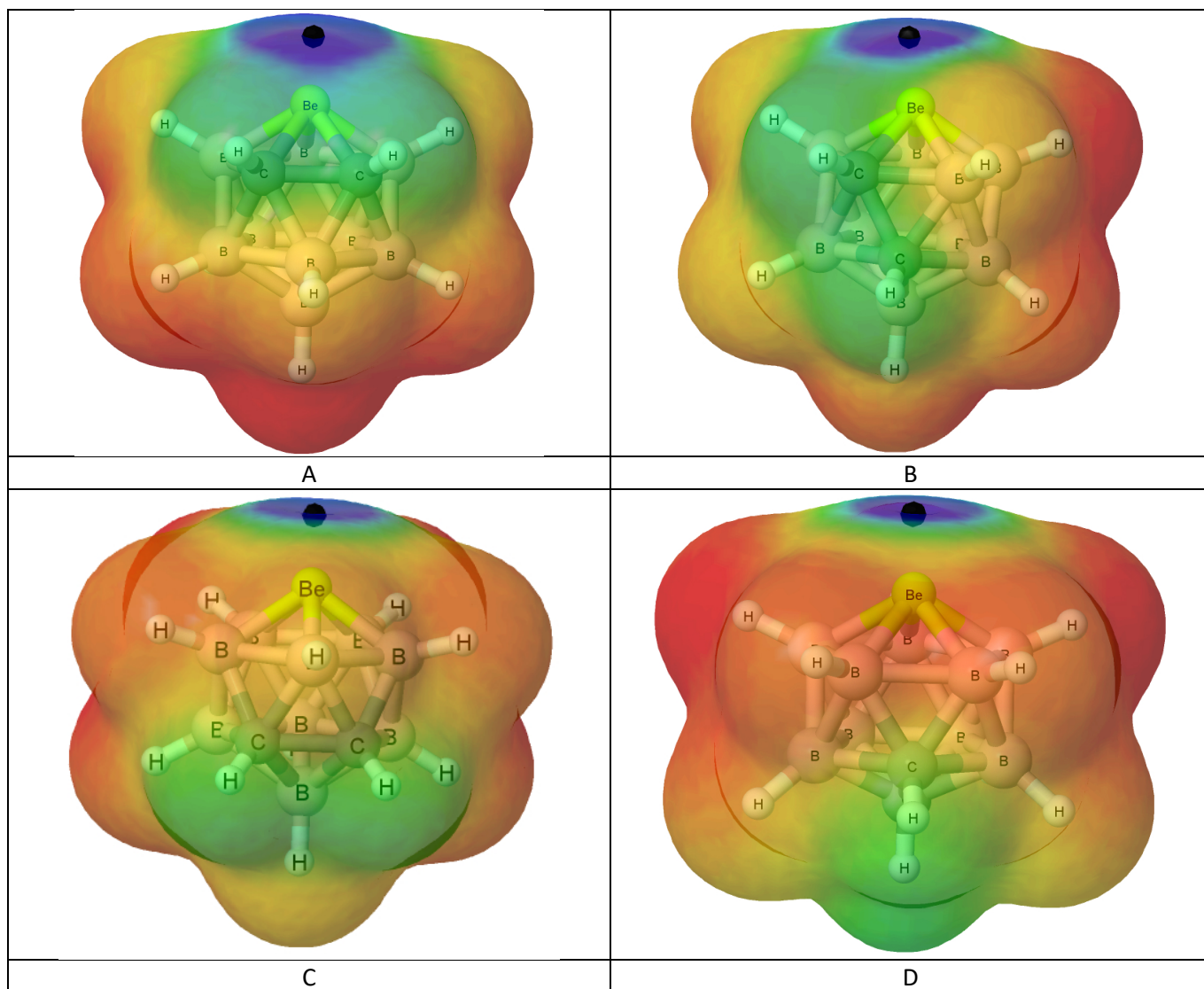


Fig. S1 Molecular electrostatic potential (MESP) on the 0.001 au electron density. Regions with $\text{MESP} > 0.1 \text{ au}$ are indicated with blue color and $\text{MESP} < -0.015 \text{ au}$ with red color. The location of the $V_{S,\text{max}}$ is indicated with a black sphere.

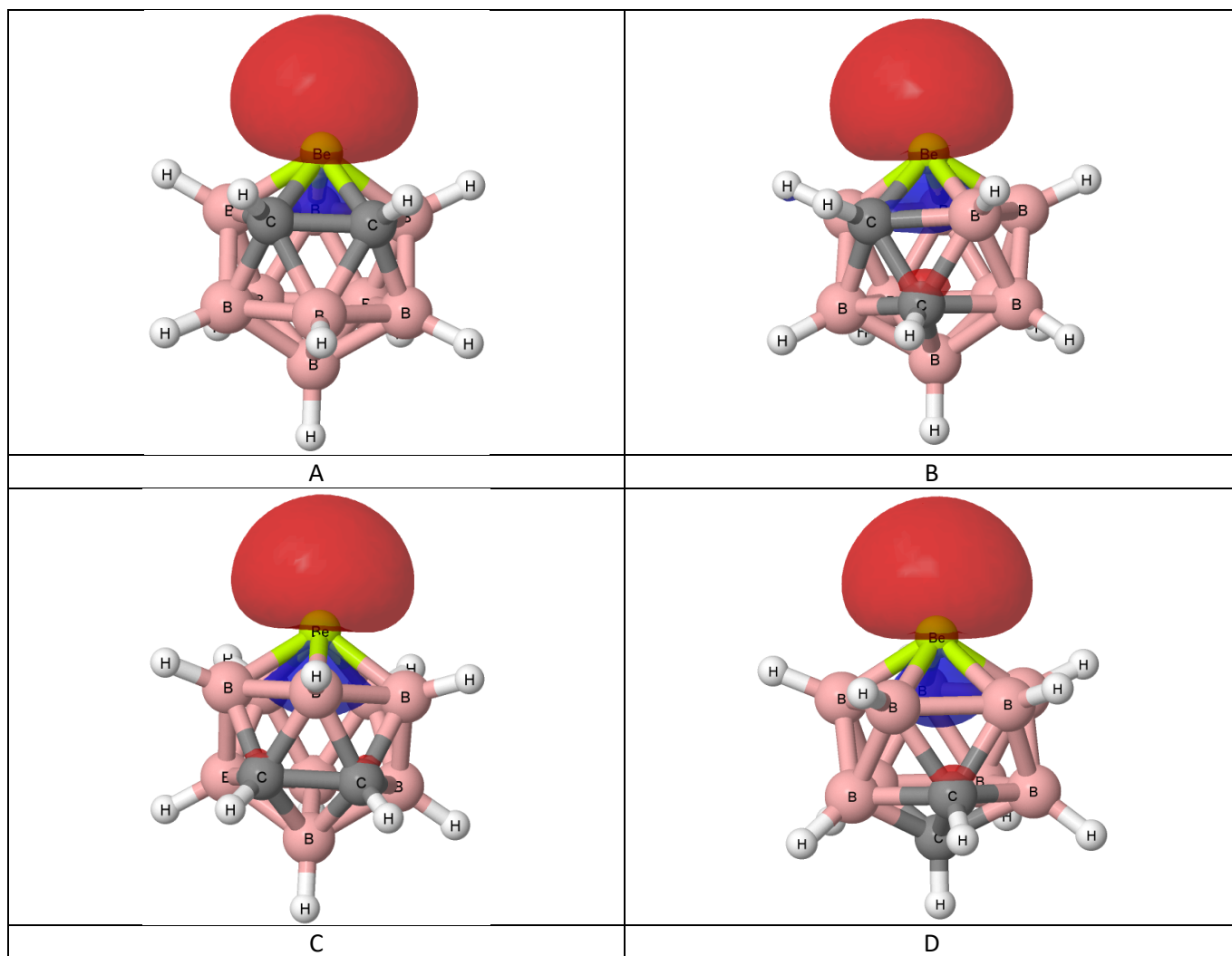


Fig. S2. LUMO of the $B_9H_{11}C_2Be$ isomers.

Table S1. Energy (a.u.) of the LUMO of the B₉H₁₁C₂Be isomers.

Isomer	LUMO
A	-0.1048
B	-0.0924
C	-0.0786
D	-0.0721

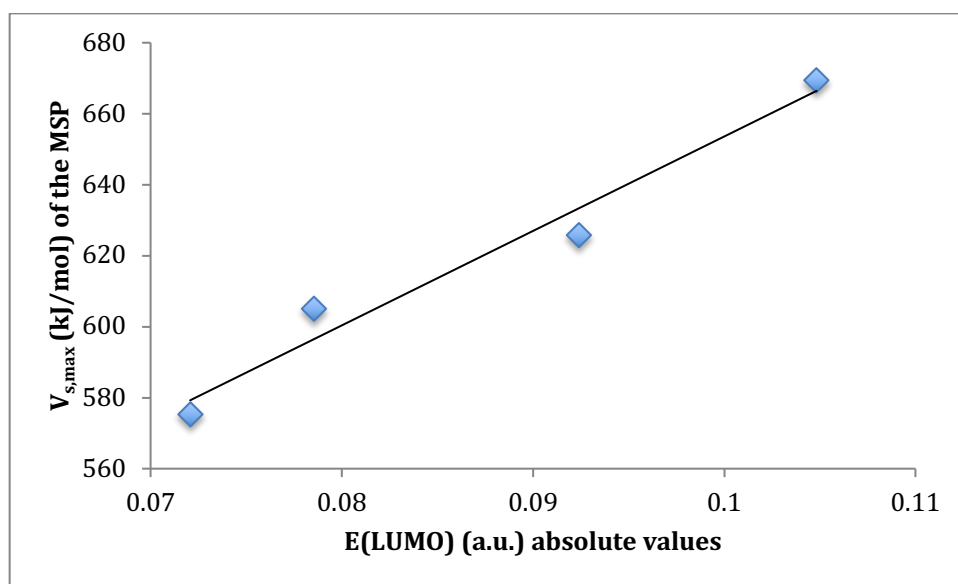
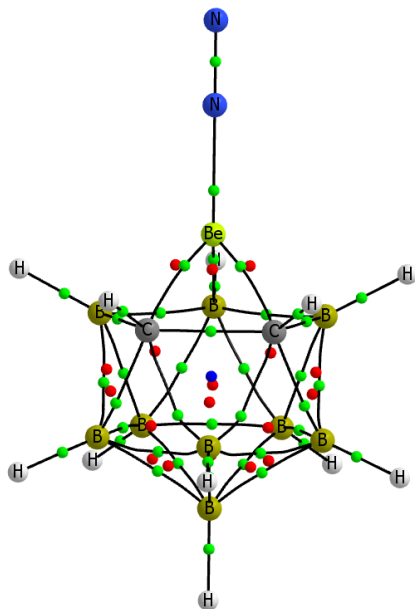


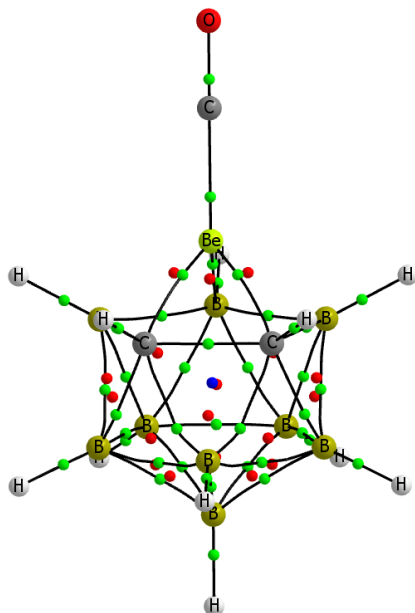
Fig. S3. Linear correlation between the V_{s,max} of the MESP and the absolute value of the energy of the LUMO.

