

Penta-coordinated or -valent: the nature of the chemical bond of some Ti-C-Al compounds

Jörg Saßmannshausen

Electronic Supplementary Information

Table of Contents

Computational details:	1
Table S1: Comparison between the observed and calculated structure 1	2
Results of 1-dft	3
Cartesian coordinates of 1-dft	3
Bader:	5
NBO:	7
NBO with less than 10 kcal/mol	12
ETS-NOVC	15
NOVC orbitals	17
NOVC pair 1:	17
NOVC pair 2:	17
NOVC pair 3:	17
NOVC pair 564:	17
NOVC pair 565:	18
NOVC pair 566:	18
Results of 3	19
Cartesian coordinates of 3	19
Bader:	21
NBO:	23
ETS-NOVC	26
NOVC orbitals	28
NOVC pair 1:	28
NOVC pair 2:	28
NOVC pair 3:	28
NOVC pair 495:	28
NOVC pair 496:	29
NOVC pair 497:	29
Results of 4	30
Cartesian coordinates of 4	30
Bader:	32
NBO:	33
NBO agostic interactions	35
NBO with less than 10 kcal/mol	36
ETS-NOVC	38
NOVC Orbitals	40
NOVC pair 1:	40
NOVC pair 2:	40
NOVC pair 3:	40
NOVC pair 514:	41
NOVC pair 515:	41
NOVC pair 516:	41
Results of Al2Me6	42
Cartesian coordinates of Al2Me6	42
Bader	43
NBO:	44
ETS-NOVC	46

Computational details:

All calculations were performed at using the PBE0 functional^{1, 2} in combination of a mixed basis set consisting of Pople's 6-311G(d,p) basis set³ for all elements apart from Ti, where the Stuttgart-Dresden effective core potential was used. This mixed basis set is abbreviated ecp11 and an expansion of the previously employed ecp1 mixed basis set.⁴ The PBE0 functional was found to give good results for transition metal complexes, specially in combination with Grimme's DFT-D method.^{5, 6}

All calculations were performed using GAMESS-US version 2019-R1 using a standard grid setting.^{7, 8} The optimised structure was subject to a numerical Hessian calculation to verify the nature of the structure being a true minimum (no imaginary frequencies).

For the ETS-NOVC properties calculation, we were using the DZVP all electron basis⁹ set instead of the effective core potential one. The larger Sapporo-DKH3-DZP basis set in combination with the all-electron scalar relativity treatment employing the local unitary transformation modification (keyword RELWFn=LUT-IOTC) with a large grid (keywords nrad=125 nleb=1202) as implemented in GAMESS-US were used for the Quantum Theory of Atoms in Molecules (QTAIM),¹⁰ and Natural Bond Orbital (NBO).^{11, 12} This way, we hope to obtain a comprehensive understanding of the way the atoms in this molecule are interacting with each other. For visualisation of the QTAIM analysis AIM2000^{13,14} was utilized, the various orbitals were generated using Jmol.¹⁵ For the ETS-NOVC analysis the program Multiwfn, version 3.8, was employed.¹⁶

References:

- 1 V. Vetere, C. Adamo, and P. Maldivi, *Chem. Phys. Lett.*, 2000, **325**, 99.
- 2 J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865
- 3 W. J. Hehre, R. Ditchfield, and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257
- 4 M. Bühl and J. Saßmannshausen, *J. Chem. Soc., Dalton Trans.*, 2001, 79.
- 5 M. Bühl and H. Kabrede, *J. Chem. Theory Comput.*, 2006, **2**, 1282.
- 6 M. Bühl, C. Reimann, D. A. Pantazis, T. Bredow, and F. Neese, *J. Chem. Theory Comput.*, 2008, **4**, 1449.
- 7 M. W. Schmidt, K. K. Baldridge, J. A. Boatz, S. T. Elbert, M. S. Gordon, J. H. Jensen, S. Koseki, N. Matsunaga, K. A. Nguyen, S. Su, T. L. Windus, M. Dupuis, and J. A. M. Jr., *J. Comp. Chem.*, 1993, **14**, 1347.
- 8 G. M.J. Barca, C. Bertoni, L. Carrington, D. Datta, N. De Silva, J. E. Deustua, D. G. Fedorov, J. R. Gour, A. O. Gunina, E. Guidez, T. Harville, S. Irle, K. J. Ivanic, Kowalski, S. S. Leang, W. L. H. Li, J. J. Lutz, I. Magoulas, J. Mato, V. Mironov, H. Nakata, B. Q. Pham, P. Piecuch, D. Poole, S. R. Pruitt, A. P. Rendell, L. B. Roskop, K. Ruedenberg, T. Sattasathuchana, M. W. Schmidt, J. Shen, L. Slipchenko, M. Sosonkina, V. Sundriyal, A. Tiwari, J. L. Galvez Vallejo, B. Westheimer, M. Wloch, P. Xu, F. Zahariev, and M. S. Gordon., *J. Chem. Phys.*, 2020, **152**, 154102.
- 9 N. Godbout, D. R. Salahub, J. Andzelm, and E. Wimmer, *Can. J. Chem.*, 1992, **70**, 560.
- 10 R. F. W. Bader, 'Atoms in Molecules: A Quantum Theory', Clarendon Press, 1990.
- 11 E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, P. Karafiloglou, C. R. Landis, and F. Weinhold, in 'NBO 7.0', Madison, WI, 2018.
- 12 E. D. Glendening, C. R. Landis, and F. Weinhold, *Journal of Computational Chemistry*, 2019, **40**, 2234.
- 13 F. Biegler-König, J. Schönbohm, and D. Bayles, *J. Comp. Chem.*, 2001, **22**, 545.
- 14 F. Biegler-König and J. Schönbohm, *J. Comput. Chem.*, 2002, **23**, 1489.
- 15 Jmol: an open-source Java viewer for chemical structures in 3D. <http://www.jmol.org/>
- 16 T. Lu and F. Chen, *Journal of Computational Chemistry*, 2012, **33**, 580.

Table S1: Comparison between the observed and calculated structure 1

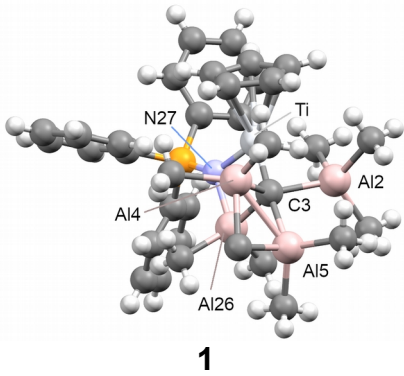
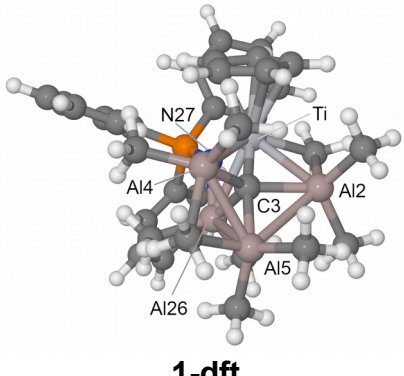
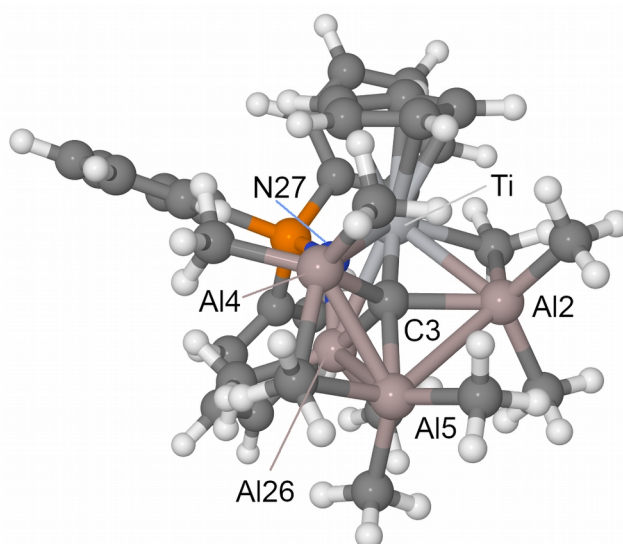
	 1	 1-dft
d(Ti-C3)	1.972(3)	1.947
d(Ti-Al26)	2.7538(9)	2.743
d(Ti-N27)	1.942(2)	1.919
d(C3-Al2)	2.095(3)	2.080
d(C3-Al4)	2.087(3)	2.119
d(C3-Al5)	2.121(3)	2.108
d(C3-Al26)	2.150(3)	2.119
d(Al26-N27)	1.943(2)	1.972
∠ (Ti-N27-Al26)		89.64°
∠ (Ti-C3-Al26)		84.72°
∠ (Ti-C3-Al5)		175.11°
∠ (Al2-C3-Al4)		129.31°
∠ (Al2-C3-Al26)		114.94°
∠ (Al4-C3-Al26)		115.16°

Table S1: Comparison between the observed and calculated structure 1

Results of 1-dft

Cartesian coordinates of 1-dft in Å

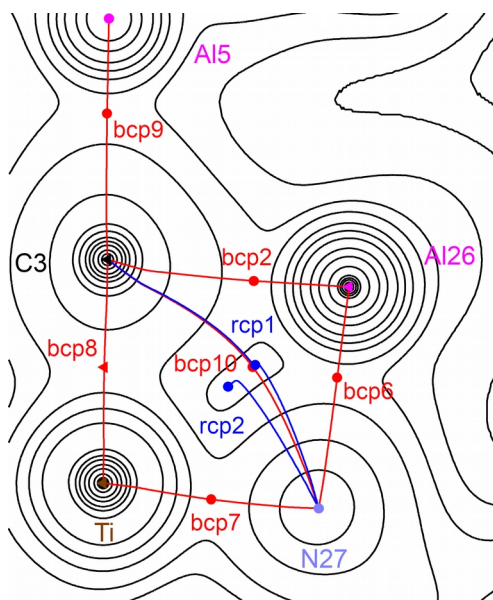
Ti	-0.908629	-1.145774	-0.153091
Al	-3.093785	-0.733589	-1.736478
C	-2.286118	0.228874	-0.078626
Al	-2.977315	0.270428	1.901834
Al	-3.822525	1.669890	-0.165710
C	-3.417250	3.408745	-1.010278
H	-2.536987	3.951850	-0.654214
H	-4.286860	4.053968	-0.822959
H	-3.331170	3.303254	-2.096346
C	-5.601355	0.893865	-0.606686
H	-5.888562	0.094077	0.083693
H	-5.736746	0.517838	-1.623130
H	-6.328662	1.707967	-0.478026
C	-4.076496	2.158718	1.897627
H	-4.919200	2.709570	1.455970
H	-3.377825	2.905375	2.281682
H	-4.555363	1.668445	2.754187
C	-4.322431	-1.129589	2.306484
H	-4.770758	-1.568931	1.409150
H	-5.145501	-0.708297	2.896870
H	-3.905860	-1.949445	2.904230
C	-1.788914	0.760930	3.421131
H	-1.197445	1.663852	3.242893
H	-1.103161	-0.019713	3.768948
H	-2.449203	0.979448	4.271578
Al	-0.699129	1.566120	-0.507009
N	0.566052	0.079316	-0.226733
P	2.152971	0.117181	-0.076216
C	2.675637	0.339149	1.645138
C	1.701320	0.395551	2.638225
H	0.655801	0.300204	2.368226
C	2.072139	0.603505	3.961384
H	1.304637	0.659467	4.725889
C	3.413588	0.751218	4.290476
H	3.703632	0.912991	5.323416
C	4.388730	0.710608	3.296466
H	5.434059	0.843951	3.553872
C	4.023127	0.515614	1.972392
H	4.780295	0.516016	1.193600
C	2.929198	1.505981	-0.950693
C	3.627823	1.352277	-2.147708
H	3.792550	0.366593	-2.566803
C	4.128443	2.468631	-2.806733
H	4.670209	2.343756	-3.738030
C	3.933477	3.737626	-2.276830
H	4.318294	4.607780	-2.798179
C	3.249117	3.893182	-1.076128
H	3.096952	4.881653	-0.656603



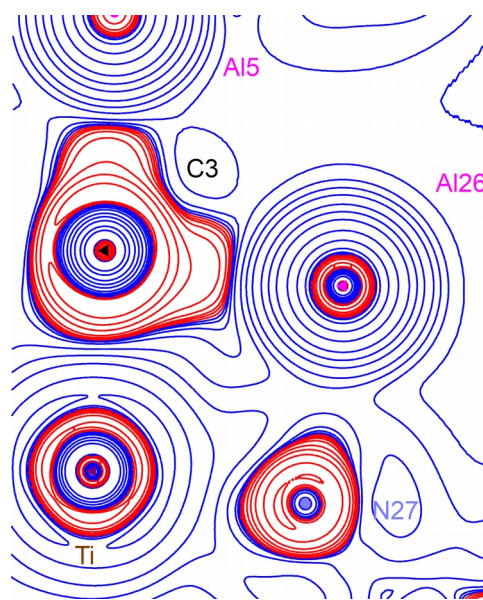
C	2.753325	2.783312	-0.409352
H	2.220858	2.913794	0.526246
C	2.898314	-1.410728	-0.712903
C	2.555727	-1.797618	-2.013715
H	1.903575	-1.168544	-2.611849
C	3.022424	-2.998617	-2.528241
H	2.751180	-3.293168	-3.536322
C	3.822755	-3.826720	-1.746049
H	4.179533	-4.770202	-2.145075
C	4.158710	-3.448873	-0.452129
H	4.773080	-4.097614	0.162726
C	3.701218	-2.242030	0.065537
H	3.956274	-1.961108	1.081506
C	-0.349464	2.200297	-2.349793
H	-0.295293	1.402922	-3.098307
H	0.620811	2.714254	-2.362867
H	-1.091641	2.926157	-2.696574
C	-0.444898	2.943976	0.908775
H	0.278072	2.664067	1.683922
H	-1.369266	3.213322	1.425934
H	-0.076830	3.862994	0.433580
C	-1.106542	-1.586584	-2.317870
H	-0.885079	-0.756656	-2.993614
H	-1.687816	-2.346554	-2.850980
H	-0.149903	-2.087493	-2.116378
C	-4.325761	-2.273261	-1.590540
H	-4.288765	-2.863533	-0.670936
H	-4.141186	-2.966779	-2.422585
H	-5.359760	-1.927815	-1.701979
C	-3.337920	0.386996	-3.347163
H	-2.596738	1.185692	-3.429209
H	-4.328342	0.850385	-3.377853
H	-3.250073	-0.241061	-4.243037
C	-1.924791	-2.971213	0.960288
C	-1.149704	-3.536517	-0.069737
C	0.213894	-3.288886	0.216925
C	0.278590	-2.551465	1.410869
H	1.178945	-2.193773	1.888960
C	-1.045960	-2.340599	1.869534
H	-1.330937	-1.825368	2.773607
H	1.056767	-3.576538	-0.396557
H	-1.538631	-4.058002	-0.932399
H	-3.000050	-2.974729	1.027991

Bader:

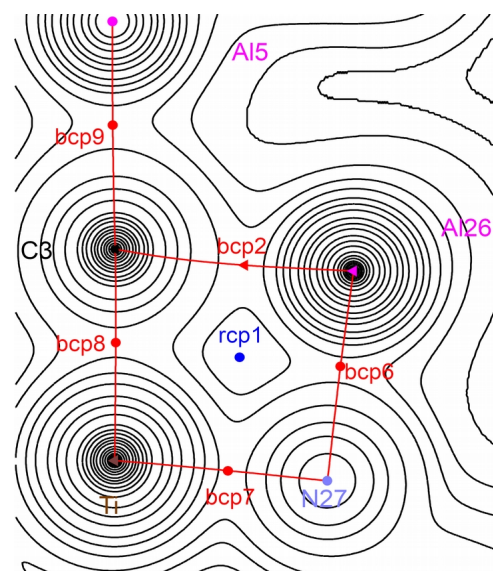
Plane through Ti-C3-Al26:



Electron density

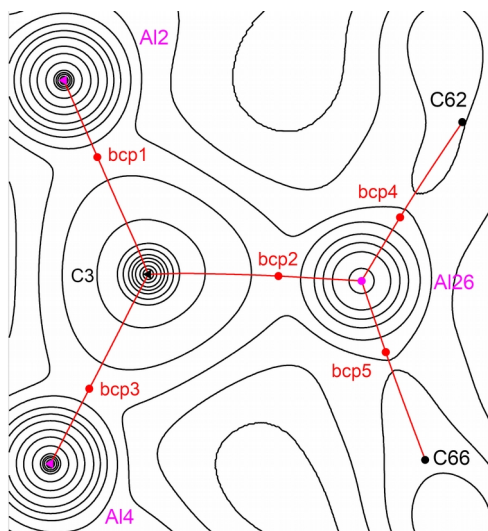


Laplacian

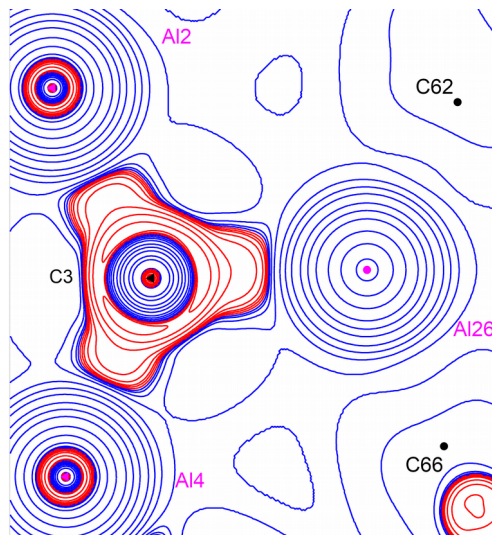


Virial

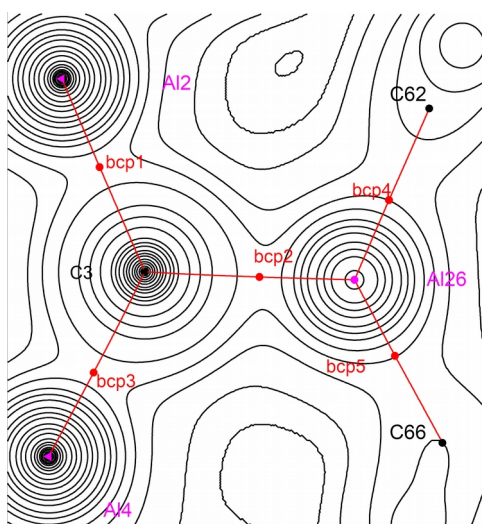
Plane through Al2-C3-Al4:



Electron density



Laplacian

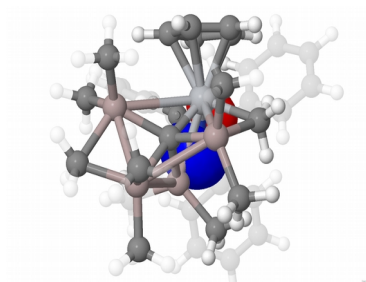


Virial

	$\varrho(\mathbf{r})$	$\nabla^2\varrho(\mathbf{r})$
bcp1	0.05876	-0.05507
bcp2	0.05547	-0.05024
bcp3	0.05523	-0.05171
bcp4	0.07941	-0.07877
bcp5	0.07716	-0.07609
bcp6	0.05668	-0.08707
bcp7	0.12260	-0.09928
bcp8	0.12857	-0.04523
bcp9	0.05558	-0.05341
bcp10	0.03766	-0.01031

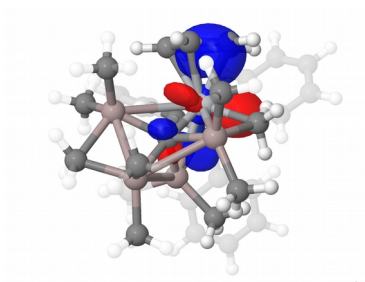
NBO:

Donororbital



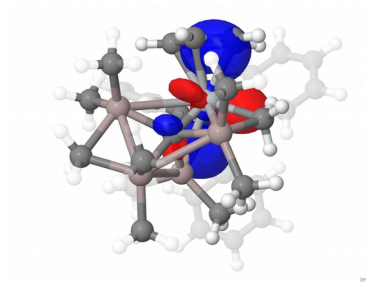
LP N 27 $sp^{6.99}$

Acceptororbital

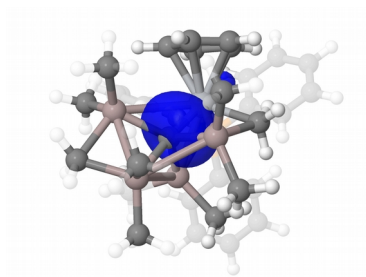


BD* Ti 1 (78.23%) $p^{0.43}d^{99.99}$ –
C 3 (21.77%) $p^{99.99}$

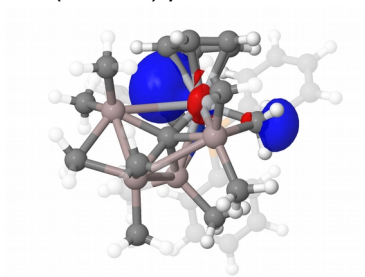
Overlaporbital



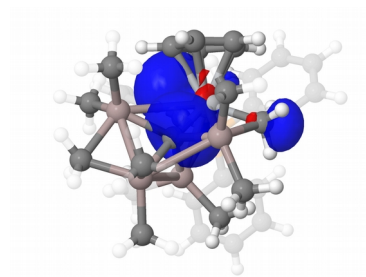
$E(2P) = 19.94 \text{ kcal/mol}$



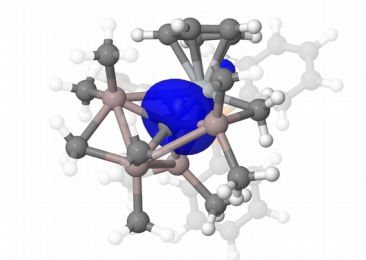
BD Ti 1 (26.17%) $sd^{5.05}$ –
C 3 (73.83%) $sp^{0.97}$



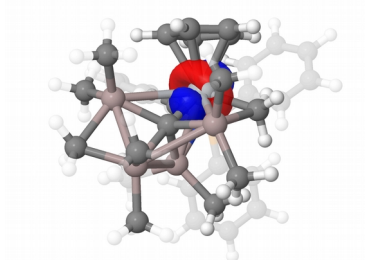
BD* Ti 1 (76.87%) $sp^{0.01}d^{6.19}$ –
C 70 (23.13%) $sp^{2.32}$



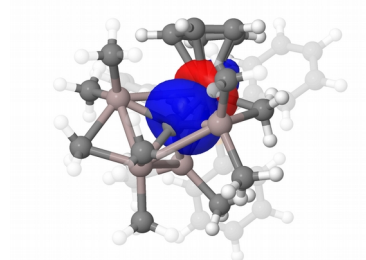
$E(2P) = 10.80 \text{ kcal/mol}$



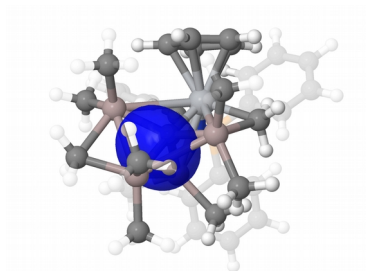
BD Ti 1 (26.17%) $sd^{5.05}$ –
C 3 (73.83%) $sp^{0.97}$



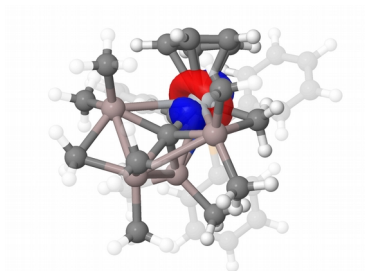
RY Ti 1 $sp^{0.31}d^{55.07}p^{0.06}$



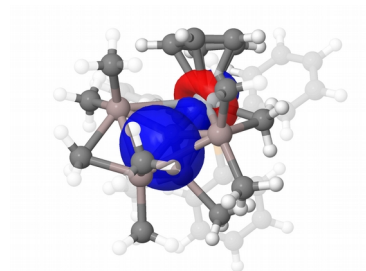
$E(2P) = 13.60 \text{ kcal/mol}$



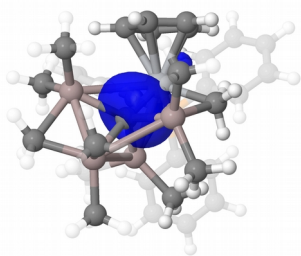
BD C 3 (87.45%) $sp^{1.05}$ –
Al 5 (12.55%) $sp^{4.62}d^{0.07}$