The correlation obeys the equation: $V_{s,max} \text{ (kJ/mol)} = 2664 |E(LUMO)| \text{ (a.u.)} + 387.48$ ($r^2 = 0.967$).

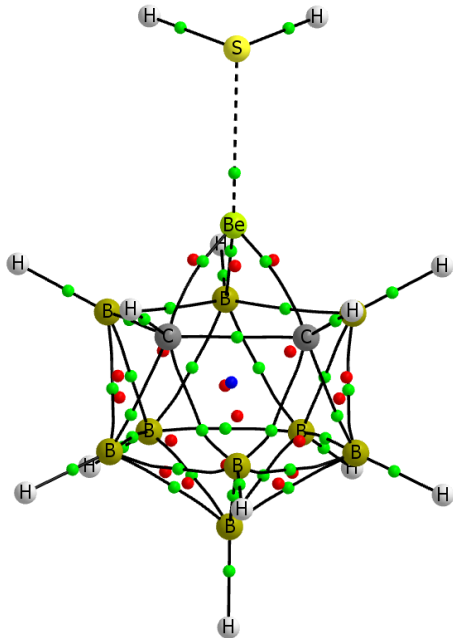
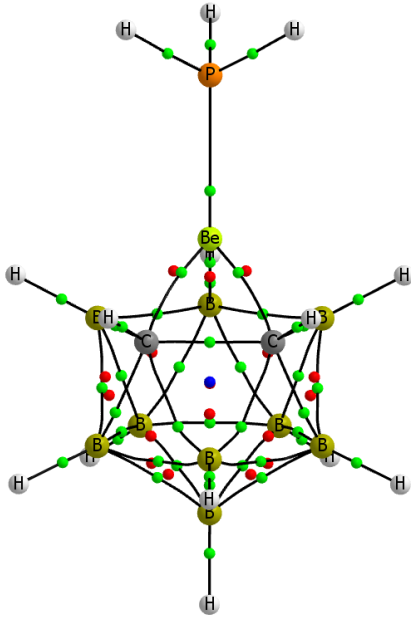
Complexes with A

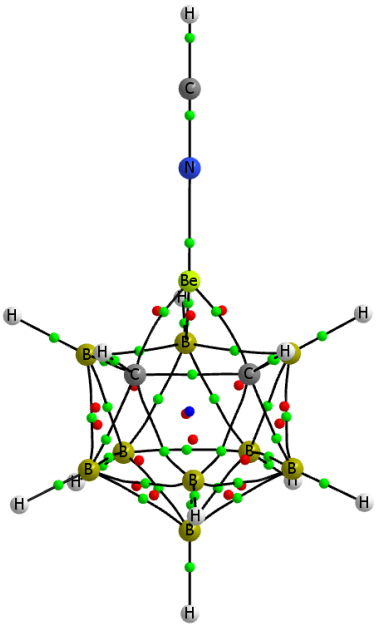


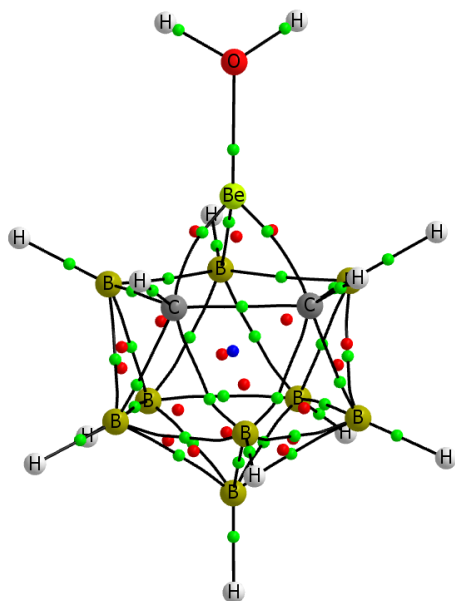
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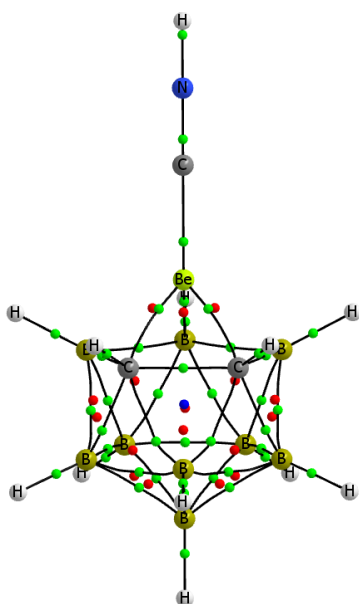
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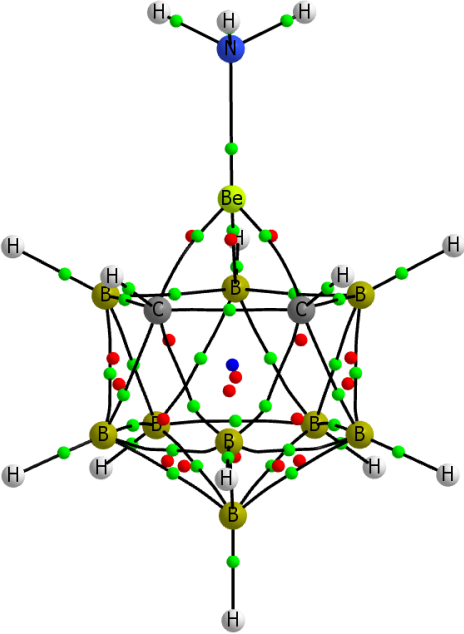
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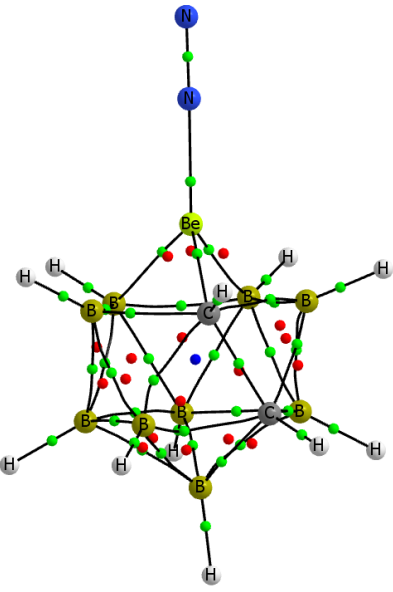
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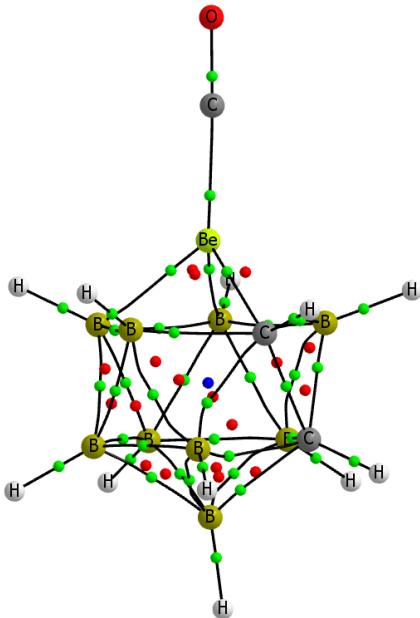