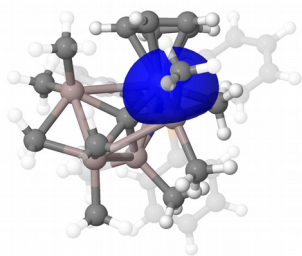
RY Ti 1 $sp^{0.31}d^{55.07}p^{0.06}$



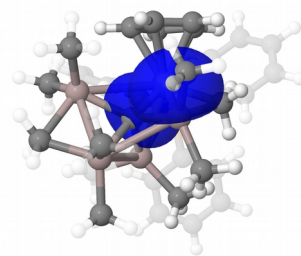
$E(2P) = 29.82 \text{ kcal/mol}$



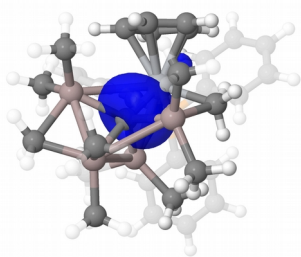
BD Ti 1 (26.17%) $sd^{5.05} -$
C 3 (73.83%) $sp^{0.97}$



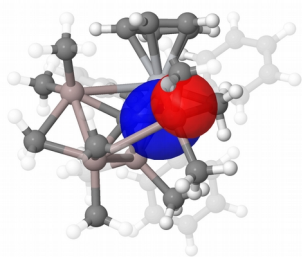
LV Al 2 $sp^{1.49}$



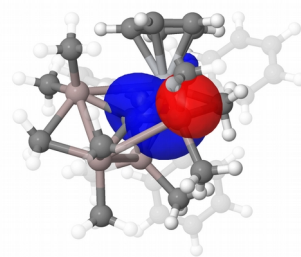
$E(2p) = 14.40$ kcal/mol



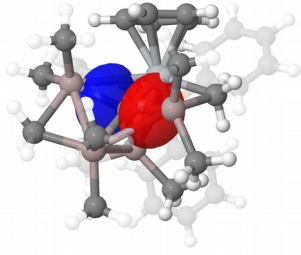
BD Ti 1 (26.17%) $sd^{5.05} -$
C 3 (73.83%) $sp^{0.97}$



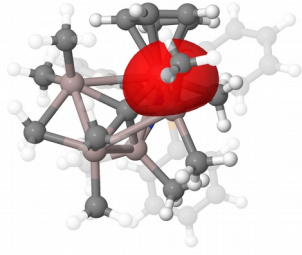
LV Al 2 $sp^{42.67}$



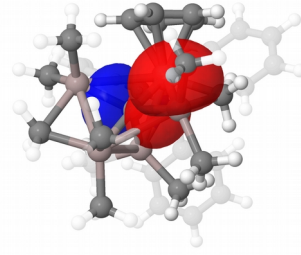
$E(2P) = 24.38$ kcal/mol



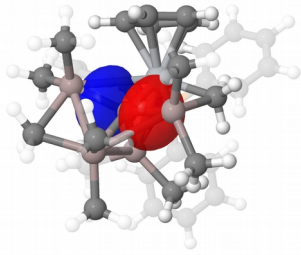
BD Ti 1 (20.56%) $sp^{0.16}d^{99.99} -$
C 3 (79.44%) $sp^{99.99}$



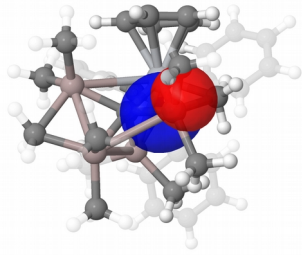
LV Al 2 $sp^{1.49}$



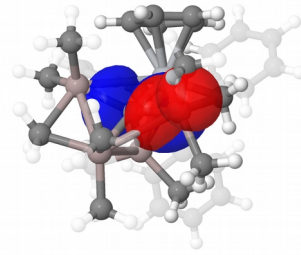
$E(2P) = 11.77$ kcal/mol



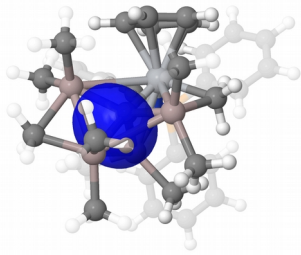
BD Ti 1 (20.56%) $sp^{0.16}d^{99.99} -$
C 3 (79.44%) $sp^{99.99}$



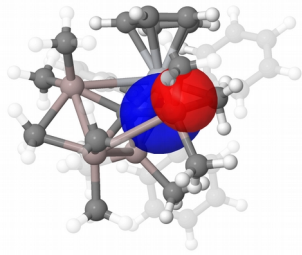
LV Al 2 $sp^{42.67}$



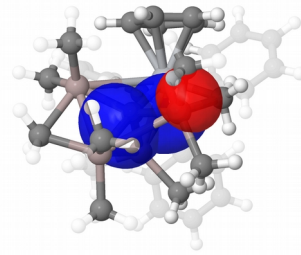
$E(2P) = 17.02$ kcal/mol



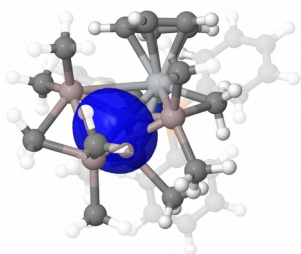
BD C 3 (87.45%) $sp^{1.05} -$
Al 5 (12.55%) $sp^{4.62}d^{0.07}$



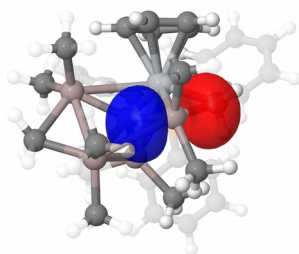
LV Al 2 $sp^{42.67}$



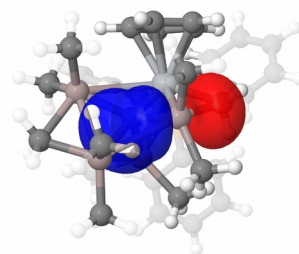
$E(2P) = 13.91$ kcal/mol



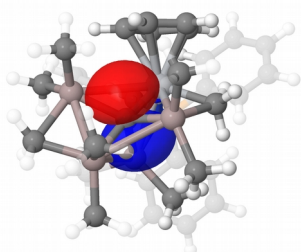
BD C 3 (87.45%) $sp^{1.05}$ –
Al 5 (12.55%) $sp^{4.62}d^{0.07}$



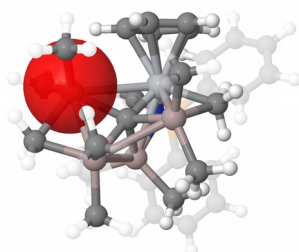
LV Al 2 $sp^{99.99}$



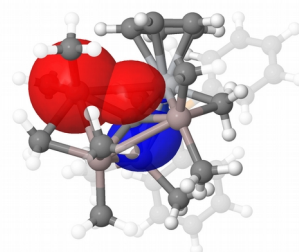
$E(2P) = 12.24 \text{ kcal/mol}$



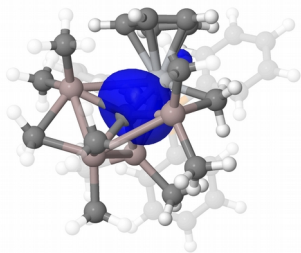
BD Ti (21.77%) $sp^{0.43}d^{99.99}$ –
C 3 (78.23%) $sp^{99.99}d^{0.89}$



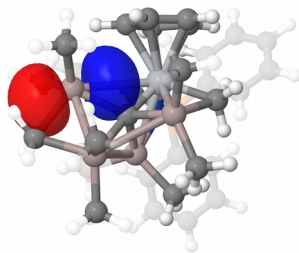
LV Al 4 $sp^{0.02}$



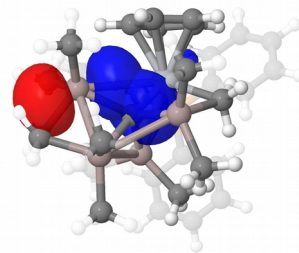
$E(2P) = 10.49 \text{ kcal/mol}$



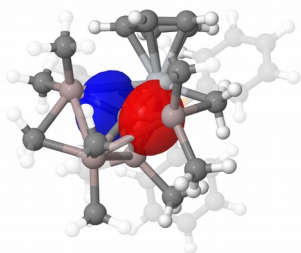
BD Ti 1 (26.17%) $sd^{5.05}$ –
C 3 (73.83%) $sp^{0.97}$



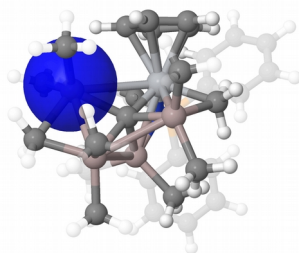
LV Al 4 $sp^{99.99}$



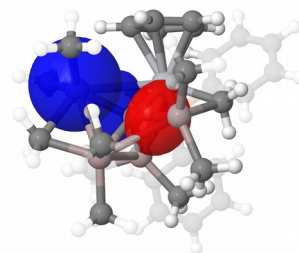
$E(2P) = 13.58 \text{ kcal/mol}$



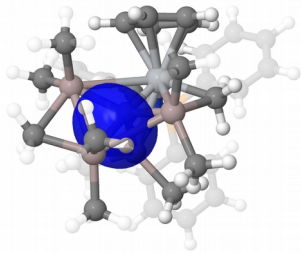
BD Ti 1 (20.56%) $sp^{0.16}d^{99.99}$ –
C 3 (79.44%) $sp^{99.99}$



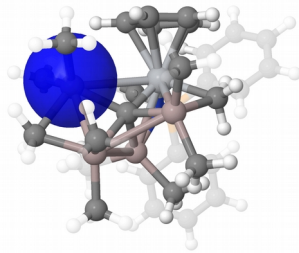
LV Al 4 $sp^{0.02}$



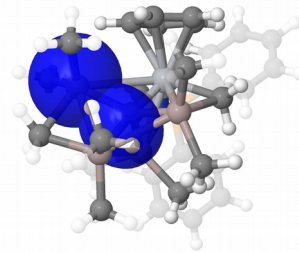
$E(2P) = 16.40 \text{ kcal/mol}$



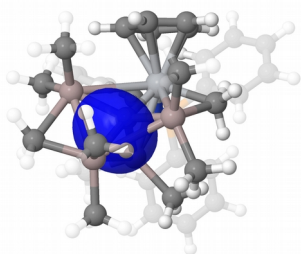
BD C 3 (87.45%) $sp^{1.05}$ –
Al 5 (12.55%) $sp^{4.62}d^{0.07}$



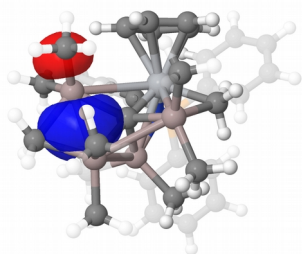
LV Al 4 $sp^{0.02}$



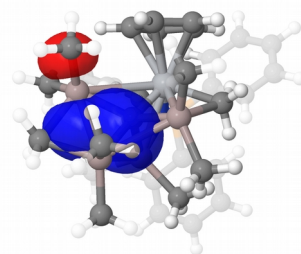
$E(2P) = 12.36 \text{ kcal/mol}$



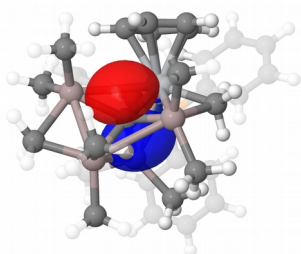
BD C 3 (87.45%) $sp^{1.05}$ –
Al 5 (12.55%) $sp^{4.62}d^{0.07}$



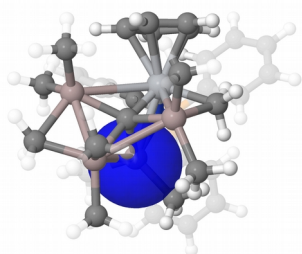
LV Al 4 $sp^{46.93}$



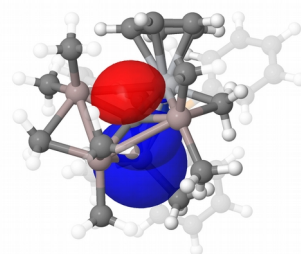
$E(2P) = 30.69 \text{ kcal/mol}$



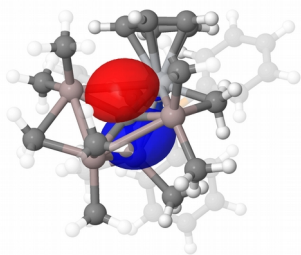
BD Ti (21.77%) $sp^{0.43}d^{99.99}$ –
C 3 (78.23%) $sp^{99.99}d^{0.89}$



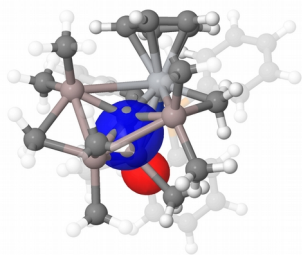
LV Al 26 $sp^{0.01}$



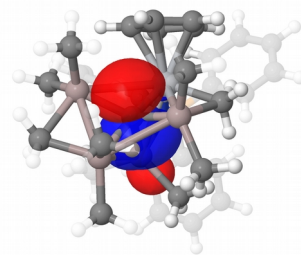
$E(2P) = 27.23 \text{ kcal/mol}$



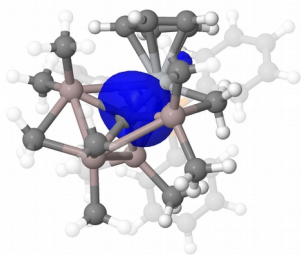
BD Ti (21.77%) $sp^{0.43}d^{99.99}$ –
C 3 (78.23%) $sp^{99.99}d^{0.89}$



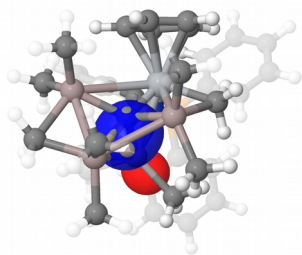
LV Al 26 $sp^{99.99}$



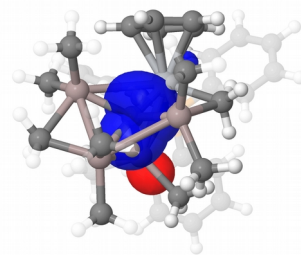
$E(2P) = 15.72 \text{ kcal/mol}$



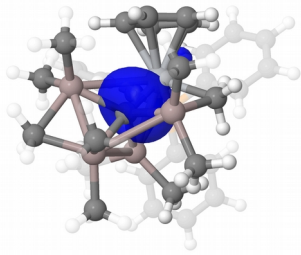
BD Ti 1 (26.17%) $sd^{5.05}$ –
C 3 (73.83%) $sp^{0.97}$



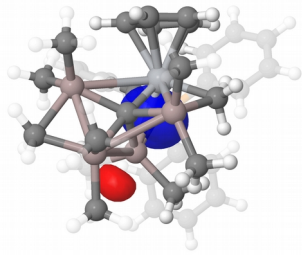
LV Al 26 $sp^{99.99}$



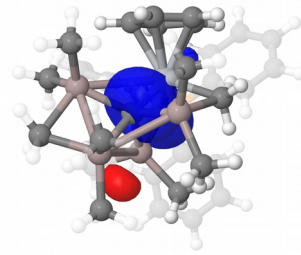
$E(2P) = 13.32 \text{ kcal/mol}$



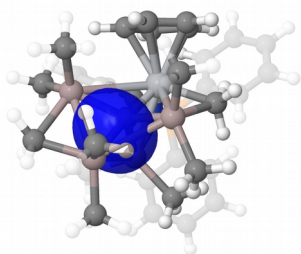
BD Ti 1 (26.17%) $sd^{5.05}$ –
C 3 (73.83%) $sp^{0.97}$



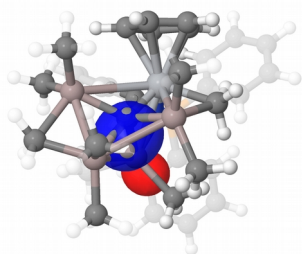
LV Al 26 $sp^{99.99}$



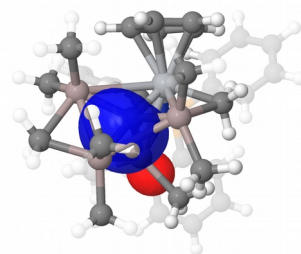
$E(2P) = 10.76 \text{ kcal/mol}$



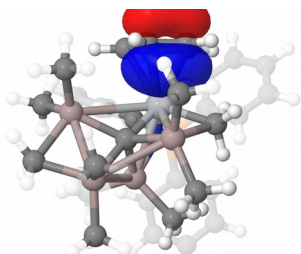
BD C 3 (87.45%) $sp^{1.05}$ –
Al 5 (12.55%) $sp^{4.62}d^{0.07}$



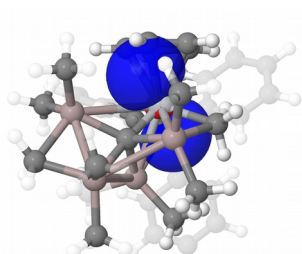
LV Al 26 $sp^{99.99}$



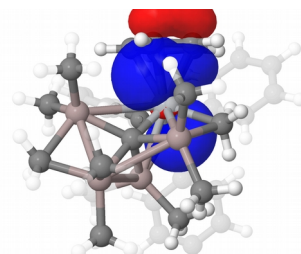
$E(2P) = 16.35 \text{ kcal/mol}$



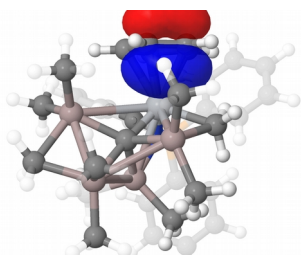
BD C 82 (50.16%) $sp^{63.00}d^{0.19}$ –
C 83 (49.84%) $sp^{68.29}d^{0.18}$



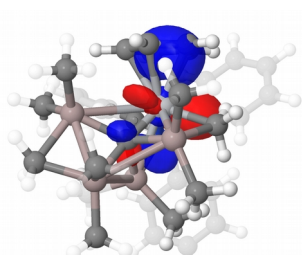
LV Ti 1 $sd^{0.58}$



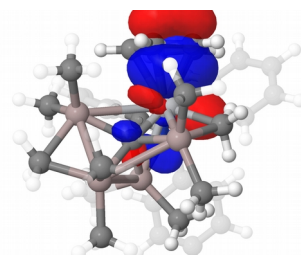
$E(2P) = 29.30 \text{ kcal/mol}$



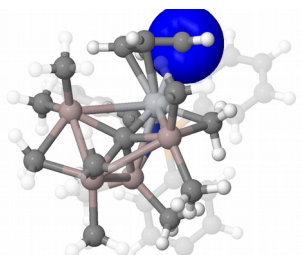
BD C 82 (50.16%) $sp^{63.00}d^{0.19}$ –
C 83 (49.84%) $sp^{68.29}d^{0.18}$



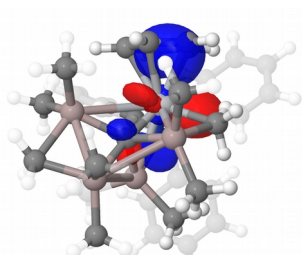
BD* Ti 1 (78.23%) $p^{0.43}d^{99.99}$ –
C 3 (21.77%) $p^{99.99}$



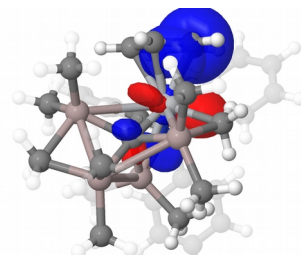
$E(2P) = 17.10 \text{ kcal/mol}$



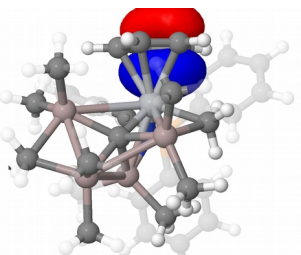
BD C 83 (49.90%) $sp^{1.96}$ –
C 84 (50.10%) $sp^{1.95}$



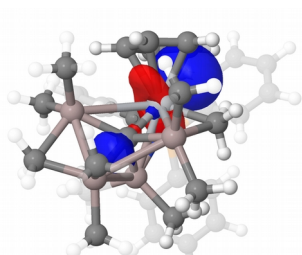
BD* Ti 1 (78.23%) $p^{0.43}d^{99.99}$ –
C 3 (21.77%) $p^{99.99}$



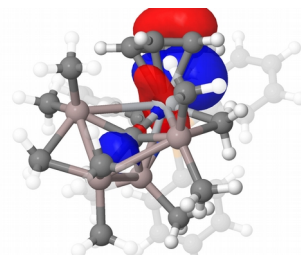
$E(2P) = 10.65 \text{ kcal/mol}$



BD C 84 (50.26%) p –
C 85 (49.74%) $sp^{82.32}$



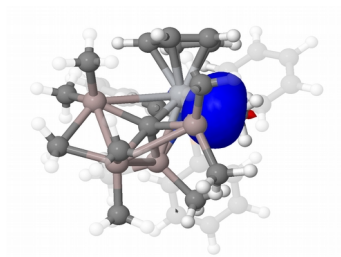
BD* Ti 1 (73.83%) $sd^{5.05}$ –
C 3 (26.17%) $sp^{0.97}$



$E(2P) = 35.90 \text{ kcal/mol}$

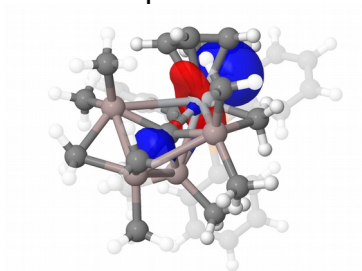
NBO with less than 10 kcal/mol

Donororbital



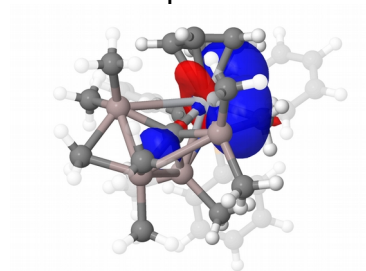
*BD Ti 1 (23.13%) $sd^{6.19}$ –
C 70 (76.87%) $sp^{2.32}$*

Acceptororbital

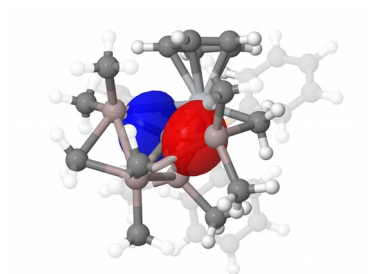


BD Ti 1 (73.83%) $sd^{5.05}$ –
C 3 (26.17%) $sp^{0.97}$*

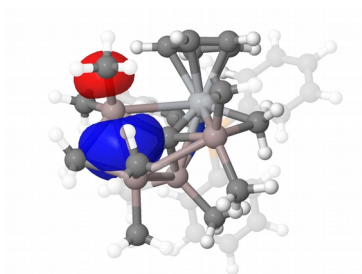
Overlaporbital



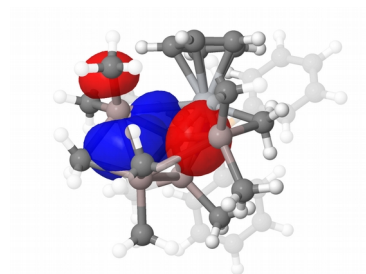
$E(2P) = 5.77$ kcal/mol



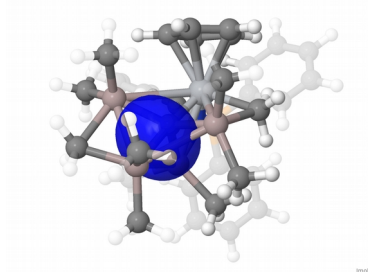
*BD Ti 1 (20.56%) $sp^{0.16}d^{99.99}p^{0.16}$ –
C 3 (79.44%) $sp^{99.99}$*