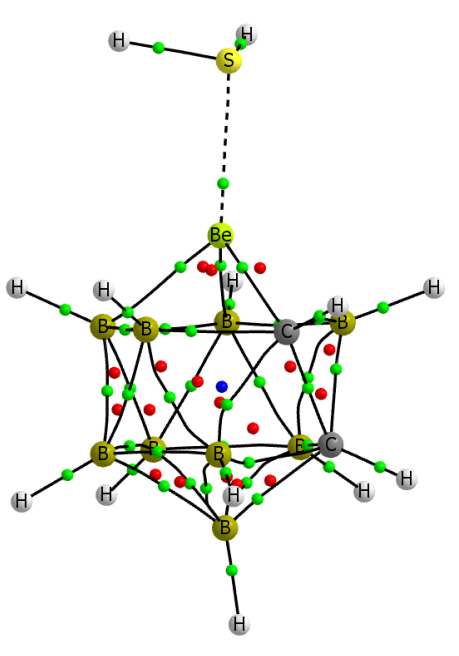
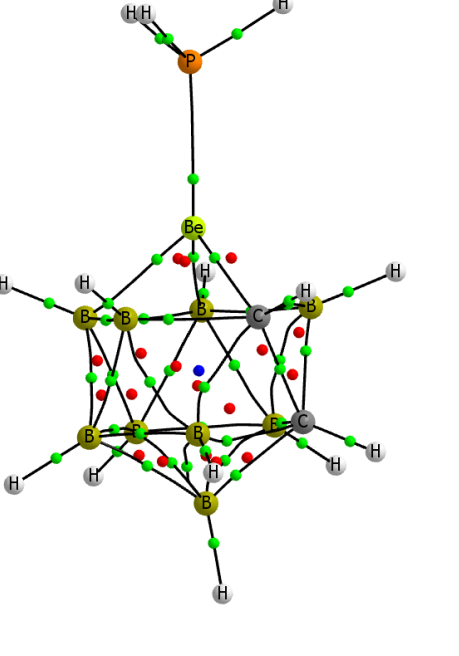
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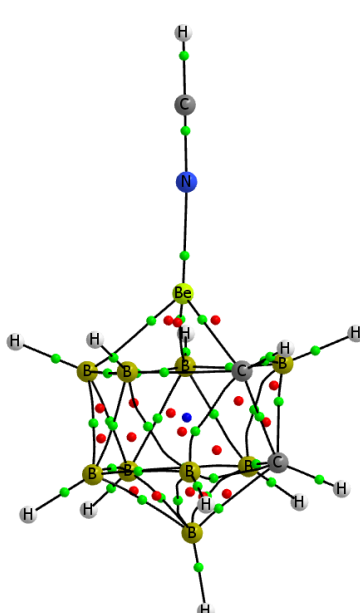
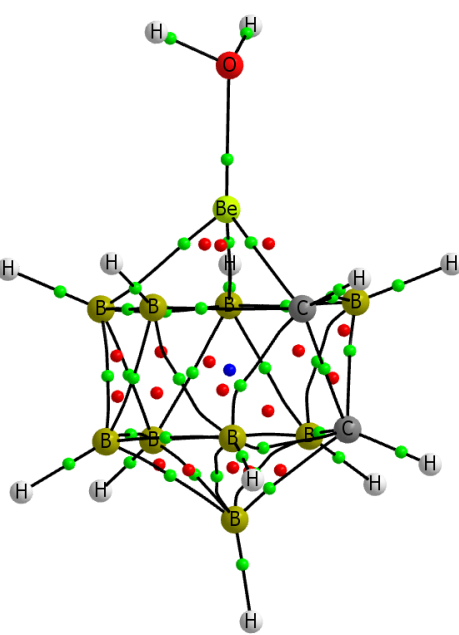
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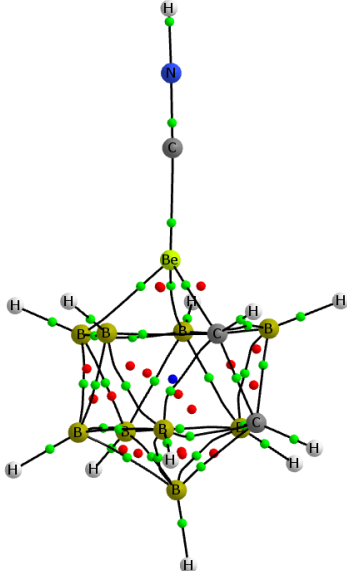
Complexes with B

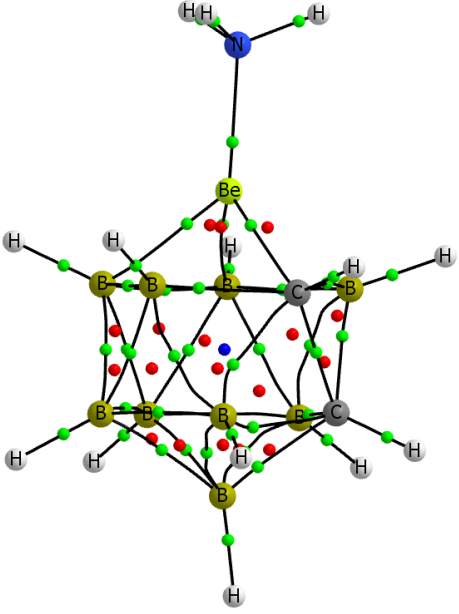
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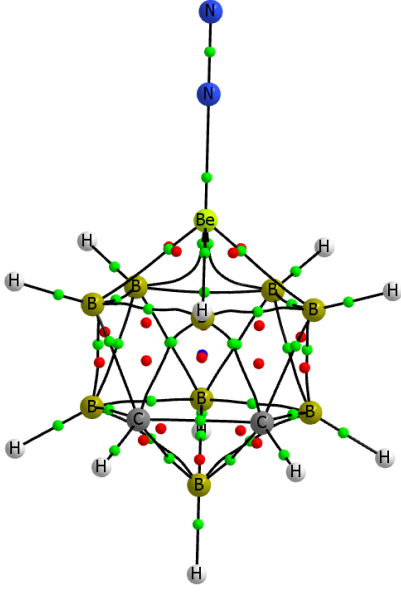
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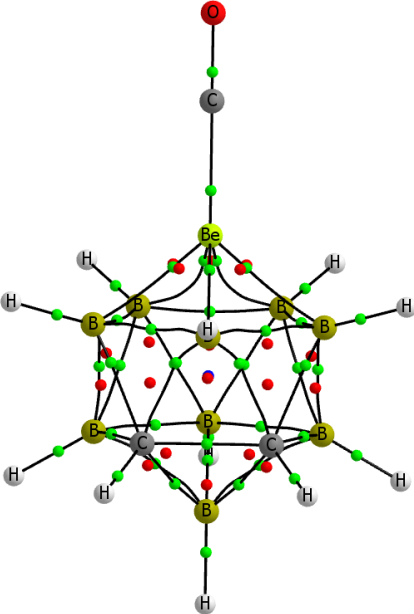
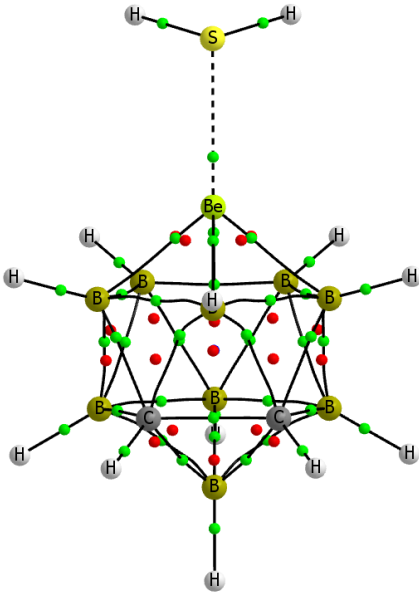
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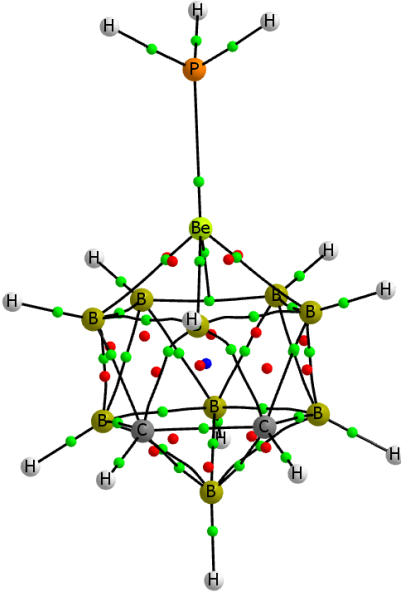
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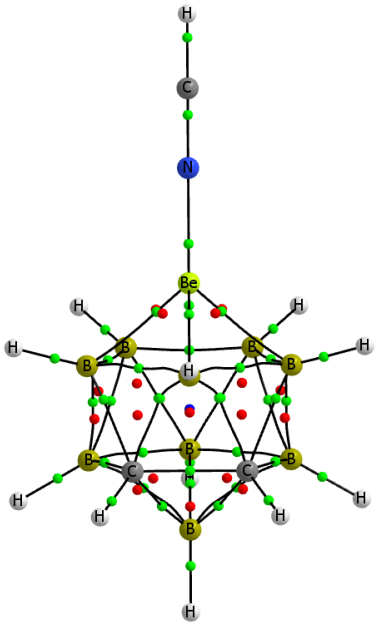
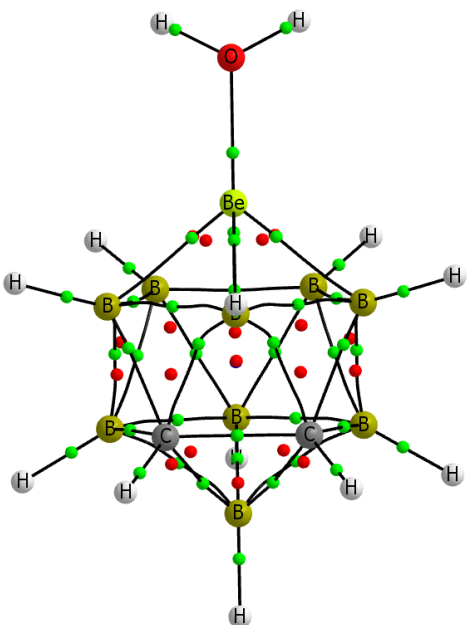
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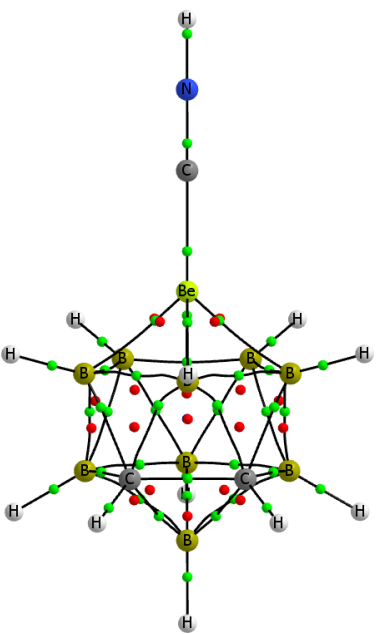
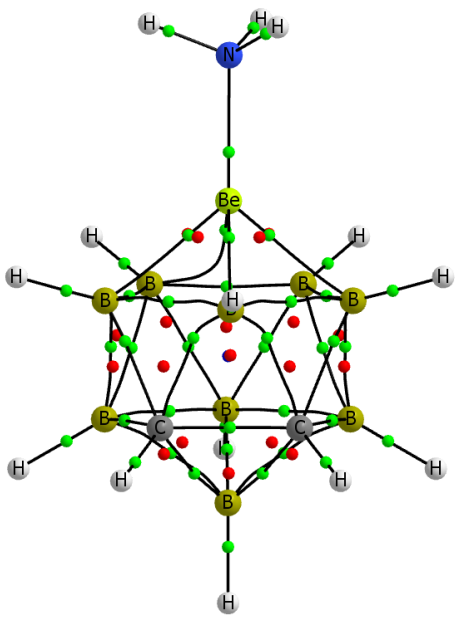
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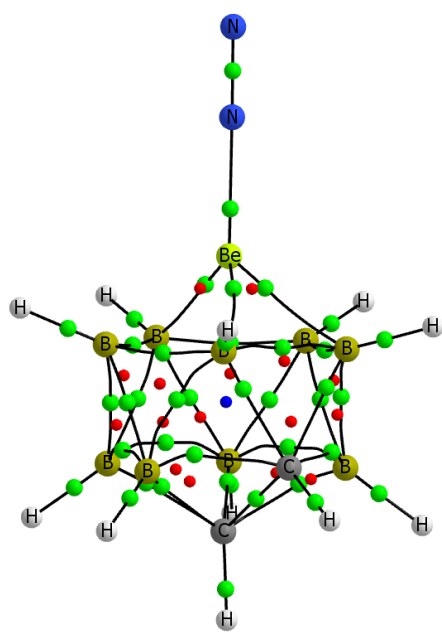
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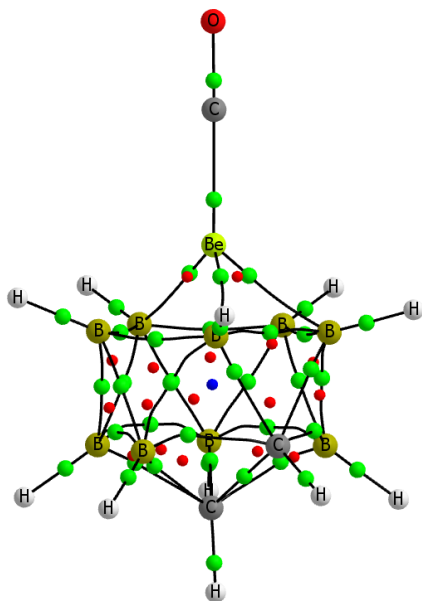
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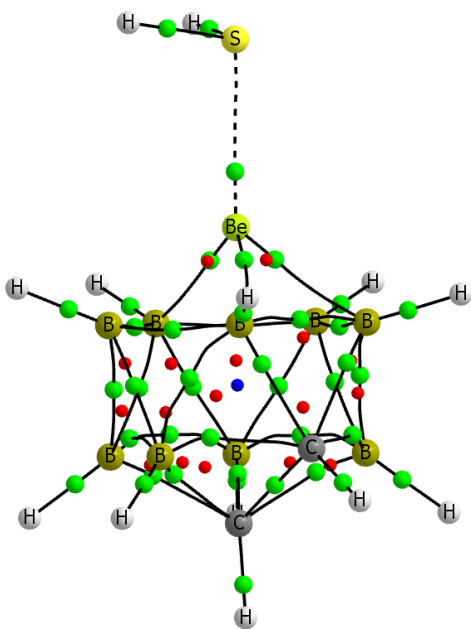
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Complexes with D