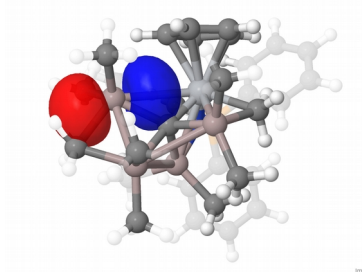
LV Al 4 $sp^{46.93}$



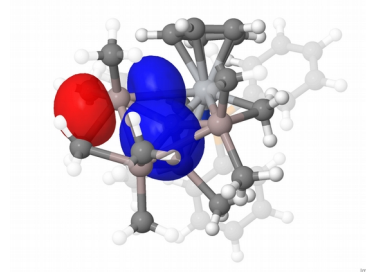
$E(2P) = 7.01$ kcal/mol



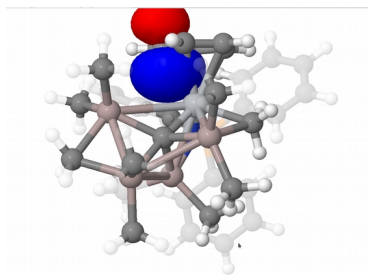
*BD C 3 (87.45%) $sp^{1.05}$ –
Al 5 (12.55%) $sp^{4.62}d^{0.07}$*



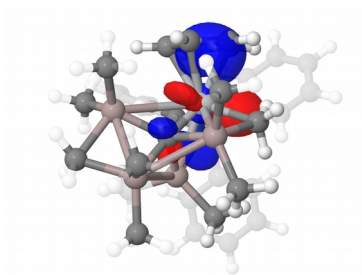
LV Al 4 $sp^{99.99}$



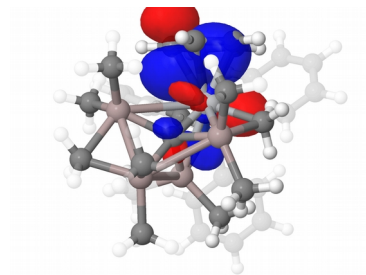
$E(2P) = 8.86$ kcal/mol



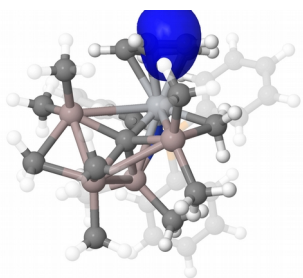
LP C 87 $sp^{15.63}d^{0.03}$



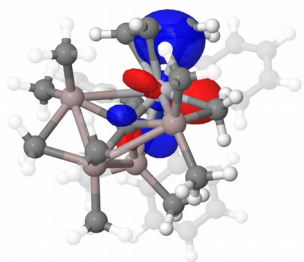
BD Ti 1 (78.23%) $p^{0.43}d^{99.99}$ –
C 3 (21.77%) $p^{99.99}$*



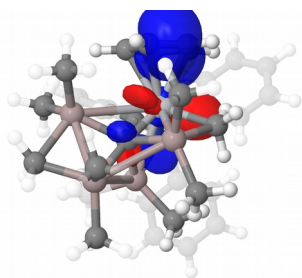
$E(2P) = 5.33$ kcal/mol



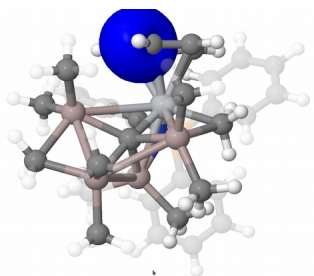
*BD C 82 (49.94%) $sp^{2.11}$ –
C 83 (50.06%) $sp^{2.06}$*



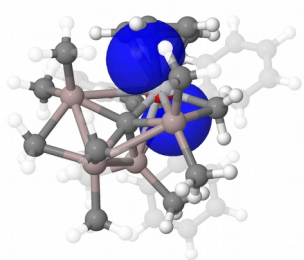
BD Ti 1 (78.23%) $p^{0.43}d^{99.99}$ –
C 3 (21.77%) $p^{99.99}$*



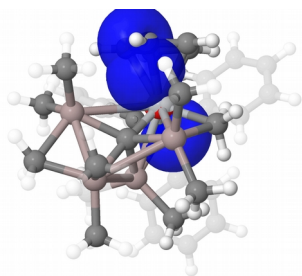
$E(2P) = 7.48 \text{ kcal/mol}$



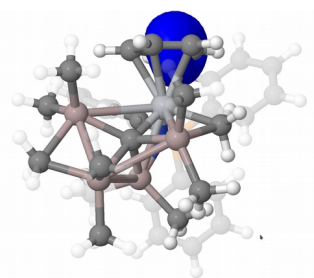
*BD C 82 (49.55%) $sp^{2.01}$ –
C 87 (50.45%) $sp^{2.22}$*



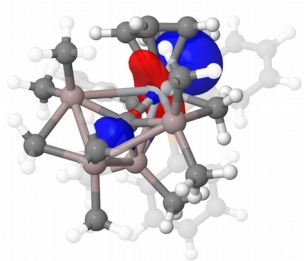
LV Ti 1 $sd^{0.58}$



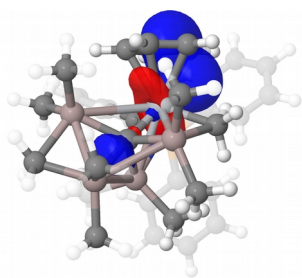
$E(2P) = 9.17 \text{ kcal/mol}$



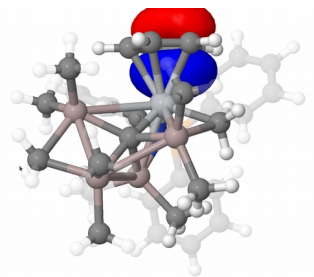
*BD C 84 (49.94%) $sp^{2.01}$ –
C 85 (50.06%) $sp^{2.03}$*



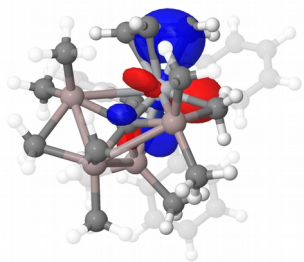
BD Ti (73.83%) $sp^{0.02}d^{5.05}$ –
C 3 (26.17%) $sp^{0.97}$*



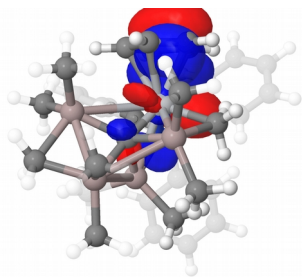
$E(2P) = 5.45 \text{ kcal/mol}$



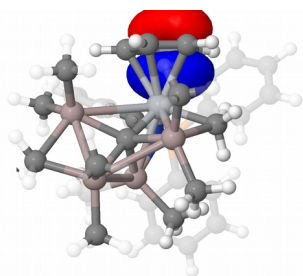
*BD C 84 (50.26%) $sp^{99.99}$ –
C 85 (49.74%) $sp^{82.32}d^{0.20}$*



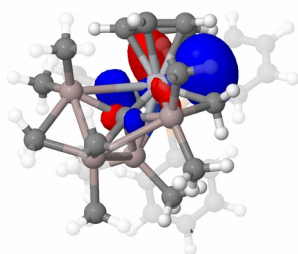
BD(1)Ti 1 (78.23%)
 $sp^{0.43}d^{99.99}p^{0.21}$ –
C 3 (21.77%) $sp^{99.99}d^{0.89}$*



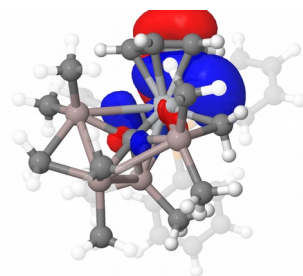
$E(2P) = 6.36 \text{ kcal/mol}$



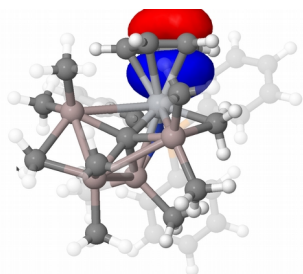
BD C 84 (50.26%) $sp^{99.99} -$
C 85 (49.74%) $sp^{82.32}d^{0.20}$



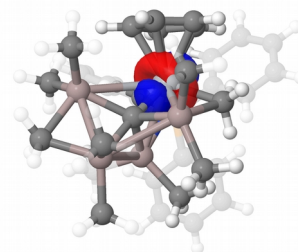
BD* Ti 1 (79.44%)
 $sp^{0.16}d^{99.99}f^{0.16} -$
C 3 (20.56%) $sp^{99.99}d^{0.30}$



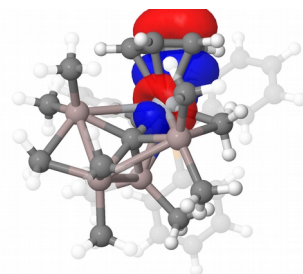
$E(2P) = 6.55 \text{ kcal/mol}$



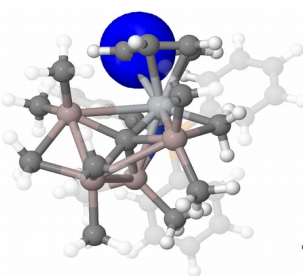
BD C 84 (50.26%) $sp^{99.99} -$
C 85 (49.74%) $sp^{82.32}d^{0.20}$