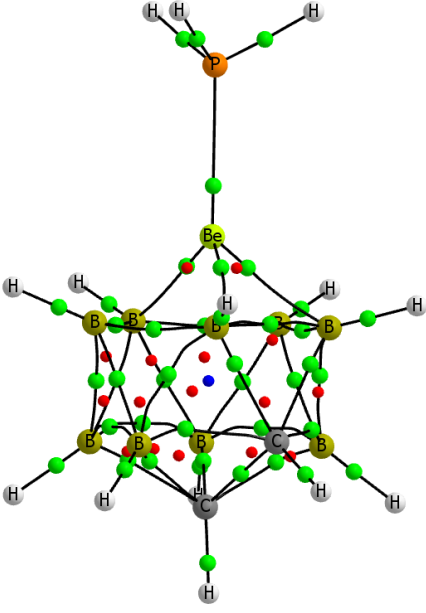
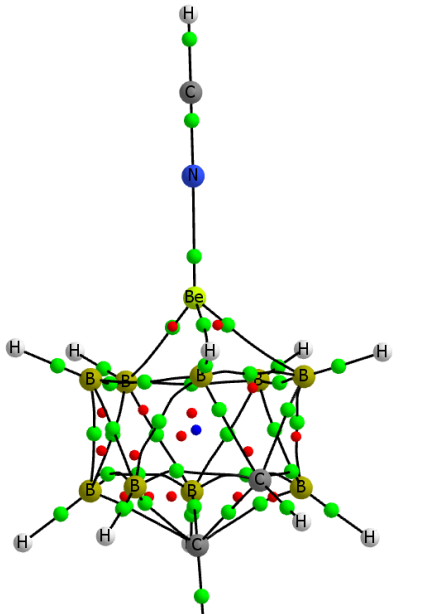
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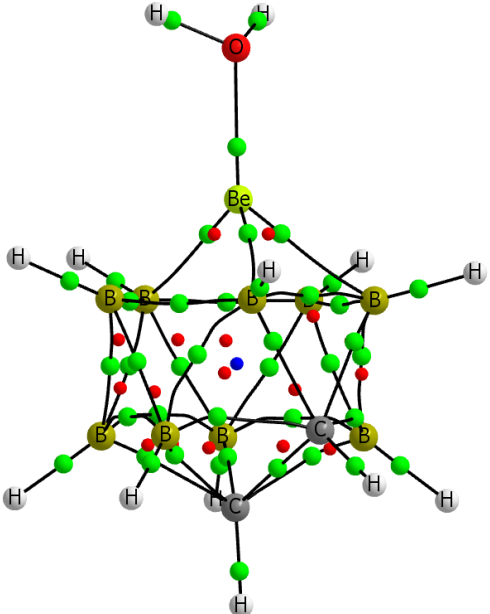
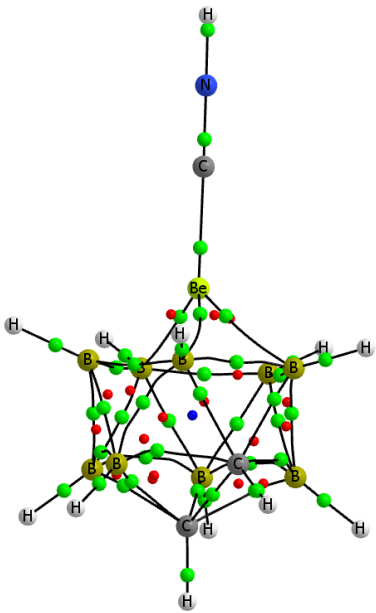


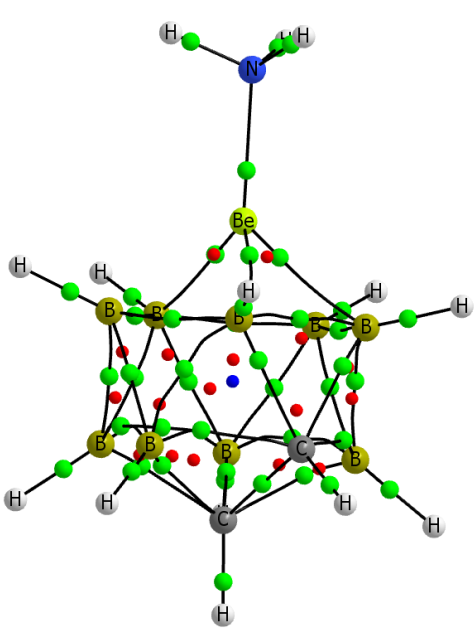
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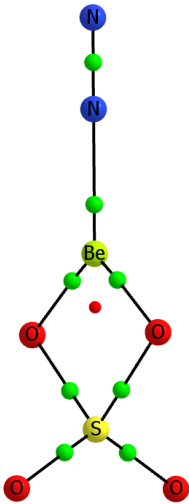
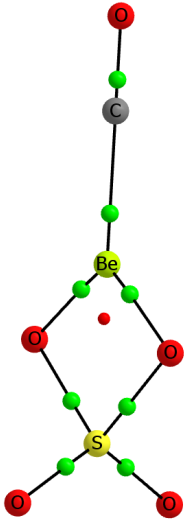
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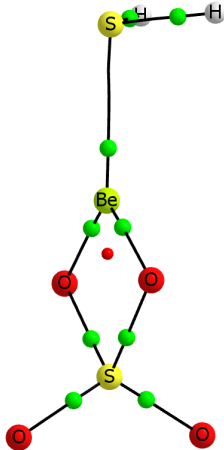
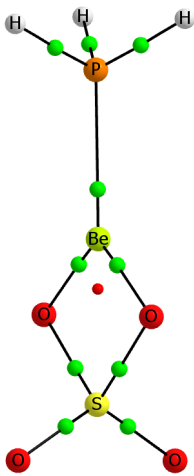
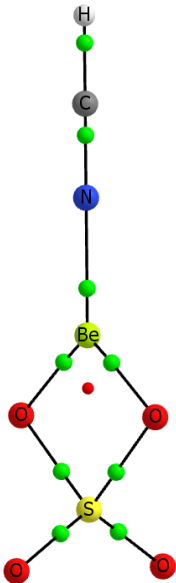
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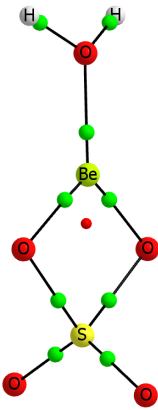
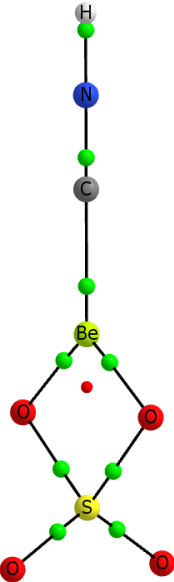
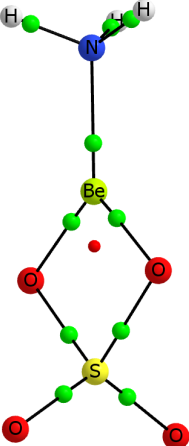
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	Be,-1.9465451141,-0.2529141225,-0.0010083761 B,-0.5899482229,-1.5689288381,0.0004308974 C,0.3004206669,1.5421394771,-0.0011993264 C,1.382873421,0.3257422091,-0.0000348499 B,-1.0788455159,1.1655544446,0.9014252462 B,-1.0781831873,1.1644344321,-0.9044112827 B,0.83504035,-1.0059758673,0.8943349356 B,0.8356771396,-1.0071059431,-0.8931244567 B,-0.7758161052,-0.5204169921,1.4703323169 B,-0.7747294349,-0.5222758709,-1.4709715887 B,0.531092745,0.6544454089,1.4573276616 B,0.5321554482,0.6526115607,-1.4584370105 H,0.7259869564,2.535030661,-0.0016717962 H,1.1381568846,1.1835034849,2.3204010148 H,2.4215524912,0.6202122587,0.0001389214 H,1.1398655398,1.180561026,-2.3217328928 H,-1.5521134168,2.0632609174,-1.5158644526 H,-1.1472370683,-0.908547539,2.5301899625