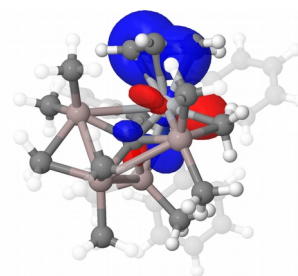
RY Ti 1 $sp^{0.31}d^{55.07}f^{0.06}$



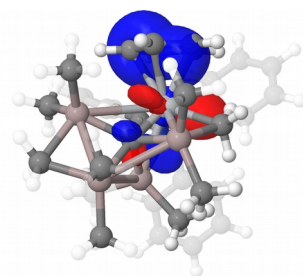
$E(2P) = 6.42 \text{ kcal/mol}$



BD C 85 (49.88%) $sp^{1.96} -$
C 87 (50.12%) $sp^{2.19}$

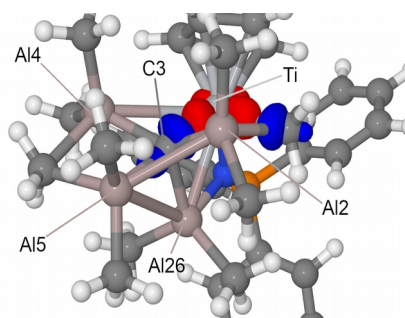


BD* Ti 1 (78.23%)
 $sp^{0.43}d^{99.99}f^{0.21} -$
C 3 (21.77%) $sp^{99.99}$

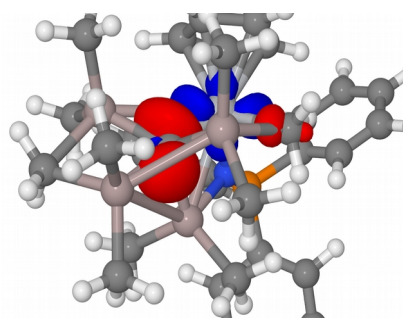


$E(2P) = 5.34 \text{ kcal/mol}$

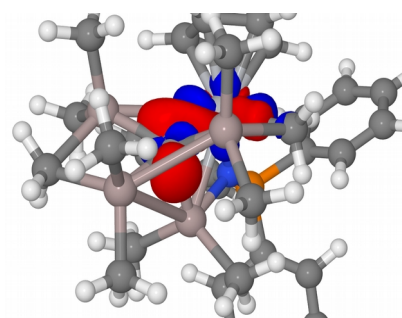
ETS-NOVC



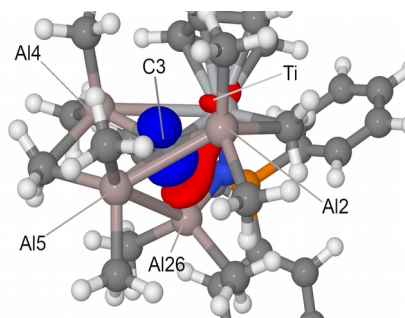
NOVC pair 1



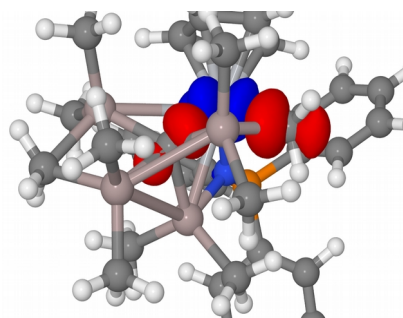
NOVC pair 564



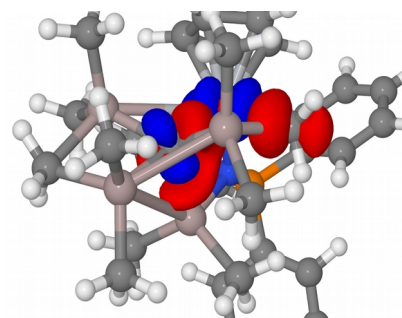
NOVC pair 1,564



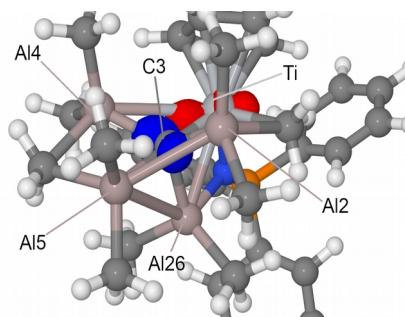
NOVC pair 2



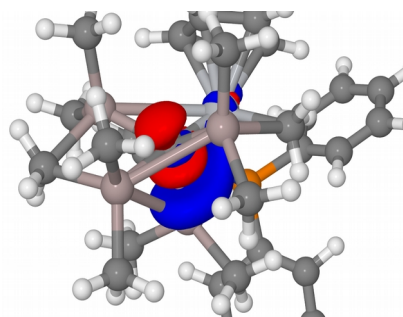
NOVC pair 565



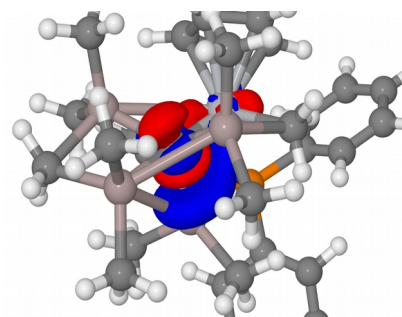
NOVC pair 2,565



NOVC pair 3



NOVC pair 566



NOVC pair 3,566

----- Pair and NOCV orbital information -----

There are totally 1126 NOCV pairs and 2252 NOCV orbitals

NOCV orbitals with absolute eigenvalues smaller than 5.0E-02 are not shown

Note: All energies are given in kcal/mol

----- Alpha NOCV orbitals -----

Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1	-39.55	1	0.43967	-126.42	1126	-0.43967	-36.46
2	-37.33	2	0.40263	-100.38	1125	-0.40263	-7.67
3	-20.87	3	0.34581	-119.57	1124	-0.34581	-59.21
4	-15.43	4	0.23558	-106.48	1123	-0.23558	-40.99
5	-2.98	5	0.12738	-120.74	1122	-0.12738	-97.34
6	-3.70	6	0.09925	-98.94	1121	-0.09925	-61.65
7	-1.70	7	0.06720	-59.11	1120	-0.06720	-33.75
8	-1.27	8	0.05576	-39.74	1119	-0.05576	-16.98

----- Beta NOCV orbitals -----

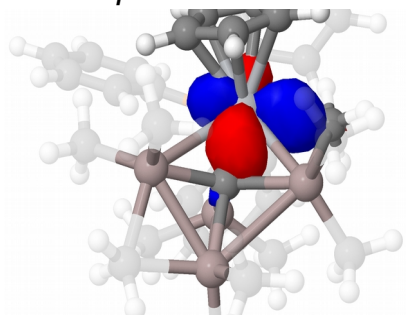
Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
564	-118.68	1127	0.87730	-153.71	2252	-0.87730	-18.43
565	-110.40	1128	0.80745	-156.93	2251	-0.80745	-20.20
566	-123.15	1129	0.64703	-118.23	2250	-0.64703	72.10
567	-11.59	1130	0.22845	-116.10	2249	-0.22845	-65.36
568	-2.60	1131	0.10426	-118.02	2248	-0.10426	-93.11
569	-1.52	1132	0.07555	-96.03	2247	-0.07555	-75.97
570	-1.38	1133	0.06013	-51.78	2246	-0.06013	-28.81

Sum of NOCV eigenvalues: Alpha= -0.00001 Beta= -0.00001

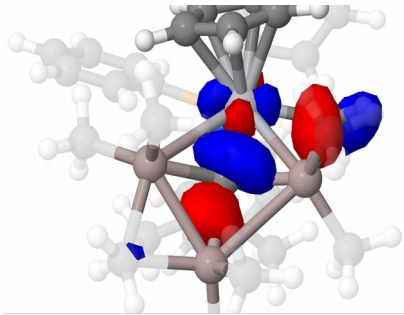
Sum of pair energies: Alpha= -122.84 Beta= -369.32 Total= -492.16

NOVC orbitals

NOVC pair 1:

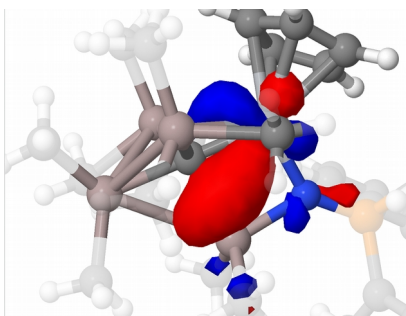


NOVC orbital 1

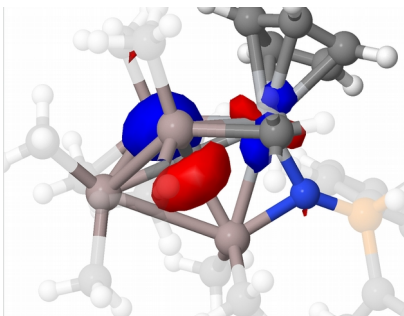


NOVC orbital 1126

NOVC pair 2:

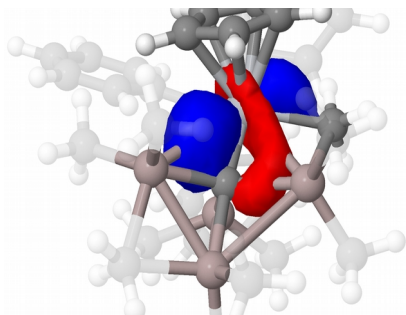


NOVC orbital 2

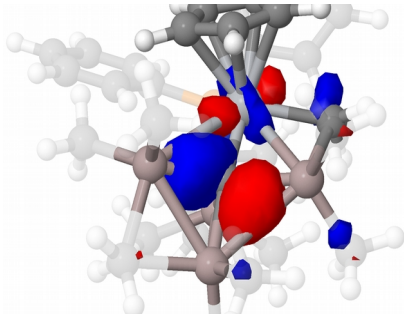


NOVC orbital 1125

NOVC pair 3:

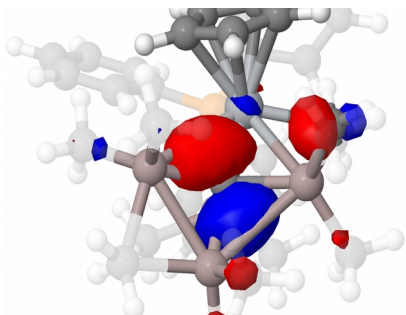


NOVC orbital 3

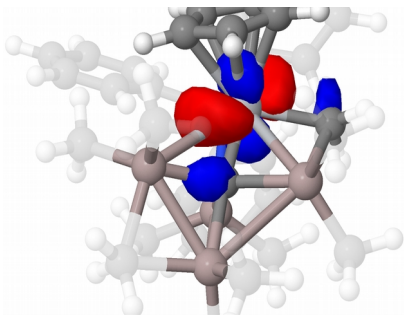


NOVC orbital 1124

NOVC pair 564

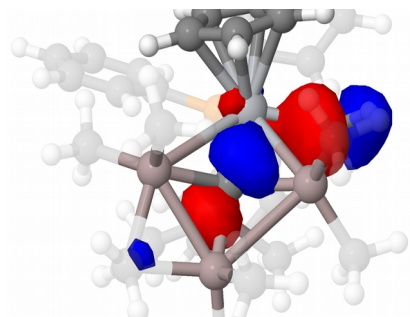


NOVC orbital 1127

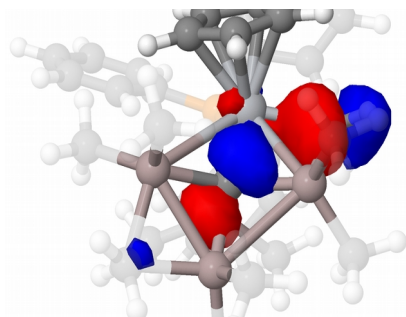


NOVC orbital 2252

NOVC pair 565:

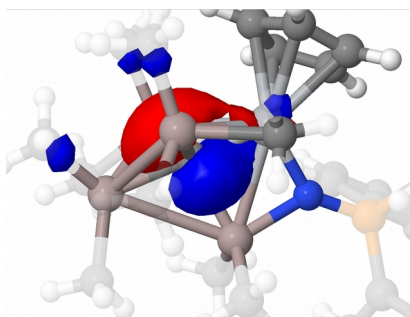


NOVC orbital 1128

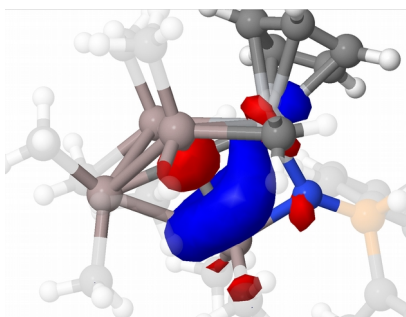


NOVC orbital 2251

NOVC pair 566:



NOVC orbital 1129

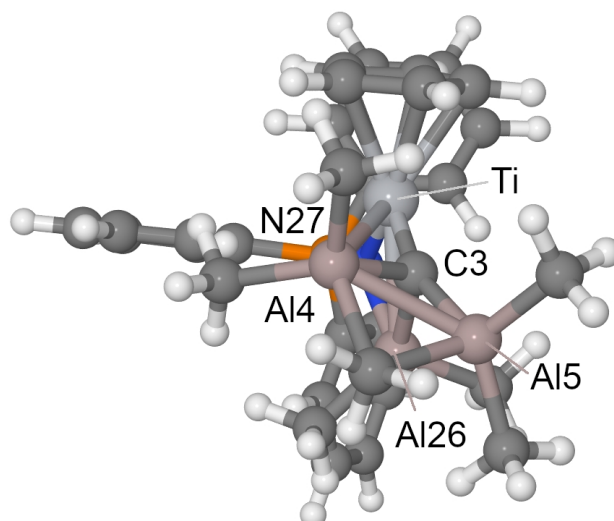


NOVC orbital 2250

Results of 3

Cartesian coordinates of 3 in Å

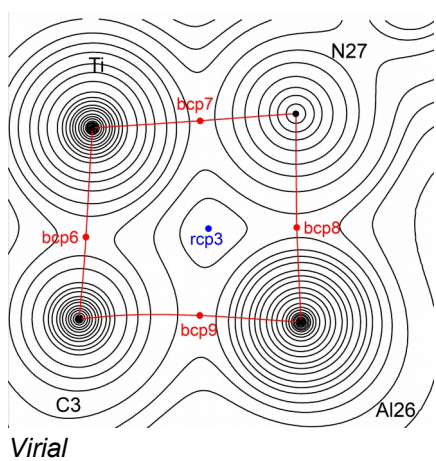
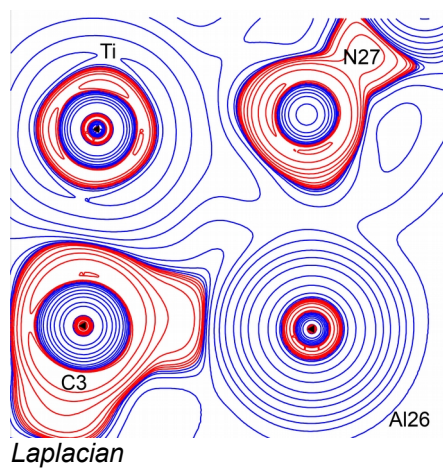
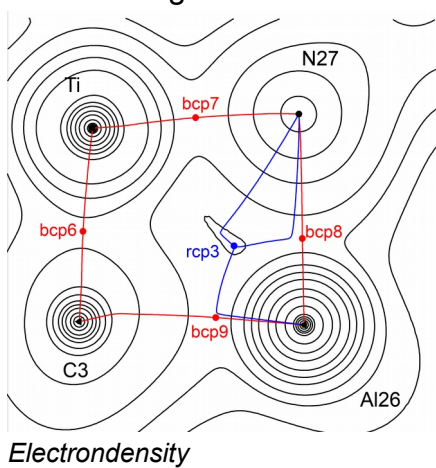
Ti	1.115823	1.055121	-0.365977
C	2.483167	-0.120251	-0.491571
Al	3.711336	0.161836	1.162213
Al	4.134883	-1.069025	-1.165574
C	3.964750	-2.953782	-1.743214
H	3.322209	-3.574811	-1.109348
H	4.965256	-3.406526	-1.723849
H	3.594665	-3.039677	-2.770521
C	5.330513	0.088871	-2.233231
H	5.628936	1.001866	-1.707767
H	4.824810	0.401356	-3.155734
H	6.248318	-0.430893	-2.535207
C	5.081522	-1.452783	0.799870
H	5.972927	-1.562503	0.166875
H	4.717857	-2.453240	1.050094
H	5.508574	-1.033235	1.721752
C	4.909607	1.746184	1.239218
H	5.408432	1.985756	0.294052
H	5.708911	1.531782	1.962018
H	4.423585	2.662534	1.593967
C	2.773565	-0.170613	2.882541
H	2.203190	-1.103479	2.905757
H	2.080904	0.651668	3.115292
H	3.492455	-0.198607	3.711719
Al	1.029465	-1.630859	-0.517074
N	-0.323588	-0.228290	-0.180909
P	-1.888826	-0.206248	0.098501
C	-2.238062	0.026309	1.862782
C	-1.170063	0.201633	2.739699
H	-0.153351	0.192346	2.359672
C	-1.407934	0.345399	4.101635
H	-0.570216	0.468028	4.779699
C	-2.709764	0.315566	4.585547
H	-2.895383	0.426117	5.648881
C	-3.778084	0.125323	3.712641
H	-4.792551	0.086378	4.095030
C	-3.545150	-0.029268	2.353643
H	-4.375771	-0.204037	1.675878
C	-2.733810	-1.749310	-0.345104
C	-3.840204	-1.791553	-1.192761
H	-4.240075	-0.877700	-1.617985
C	-4.430780	-3.012802	-1.498346
H	-5.288435	-3.043653	-2.161855
C	-3.920924	-4.188040	-0.961950
H	-4.379408	-5.139890	-1.208690
C	-2.822616	-4.146450	-0.108477
H	-2.420199	-5.061893	0.311317
C	-2.231975	-2.932393	0.204650



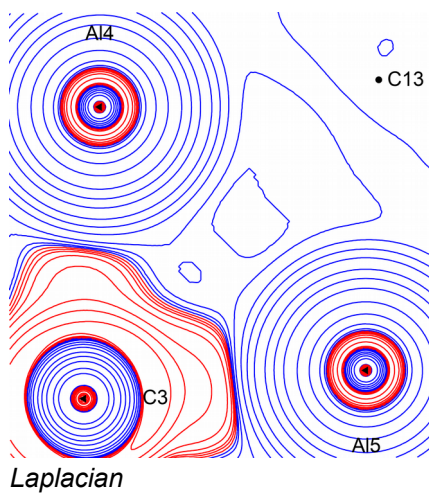
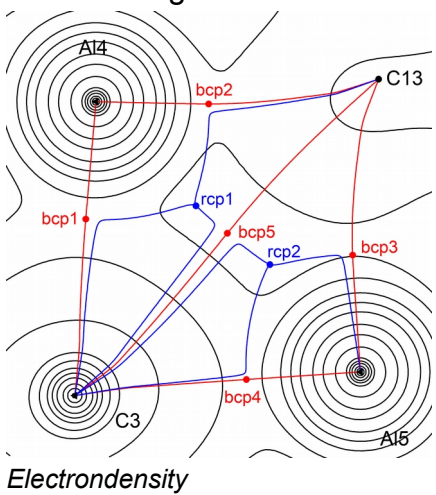
H	-1.372503	-2.907491	0.866399
C	-2.705205	1.118027	-0.835908
C	-2.542127	1.095419	-2.225702
H	-1.989084	0.284612	-2.691702
C	-3.065855	2.117565	-3.002686
H	-2.939484	2.095256	-4.079755
C	-3.740004	3.175618	-2.397586
H	-4.140410	3.980193	-3.005153
C	-3.891808	3.206621	-1.017062
H	-4.407698	4.035957	-0.545194
C	-3.379191	2.177548	-0.233287
H	-3.493057	2.208608	0.845089
C	0.586644	-2.333754	-2.315782
H	0.741947	-1.580224	-3.098659
H	-0.467698	-2.638201	-2.360782
H	1.188112	-3.207062	-2.586730
C	1.211713	-2.913796	0.987500
H	0.706987	-2.587821	1.905543
H	2.266298	-3.057002	1.247813
H	0.817109	-3.902429	0.720829
C	2.394191	3.015325	-0.641349
C	1.423089	3.007769	-1.665864
C	0.140033	3.150600	-1.070558
C	0.314129	3.209095	0.323925
H	-0.472646	3.286764	1.062551
C	1.705829	3.107221	0.592508
H	2.169651	3.116452	1.570047
H	-0.805956	3.177568	-1.593343
H	1.628111	2.917149	-2.724756
H	3.460693	2.907922	-0.764085

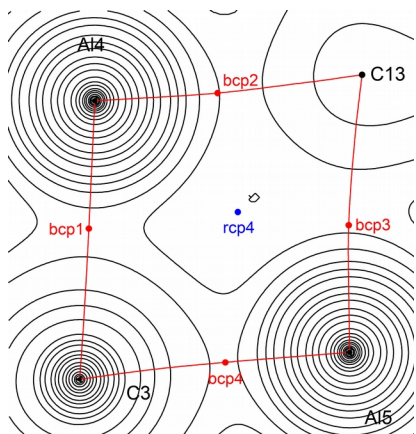
Bader:

Plane through Ti-C3-Al26:



Plane through C3-Al4-Al5:

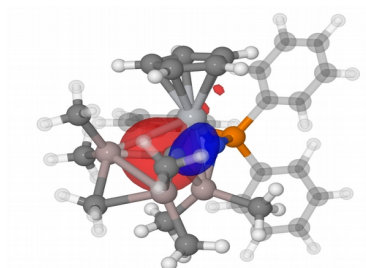




	$q(\mathbf{r})$	$\nabla^2 q(\mathbf{r})$
bcp1	0.05519	-0.05373
bcp2	0.05049	-0.04596
bcp3	0.04222	-0.03666
bcp4	0.06564	-0.06874
bcp5	0.03649	-0.00326
bcp6	0.17548	-0.04831
bcp7	0.11419	-0.10539
bcp8	0.05528	-0.08518
bcp9	0.05766	-0.05387
rcp1	0.03609	-0.00660
rcp2	0.03573	-0.00844
rcp3	0.03952	-0.01493
rcp4	0.03788	-0.00290

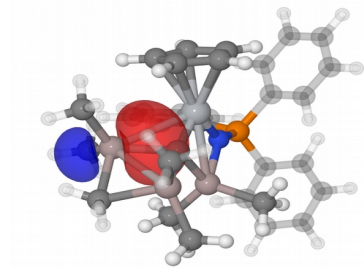
NBO:

Donororbital



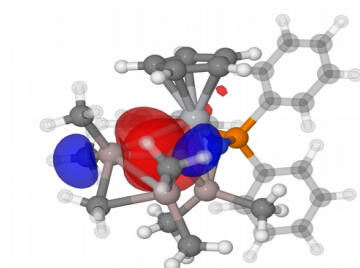
BD Ti 1 (29.64%) $sp^{0.05}d^{40.95}p^{0.03}$
C 2 (29.64%) $sp^{5.95}$

Acceptororbital

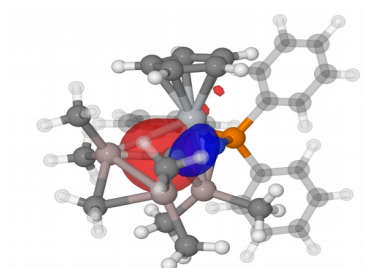


LV Al 3 $sp^{13.46}d^{0.11}$

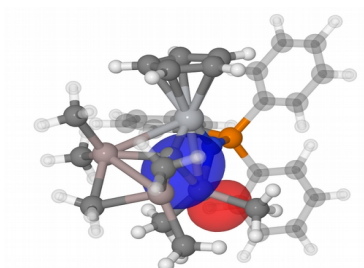
Overlaporbital



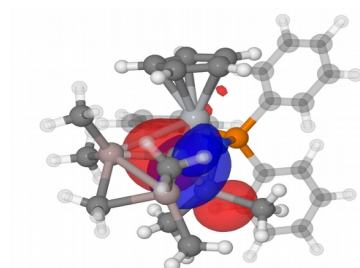
$E(2P) = 28.33 \text{ kcal/mol}$



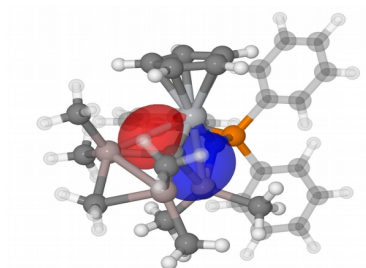
BD Ti 1 (29.64%) $sp^{0.05}d^{40.95}p^{0.03}$
C 2 (29.64%) $sp^{5.95}$



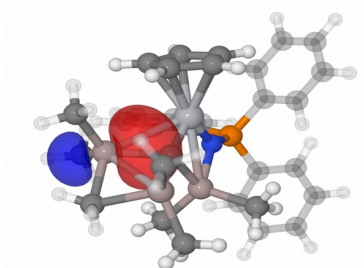
LV Al 25 $sp^{41.41}d^{0.45}$



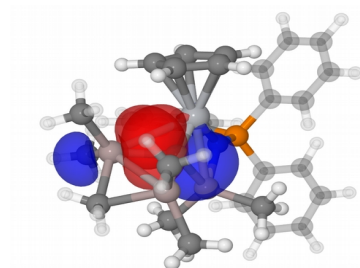
$E(2P) = 20.26 \text{ kcal/mol}$



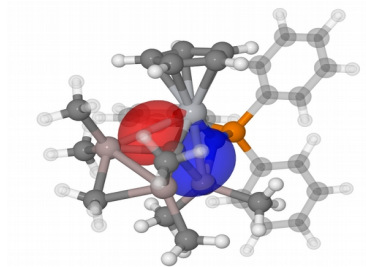
BD Ti 1 (25.38%) $sp^{0.05}d^{99.99}p^{0.11}$
C 2 (74.62%) $sp^{79.60}d^{0.15}$



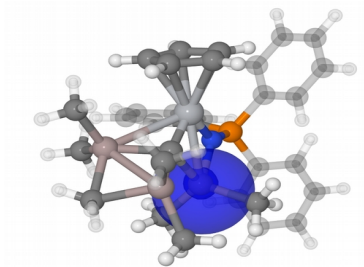
LV Al 3 $sp^{13.46}d^{0.11}$



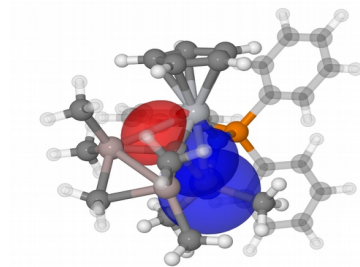
$E(2P) = 19.19 \text{ kcal/mol}$



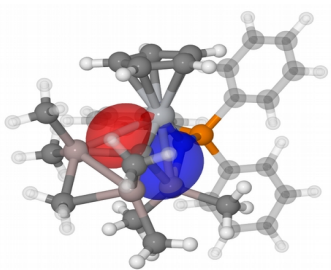
BD Ti 1 (25.38%) $sp^{0.05}d^{99.99}p^{0.11}$
C 2 (74.62%) $sp^{79.60}d^{0.15}$