	H,1.6473619045,-1.6382170452,1.4764007263 H,1.6484248738,-1.6400762748,-1.4738003575 H,-1.1452921496,-0.9117631955,-2.5306262382 H,-0.8292757639,-2.7334650768,0.0010879476 H,-1.553244624,2.0651248793,1.5114241647 C,-3.6485457959,-0.5651319122,0.0011765918 N,-4.7804909239,-0.7968979036,0.0031046171 H,-5.7561698756,-1.007875263,0.0051076295
	Be,-1.8970907874,-0.5869237864,0.0000000069 B,-0.3746179555,-1.7073896763,0.0000000179 C,0.1139577267,1.4860702399,-0.0000000154 C,1.3431731453,0.4189047112,-0.0000000049 B,-1.206318822,0.9329760246,0.8993816717 B,-1.2063188228,0.932976006,-0.8993816899 B,0.9701696491,-0.9732736589,0.8940358753 B,0.9701696483,-0.9732736774,-0.8940358556 B,-0.690207318,-0.6957347691,1.4653975728 B,-0.6902073193,-0.6957347994,-1.4653975578 B,0.4572109663,0.6336318225,1.4582046568 B,0.457210965,0.6336317923,-1.4582046703 H,0.4107974778,2.5247265203,-0.0000000263 H,0.9922183257,1.2369043742,2.3206218947 H,2.3351112794,0.8446270877,-0.0000000098 H,0.9922183236,1.2369043262,-2.3206219211 H,-1.7895747852,1.7659452184,-1.5136982882 H,-1.0121265265,-1.1304835858,2.5264349908 H,1.8577666728,-1.4967644072,1.474701034 H,1.8577666715,-1.4967644378,-1.4747010046 H,-1.0121265287,-1.1304836381,-2.5264349665 H,-0.463932951,-2.8956434714,0.0000000302 H,-1.7895747839,1.7659452497,1.5136982533 N,-3.5316042295,-1.1209994631,0.0000000132 H,-4.1991619787,-0.3530403048,0.0000000055 H,-3.7248223369,-1.6926378524,-0.8198176976 H,-3.7248223362,-1.6926378354,0.8198177359

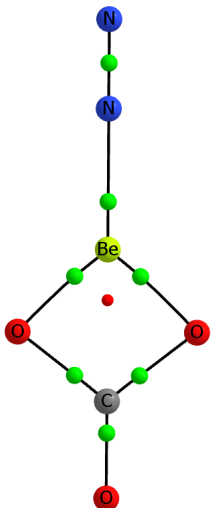
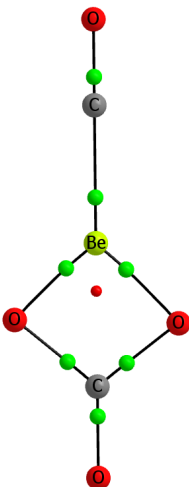
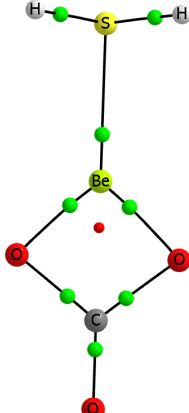
Complexes with SO₄Be

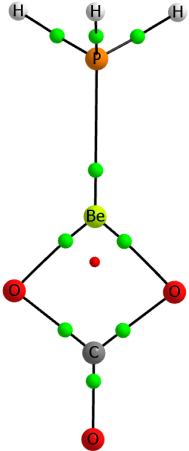
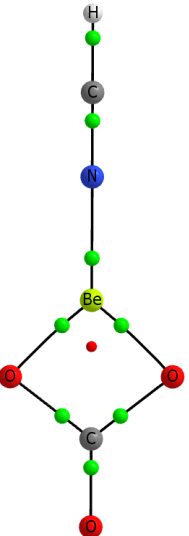
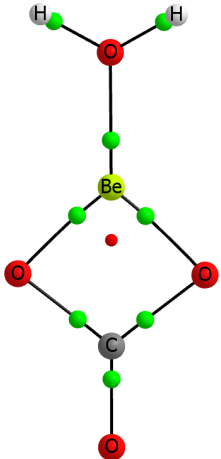
	Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 S,1,r2,3,90.,2,0.,0 O,6,r11,1,a11,3,0.,0 O,6,r11,1,a11,3,180.,0 N,1,r20,3,90.,2,180.,0 N,1,r21,3,90.,2,180.,0 r1=1.49184134 a1=50.16290343 r11=1.42969953 a11=119.68336993 r2=2.10148417 r20=1.72944741 r21=2.82474555
	Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 S,1,r2,3,90.,2,0.,0 O,6,r11,1,a11,3,0.,0 O,6,r11,1,a11,3,180.,0 C,1,r20,3,90.,2,180.,0 O,1,r21,3,90.,2,180.,0 r1=1.49717897 a1=49.90596691 r11=1.42997602 a11=119.71694721 r2=2.10786612 r20=1.80188171 r21=2.9197351

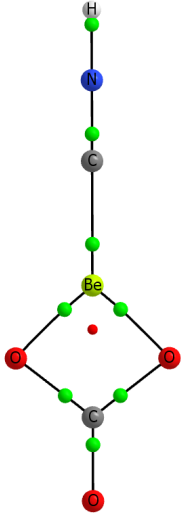
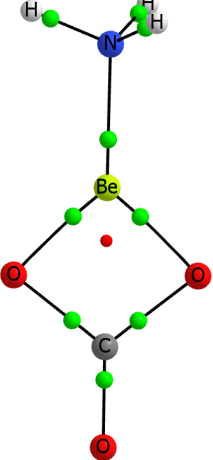
 The structure shows a central Be atom (yellow) coordinated to a sulfonate group (S, green; O, red) and a hydrogen sulfide molecule (S, green; H, white). The sulfonate group is a tetrahedral structure with a central S atom bonded to three O atoms and one Be atom. The Be atom is also bonded to a hydrogen sulfide molecule.	Be,-0.1963680949,0.,-1.1488441609 O,-0.0994294136,1.1441795513,-0.1796836494 O,-0.0994294136,-1.1441795513,-0.1796836494 S,0.0153593334,0.,0.9528122063 O,-1.1447962425,0.,1.7910113839 O,1.3230439272,0.,1.5361132929 S,-0.3176724137,0.,-3.2578717928 H,0.5794228482,0.9875198576,-3.4629891295 H,0.5794228482,-0.9875198576,-3.4629891295
 The structure shows a central Be atom (yellow) coordinated to a phosphonate group (P, orange; O, red) and a hydrogen phosphide molecule (P, orange; H, white). The phosphonate group is a tetrahedral structure with a central P atom bonded to three O atoms and one Be atom. The Be atom is also bonded to a hydrogen phosphide molecule.	Be,0.7719706738,0.0248460201,0.0014551413 O,-0.2099194018,0.1758091404,-1.1309645684 O,-0.2081075657,-0.1478012741,1.1323494185 S,-1.344805731,-0.0006366674,-0.0004888376 O,-2.0450395696,-1.2373786899,-0.1767591221 O,-2.0770687689,1.2175569676,0.1742750849 P,2.9356601555,-0.0031617863,-0.0042550283 H,3.5925490435,0.7476228862,-0.9953266301 H,3.5942218813,0.4399224733,1.1565105361 H,3.5381282828,-1.26170507,-0.1846869944
 The structure shows a central Be atom (yellow) coordinated to a sulfonate group (S, green; O, red) and a hydrogen sulfide molecule (S, green; H, white). The sulfonate group is a tetrahedral structure with a central S atom bonded to three O atoms and one Be atom. The Be atom is also bonded to a hydrogen sulfide molecule.	Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 S,1,r2,3,90.,2,0.,0 O,6,r11,1,a11,3,0.,0 O,6,r11,1,a11,3,180.,0 N,1,r20,3,90.,2,180.,0 C,1,r21,3,90.,2,180.,0 H,1,r22,3,90.,2,180.,0 r1=1.50761796 a1=49.26302413 r11=1.43250865 a11=120.09561047 r2=2.11693735 r20=1.66955813 r21=2.81134635 r22=3.88250424

 The structure shows a central Be atom (yellow) coordinated to a sulfonate group (S in yellow, O in red, green spheres for other atoms) and a water molecule (H in white, O in red). The Be atom is also bonded to two green spheres. The sulfonate group consists of a central S atom bonded to three O atoms, with additional green spheres representing other atoms in the chain.	Be,-0.0367074401,0.,-1.2654795202 O,-0.0260328731,1.1442473587,-0.287684158 O,-0.0260328731,-1.1442473587,-0.287684158 S,-0.0027130175,0.,0.8459390767 O,-1.2252459373,0.,1.5912813074 O,1.2536522417,0.,1.5343034573 O,0.0591663,0.,-2.8592109182 H,0.3219765561,0.7937796942,-3.3417783701 H,0.3219765561,-0.7937796942,-3.3417783701
 The structure shows a central Be atom (yellow) coordinated to a sulfonate group (S in yellow, O in red, green spheres for other atoms) and a water molecule (H in white, O in red). The Be atom is also bonded to two green spheres. The sulfonate group consists of a central S atom bonded to three O atoms, with additional green spheres representing other atoms in the chain. A nitrogen-containing chain (N in blue, C in grey, H in white) is also present, connected to the sulfonate group.	Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 S,1,r2,3,90.,2,0.,0 O,6,r11,1,a11,3,0.,0 O,6,r11,1,a11,3,180.,0 C,1,r20,3,90.,2,180.,0 N,1,r21,3,90.,2,180.,0 H,1,r22,3,90.,2,180.,0 r1=1.50856025 a1=49.23879426 r11=1.43226129 a11=120.06010634 r2=2.11879626 r20=1.77121222 r21=2.92090301 r22=3.92270494
 The structure shows a central Be atom (yellow) coordinated to a sulfonate group (S in yellow, O in red, green spheres for other atoms) and a water molecule (H in white, O in red). The Be atom is also bonded to two green spheres. The sulfonate group consists of a central S atom bonded to three O atoms, with additional green spheres representing other atoms in the chain.	Be,0.0028421533,-1.2448211107,-0.0085991001 O,0.0921308299,-0.2587050614,1.1341917824 O,-0.0900234983,-0.2513403005,-1.1431925605 S,-0.0010059546,0.8761781677,0.0000524736 O,1.2330156366,1.598116754,-0.0966484693 O,-1.2377765183,1.5928184107,0.100959262 N,0.0075496475,-2.9361237383,0.0048290775 H,-0.768558967,-3.3062992556,0.5532987562 H,-0.0660797183,-3.326944472,-0.9338377169 H,0.8620103893,-3.3027723939,0.4239464953

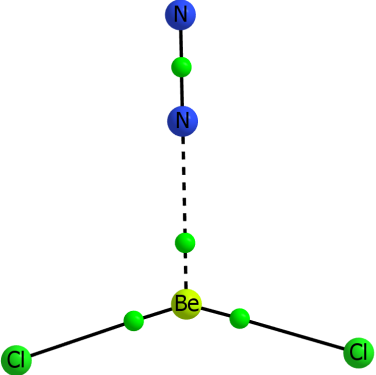
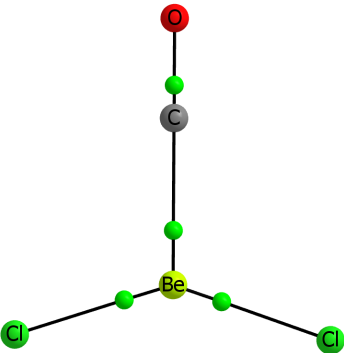
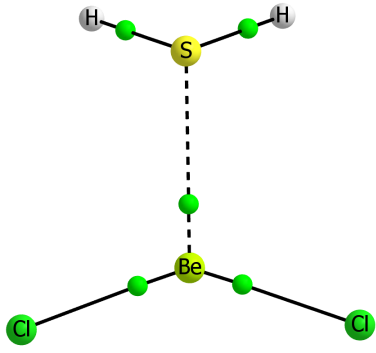
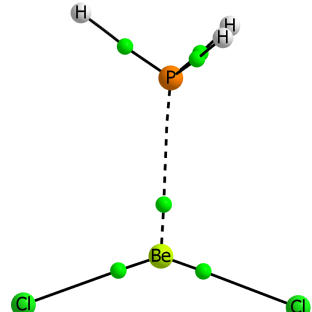
Complexes with CO₃Be

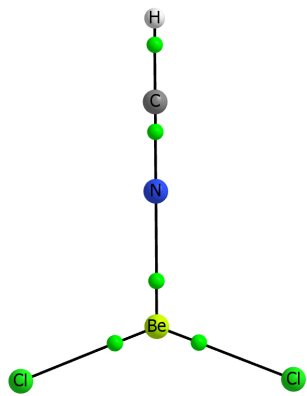
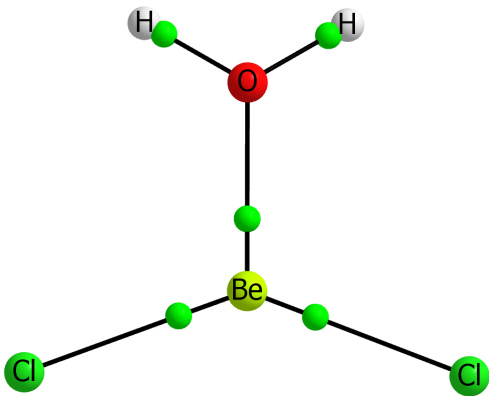
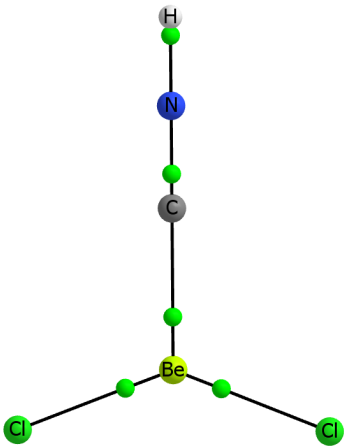
	Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 C,1,r2,3,90.,2,0.,0 O,1,r21,3,90.,2,0.,0 N,1,r10,3,90.,2,180.,0 N,1,r11,3,90.,2,180.,0 r1=1.48835342 a1=47.22160079 r2=1.85829487 r21=3.04657425 r10=1.72418875 r11=2.82032273
	Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 C,1,r2,3,90.,2,0.,0 O,1,r21,3,90.,2,0.,0 C,1,r10,3,90.,2,180.,0 O,1,r11,3,90.,2,180.,0 r1=1.49437121 a1=46.93238639 r2=1.86529118 r21=3.0542137 r10=1.79407564 r11=2.91337923
	Be,-0.1753354445,0.,0.6738509965 O,-0.0632650038,1.0917854588,-0.342672081 O,-0.0632650038,-1.0917854588,-0.342672081 C,0.0315601879,0.,-1.1828198926 O,0.168134488,0.,-2.3651209044 S,-0.3451001131,0.,2.784716655 H,0.5437824832,0.9870772072,3.0224716511 H,0.5437824832,-0.9870772072,3.0224716511

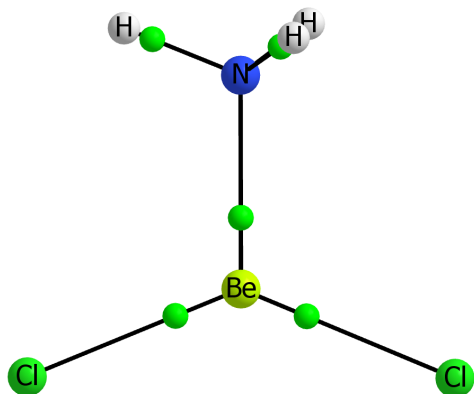
	Be,-0.011335693,0.2168309779,0.0253920571 O,1.1173961396,-0.7412142493,-0.2156192382 O,-1.0116627624,-0.8808007436,0.2363567247 C,0.105216917,-1.6528265998,-0.0030324134 O,0.1791039991,-2.8413623689,-0.0220369927 P,-0.1585087605,2.3788424346,-0.0004734139 H,-1.137541563,2.9838577947,0.8085886228 H,-0.4602763333,2.9642900853,-1.244364531 H,0.9798640564,3.1225906692,0.3601891848
	Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 C,1,r2,3,90.,2,0.,0 O,1,r21,3,90.,2,0.,0 N,1,r10,3,90.,2,180.,0 C,1,r11,3,90.,2,180.,0 H,1,r12,3,90.,2,180.,0 r1=1.50178367 a1=46.47869219 r2=1.87553959 r21=3.06772195 r10=1.67073546 r11=2.81318081 r12=3.88367789
	Be,-0.0299173482,0.,0.8109471756 O,-0.0169609194,1.0912686981,-0.2154808921 O,-0.0169609194,-1.0912686981,-0.2154808921 C,0.0009514699,0.,-1.0589386034 O,0.025654713,0.,-2.2501088839 O,0.0492623368,0.,2.4115166066 H,0.3139861509,0.7930390062,2.8933077959 H,0.3139861509,-0.7930390062,2.8933077959

	Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 C,1,r2,3,90.,2,0.,0 O,1,r21,3,90.,2,0.,0 C,1,r10,3,90.,2,180.,0 N,1,r11,3,90.,2,180.,0 H,1,r12,3,90.,2,180.,0 r1=1.50339133 a1=46.41851026 r2=1.87741437 r21=3.06930933 r10=1.76962864 r11=2.92059503 r12=3.92159201
	Be,-0.00007441,0.7812307151,0.0009239622 O,1.083408394,-0.2501166396,0.1569687397 O,-1.0722084264,-0.2629233971,-0.156779457 C,0.0101708496,-1.0989512669,-0.0005883126 O,0.0177023946,-2.2913813414,-0.0013997488 N,-0.0255684319,2.4779957409,-0.0000951477 H,-0.628515251,2.8408966931,0.7375580579 H,-0.3886888713,2.8435373831,-0.8798111982 H,0.9032957523,2.8737581129,0.1382231045

Complexes with Cl₂Be

	Be X,1,1. Cl,1,r1,2,a1 Cl,1,r1,2,a1,3,180.,0 N,1,r2,3,a1,2,0.,0 N,1,r3,3,a1,2,0.,0 r1=1.84266688 r2=1.88424314 r3=2.98085024 a1=107.10147857
	Be X,1,1. Cl,1,r1,2,a1 Cl,1,r1,2,a1,3,180.,0 C,1,r2,3,a1,2,0.,0 O,1,r3,3,a1,2,0.,0 r1=1.85398427 r2=1.87414442 r3=2.99642107 a1=108.51427732
	Be X,1,1. Cl,1,r1,2,a1 Cl,1,r1,2,a1,3,180.,0 S,1,r2,3,a1,2,0.,0 H,5,r4,1,a4,3,d4,0 H,5,r4,1,a4,4,-d4,0 r1=1.8572488 r2=2.24956836 r4=1.34671404 a1=109.46201323 a4=99.15363265 d4=41.99516344
	Be,0.0564350757,-0.0131945912,0.0366609623 Cl,1.6928658127,-0.4755215687,-0.7269386539 Cl,-1.714799149,0.2585381715,-0.4536131029 P,0.4151213495,0.300406836,2.2639378646 H,-0.6141525977,0.6641697281,3.156597353 H,1.3758817726,1.2713231648,2.6137818464 H,0.9560234527,-0.792879245,2.9712674345

	Be X,1,1. Cl,1,r1,2,a1 Cl,1,r1,2,a1,3,180.,0 N,1,r2,3,a1,2,0.,0 C,1,r3,3,a1,2,0.,0 H,1,r4,3,a1,2,0.,0 r1=1.8676787 r2=1.73035406 r3=2.87350644 r4=3.94276406 a1=111.56446494
	Be X,1,1. Cl,1,r1,2,a1 Cl,1,r1,2,a1,3,180.,0 O,1,r2,3,a1,2,0.,0 H,5,r4,1,a4,3,d4,0 H,5,r4,1,a4,4,-d4,0 r1=1.87217475 r2=1.64178731 r4=0.9648764 a1=110.48676626 a4=120.15816917 d4=16.35346049
	Be X,1,1. Cl,1,r1,2,a1 Cl,1,r1,2,a1,3,180.,0 C,1,r2,3,a1,2,0.,0 N,1,r3,3,a1,2,0.,0 H,1,r4,3,a1,2,0.,0 r1=1.86972985 r2=1.81752714 r3=2.97136244 r4=3.9704857 a1=111.4380413



Be
 X,1,1.
 Cl,1,r1,2,a1
 Cl,1,r1,2,a1,3,180.,0
 N,1,r2,3,a1,2,0.,0
 H,5,r3,1,a3,3,0.,0
 H,5,r4,1,a4,3,d4,0
 H,5,r4,1,a4,3,-d4,0

 r1=1.87966239
 r2=1.73906264
 r3=1.01809737
 r4=1.01882542
 a1=112.56398
 a3=111.8729243
 a4=110.89414617
 d4=121.10556264

Table S3. Electron density (au) at the BCP between the Be atom and the Lewis base.

LB	A:LB	B:LB	C:LB	D:LB	CO ₃ Be:LB	SO ₄ Be:LB	Cl ₂ Be:LB
N ₂	0.0634	0.0633	0.0633	0.0626	0.0585	0.0583	0.0379
CO	0.0699	0.0705	0.0712	0.0706	0.0612	0.0607	0.0507
SH ₂	0.0486	0.0481	0.0464	0.0459	0.0503	0.0519	0.0383
PH ₃	0.0534	0.0527	0.0520	0.0515	0.0517	0.0532	0.0412
NCH	0.0735	0.0729	0.0721	0.0716	0.0720	0.0730	0.0616
OH ₂	0.0711	0.0694	0.0666	0.0663	0.0774	0.0795	0.0695
CNH	0.0728	0.0730	0.0732	0.0727	0.0678	0.0685	0.0612
NH ₃	0.0744	0.0731	0.0714	0.0711	0.0771	0.0792	0.0702

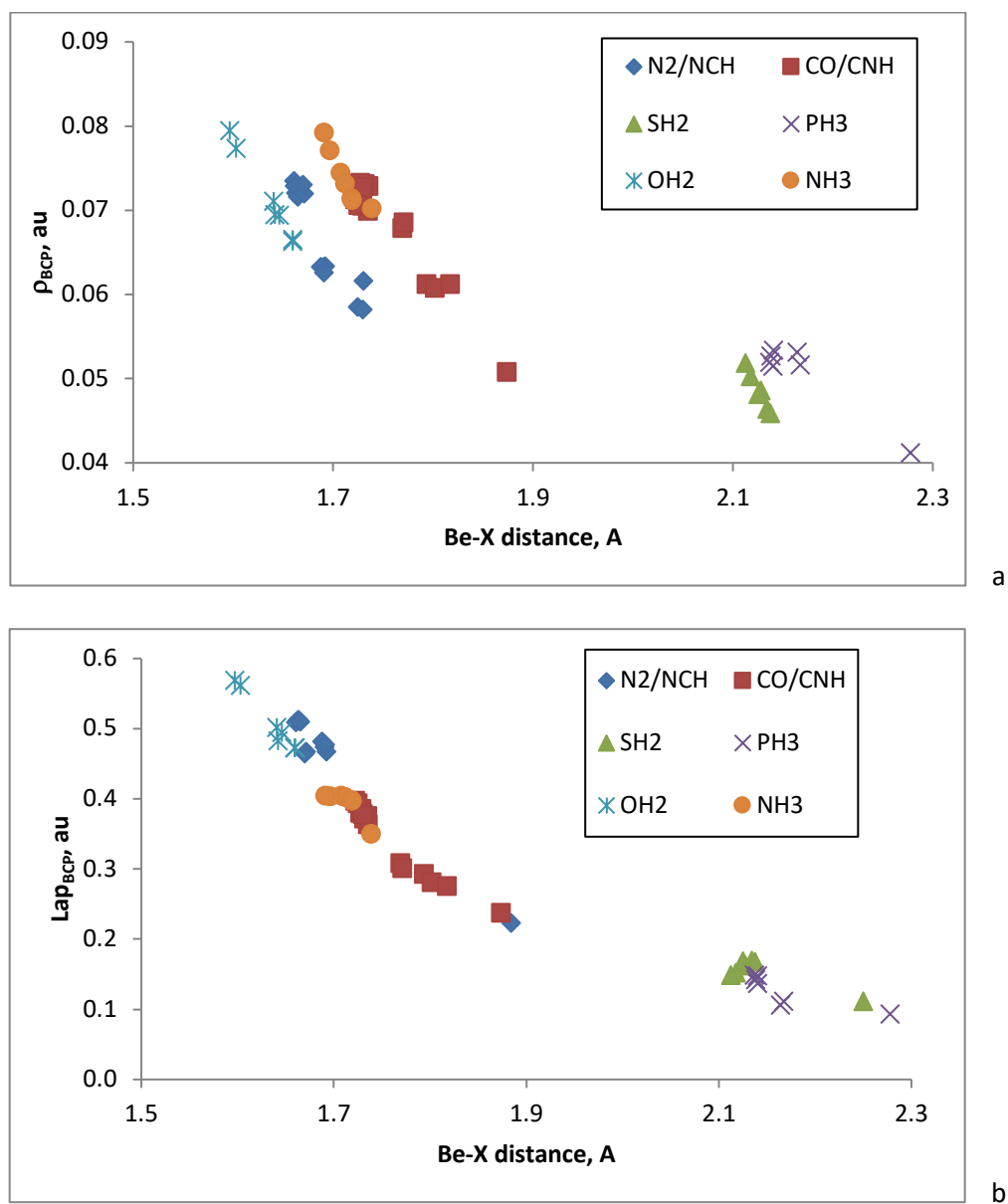


Fig. S4. Electron density properties (ρ_{BCP} and $\nabla^2\rho_{\text{BCP}}$) at the intermolecular BCPs (au) vs. the interatomic distance (Å).

Table S4. LMOEDA energy terms (kJ mol⁻¹)

Complexes with A	N ₂	CO	SH ₂	PH ₃	NCH	OH ₂	CNH	NH ₃
Electrostatic energy	-99.3	-136.9	-139.2	-157.0	-186.5	-213.3	-208.7	-274.6
Exchange energy	-61.2	-75.7	-71.1	-86.2	-73.1	-64.1	-82.6	-81.9
Repulsion energy	231.1	273.3	242.5	279.1	271.4	245.8	292.6	302.7
Polarization energy	-147.2	-176.6	-132.9	-154.5	-167.1	-142.3	-177.4	-151.6
Dispersion energy	-26.7	-27.9	-28.2	-28.4	-29.4	-29.2	-28.7	-31.5
Total LMOEDA energy	-103.4	-143.8	-128.9	-147.0	-184.7	-203.0	-204.8	-236.9

Complexes with B	N ₂	CO	SH ₂	PH ₃	NCH	OH ₂	CNH	NH ₃
Electrostatic energy	-97.5	-133.8	-135.6	-151.4	-179.7	-205.1	-202.8	-266.7
Exchange energy	-60.9	-75.0	-71.1	-85.8	-72.7	-62.3	-83.0	-80.5
Repulsion energy	228.8	269.1	240.2	275.1	268.3	239.1	291.8	296.9
Polarization energy	-144.4	-173.8	-127.9	-148.7	-161.9	-136.4	-174.2	-145.4
Dispersion energy	-27.2	-28.7	-28.3	-28.6	-29.7	-29.2	-29.2	-31.6
Total LMOEDA energy	-101.2	-142.2	-122.7	-139.4	-175.7	-193.8	-197.4	-227.3

Complexes with C	N ₂	CO	SH ₂	PH ₃	NCH	OH ₂	CNH	NH ₃
Electrostatic energy	-94.7	-131.2	-127.4	-144.3	-171.5	-192.1	-195.9	-255.7
Exchange energy	-59.8	-74.8	-68.5	-84.4	-71.0	-58.7	-82.5	-77.2
Repulsion energy	224.2	266.6	229.6	267.1	261.3	226.7	288.4	284.9
Polarization energy	-141.9	-172.8	-119.7	-142.2	-156.3	-128.0	-171.1	-137.7
Dispersion energy	-27.5	-29.2	-28.1	-28.7	-29.7	-29.0	-29.6	-31.4
Total LMOEDA energy	-99.7	-141.4	-114.2	-132.4	-167.2	-181.0	-190.7	-217.0

Complexes with D	N ₂	CO	SH ₂	PH ₃	NCH	OH ₂	CNH	NH ₃
Electrostatic energy	-94.6	-130.8	-125.9	-142.8	-170.0	-190.0	-194.1	-254.3
Exchange energy	-60.1	-75.1	-68.4	-84.3	-71.3	-58.7	-82.8	-77.6
Repulsion energy	225.1	267.4	229.6	267.3	262.3	226.8	289.2	285.9
Polarization energy	-139.8	-170.3	-117.8	-139.9	-154.6	-127.3	-169.0	-136.4
Dispersion energy	-27.4	-29.2	-28.0	-28.6	-29.7	-28.9	-29.6	-31.4
Total LMOEDA energy	-96.9	-137.9	-110.5	-128.4	-163.3	-178.1	-186.2	-213.8

Complexes with SO₄Be	N ₂	CO	SH ₂	PH ₃	NCH	OH ₂	CNH	NH ₃
Electrostatic energy	-81.5	-111.3	-130.7	-145.6	-186.3	-220.1	-201.4	-286.2
Exchange energy	-36.1	-40.8	-48.7	-54.6	-49.0	-46.3	-51.5	-59.3
Repulsion energy	154.3	169.5	187.5	201.0	207.4	203.6	210.1	251.8
Polarization energy	-128.0	-142.6	-137.5	-149.0	-157.8	-151.2	-157.2	-151.3
Dispersion energy	-21.2	-21.3	-25.5	-25.0	-26.5	-28.5	-24.7	-30.0
Total LMOEDA energy	-112.6	-146.6	-155.0	-173.1	-212.4	-242.4	-224.7	-275.0

Complexes with CO₃Be	N ₂	CO	SH ₂	PH ₃	NCH	OH ₂	CNH	NH ₃
Electrostatic energy	-82.6	-112.1	-129.2	-141.9	-182.5	-214.9	-197.7	-279.2

Exchange energy	-38.7	-43.8	-50.5	-56.2	-51.2	-47.7	-54.0	-61.0
Repulsion energy	161.0	177.5	189.3	202.5	210.9	203.8	215.3	252.2
Polarization energy	-127.8	-143.3	-129.7	-141.4	-152.9	-144.3	-153.6	-143.5
Dispersion energy	-21.5	-21.6	-25.1	-24.6	-26.5	-28.2	-24.8	-29.8
Total LMOEDA energy	-109.6	-143.3	-145.3	-161.6	-202.1	-231.3	-214.8	-261.3

Complexes with Cl₂Be	N ₂	CO	SH ₂	PH ₃	NCH	OH ₂	CNH	NH ₃
Electrostatic energy	-94.7	-135.2	-139.2	-149.9	-193.6	-242.1	-208.2	-291.3
Exchange energy	-69.8	-90.3	-85.8	-95.9	-100.8	-104.8	-106.4	-117.6
Repulsion energy	251.8	322.6	290.6	318.4	356.4	370.7	371.1	411.0
Polarization energy	-101.2	-144.2	-111.2	-127.2	-155.3	-155.7	-165.2	-157.4
Dispersion energy	-23.8	-26.8	-27.7	-27.7	-30.1	-33.1	-29.3	-34.0
Total LMOEDA energy	-37.7	-73.9	-73.2	-82.3	-123.3	-165.0	-137.9	-189.2

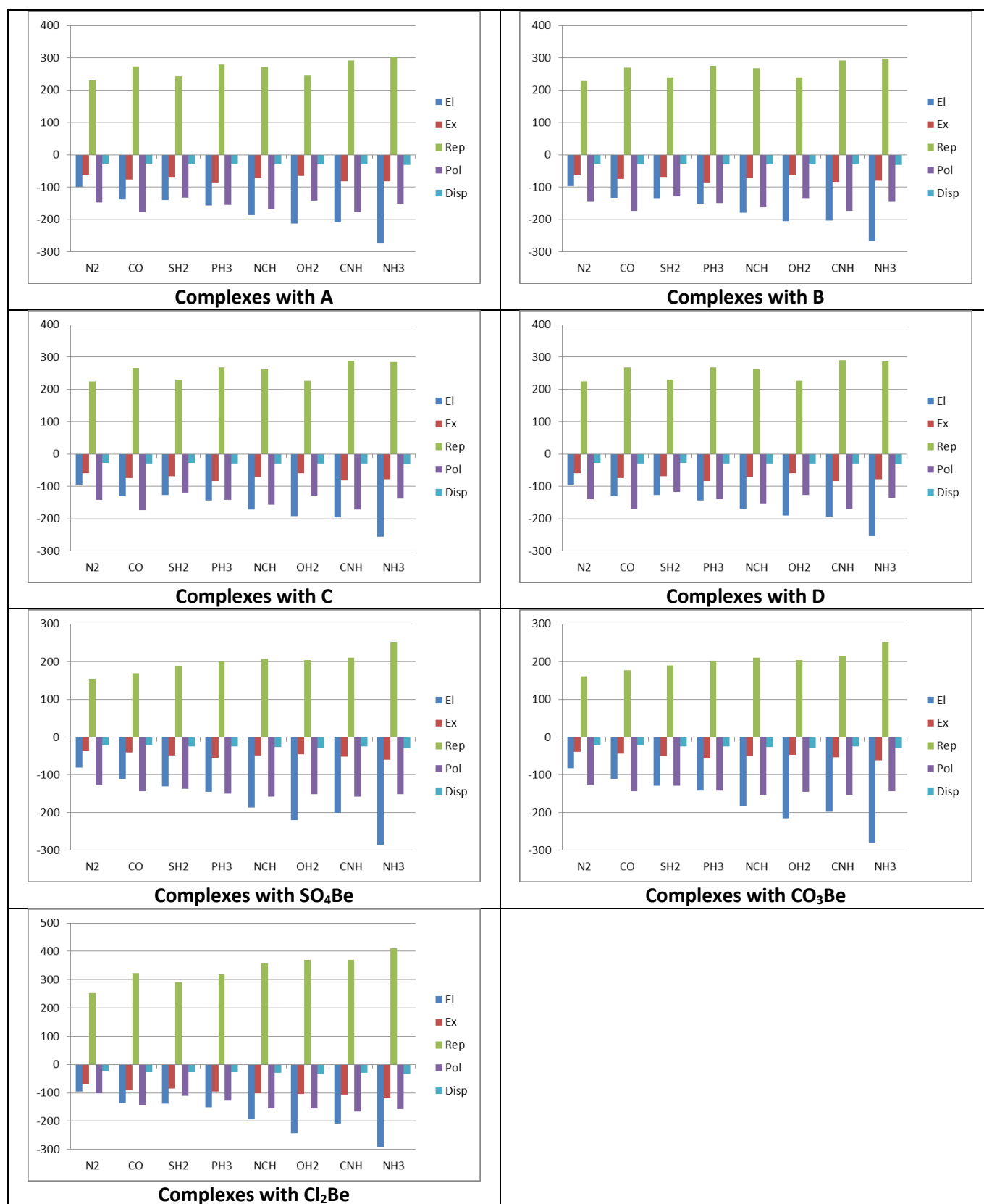


Fig. S5. Graphical representation of the LMOEDA energy terms (kJ mol^{-1})

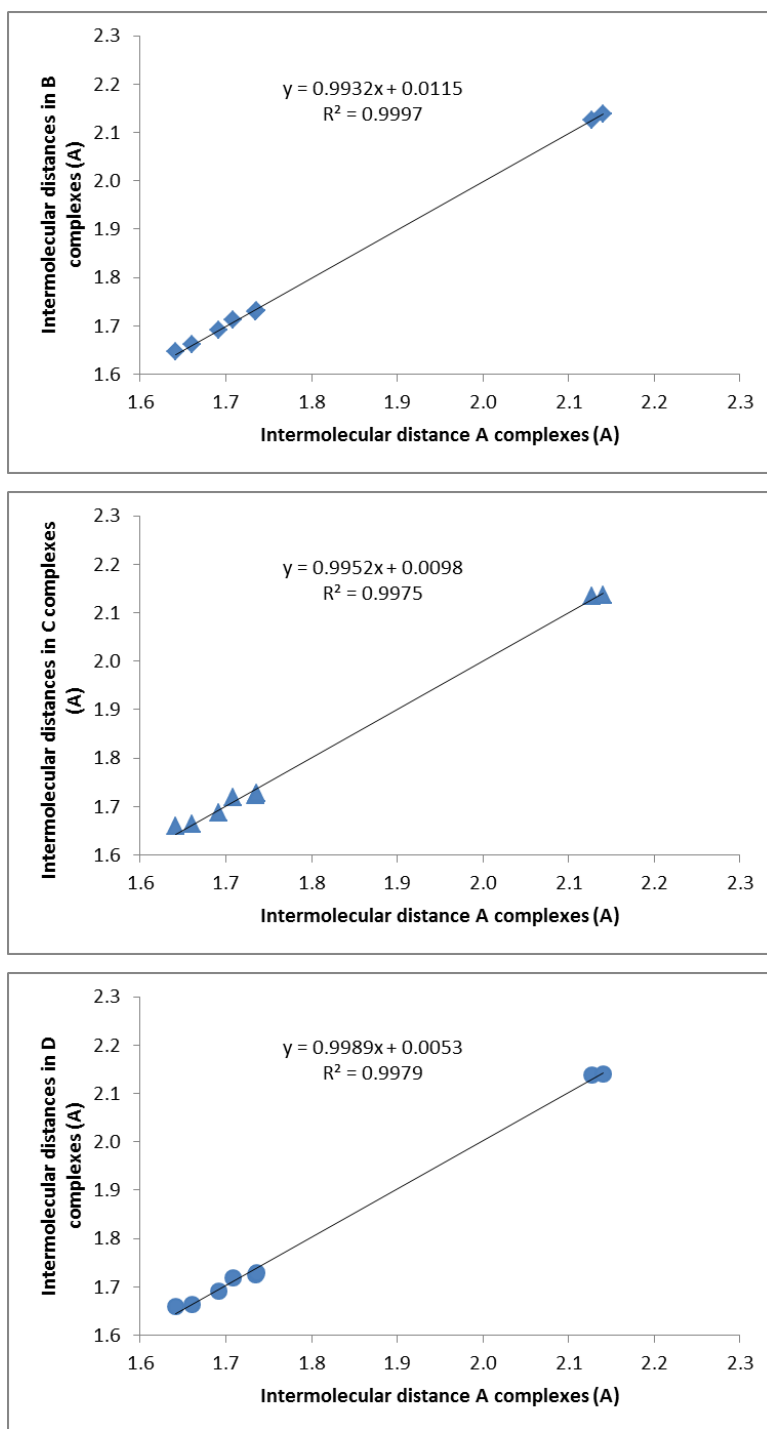


Fig. S6. Intermolecular distances in A complexes vs. B-D complexes (Å)

Table S5. Dissociation ΔG energies (kJ mol^{-1})

LB	A:LB	B:LB	C:LB	D:LB	CO ₃ Be:LB	SO ₄ Be:LB	Cl ₂ Be:LB
N ₂	72.3	69.3	44.4	18.3	56.8	66.5	-25.3
CO	102.3	100.1	76.0	49.2	78.6	88.9	-9.0
SH ₂	121.5	113.9	85.3	58.0	109.8	123.7	12.3
PH ₃	132.0	129.7	100.6	71.9	118.7	133.3	15.9
NCH	151.3	142.2	111.4	83.8	145.2	160.9	35.8
OH ₂	152.7	143.4	115.9	83.6	150.8	166.3	42.5
CNH	165.0	157.5	128.1	100.0	159.5	173.9	62.7
NH ₃	201.8	191.5	160.3	133.3	208.1	223.6	95.8

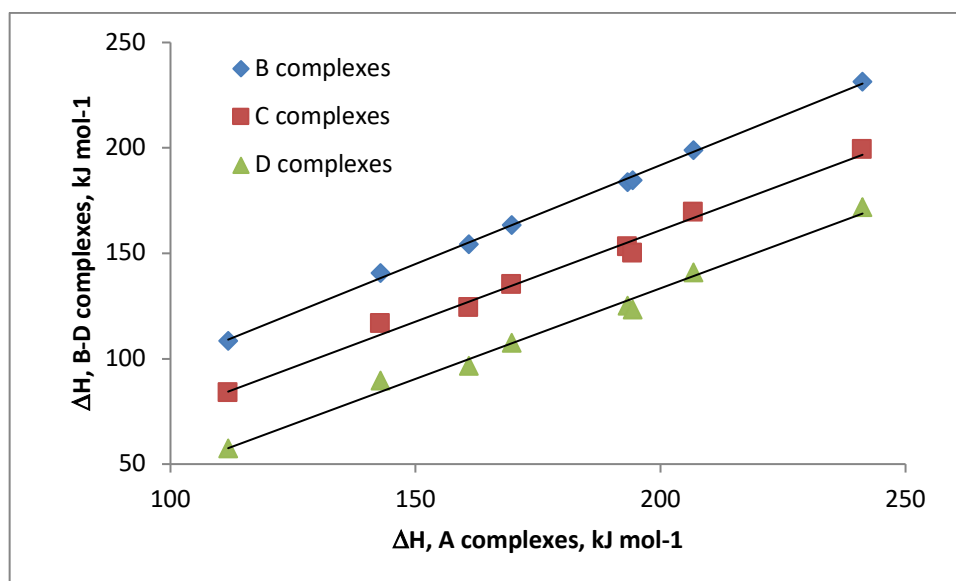


Fig. S7. Dissociation enthalpies of A complexes vs. B-D complexes (kJ mol^{-1})