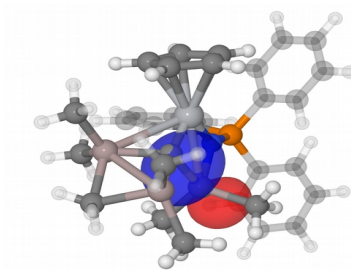
LV Al 25 $sp^{0.04}$



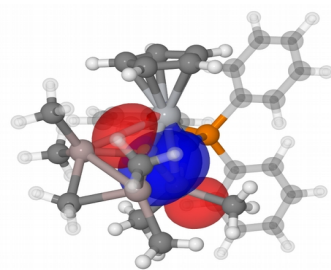
$E(2P) = 25.54 \text{ kcal/mol}$



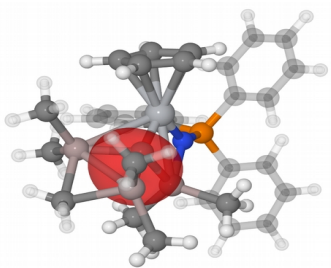
BD Ti 1 (25.38%) $sp^{0.05}d^{99.99}p^{0.11}$
C 2 (74.62%) $sp^{79.60}d^{0.15}$



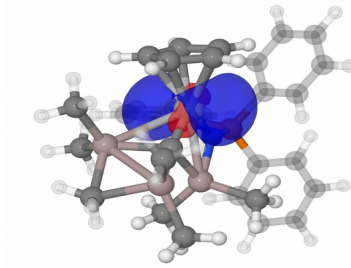
LV Al 25 $sp^{41.41}d^{0.45}$



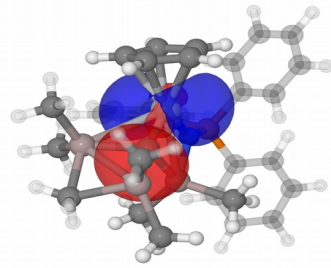
$E(2P) = 38.10 \text{ kcal/mol}$



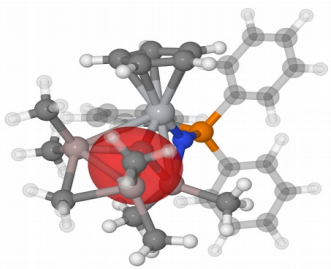
BD C 2 (84.59%) $sp^{0.84} -$
Al 4 (15.41%) $sp^{2.87}d^{0.05}$



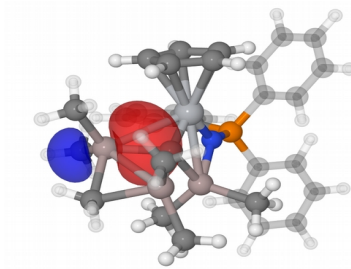
LV Ti 1 $sp^{0.01}d^{0.80}$



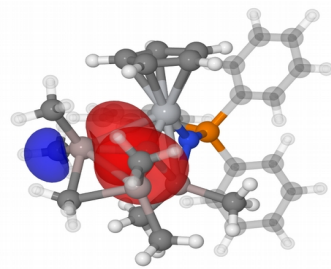
$E(2P) = 17.23 \text{ kcal/mol}$



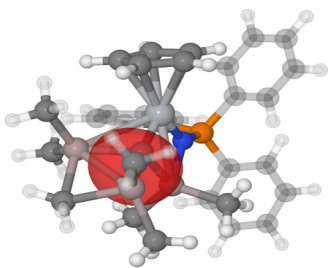
BD C 2 (84.59%) $sp^{0.84} -$
Al 4 (15.41%) $sp^{2.87}d^{0.05}$



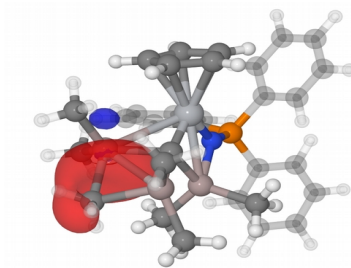
LV Al 3 $sp^{13.46}d^{0.11}$



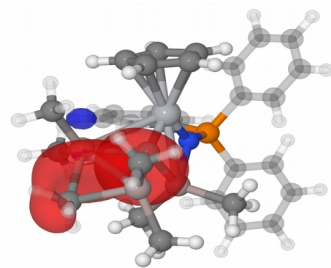
$E(2P) = 51.82 \text{ kcal/mol}$



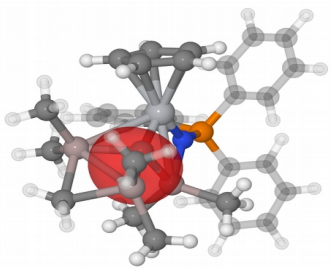
BD C 2 (84.59%) $sp^{0.84} -$
Al 4 (15.41%) $sp^{2.87}d^{0.05}$



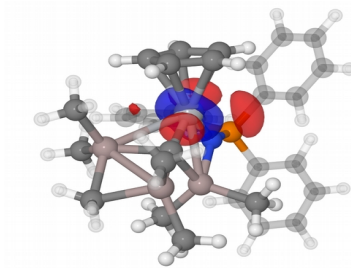
BD* Al 3 (87.45%) $sp^{3.59}d^{0.08} -$
C 13 (12.55%) $sp^{2.21}$



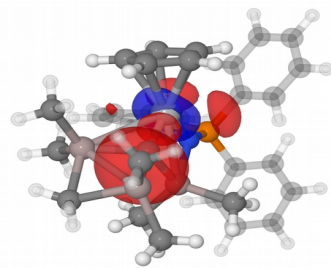
$E(2P) = 15.22 \text{ kcal/mol}$



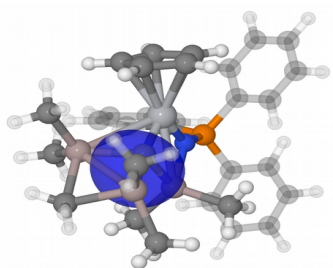
BD C 2 (84.59%) $sp^{0.84} -$
Al 4 (15.41%) $sp^{2.87}d^{0.05}$



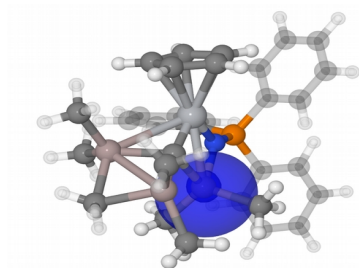
RY Ti 1 $sp^{0.18}d^{15.03}p^{0.03}$



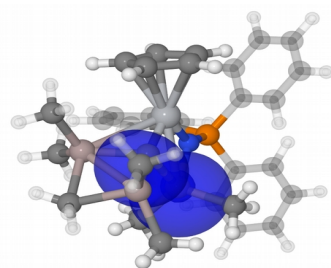
$E(2P) = 16.21 \text{ kcal/mol}$



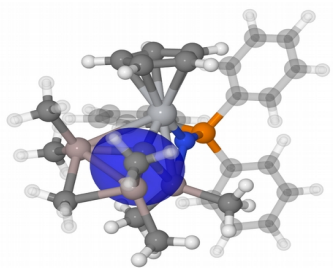
BD C 2 (84.59%) $sp^{0.84}$ –
Al 4 (15.41%) $sp^{2.87}d^{0.05}$



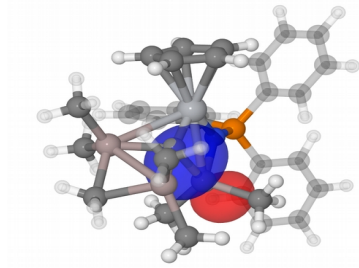
LV Al 25 $sp^{0.04}$



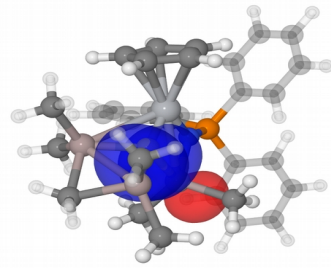
$E(2P) = 5.22$ kcal/mol



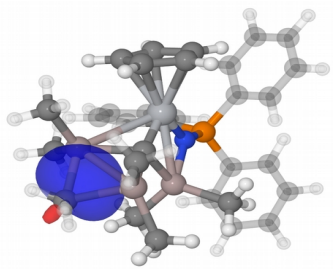
BD C 2 (84.59%) $sp^{0.84}$ –
Al 4 (15.41%) $sp^{2.87}d^{0.05}$



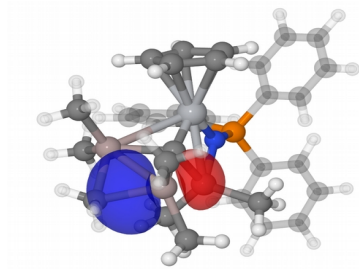
LV Al 25 $sp^{41.41}d^{0.45}$



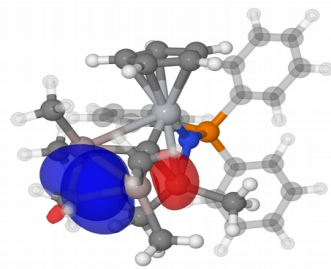
$E(2P) = 23.50$ kcal/mol



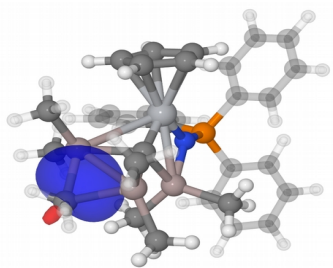
BD Al 3 (12.55%) $sp^{3.59}d^{0.08}$ –
C 13 (87.45%) $sp^{2.21}$



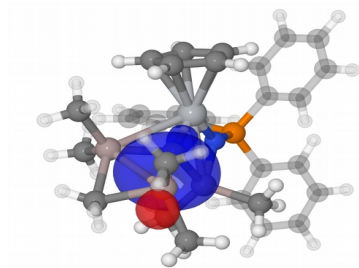
LV Al 4 $sp^{21.41}d^{0.30}$



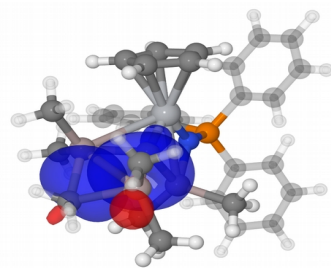
$E(2P) = 67.61$ kcal/mol



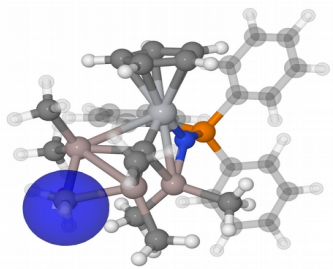
BD Al 3 (12.55%) $sp^{3.59}d^{0.08}$ –
C 13 (87.45%) $sp^{2.21}$



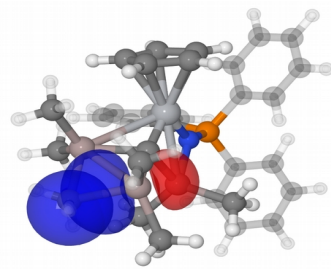
BD* C 2 (15.41%) $sp^{0.84}$ –
Al 4 (84.59%) $sp^{2.87}d^{0.05}$



$E(2P) = 11.30$ kcal/mol



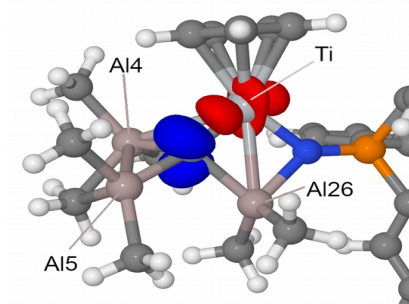
LV Al 4 $sp^{21.41}d^{0.30}$



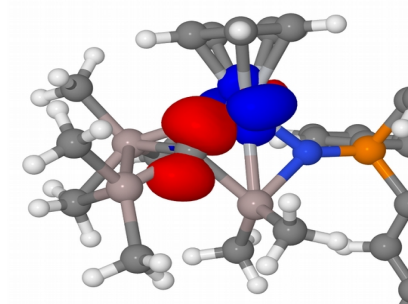
$E(2P) = 13.61$ kcal/mol

Note: For the NBO the atomic numbers from the output file were used. They are not the same as the one in the manuscript.

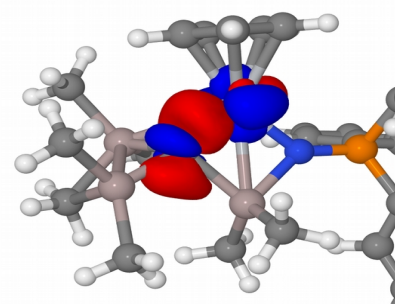
ETS-NOVC



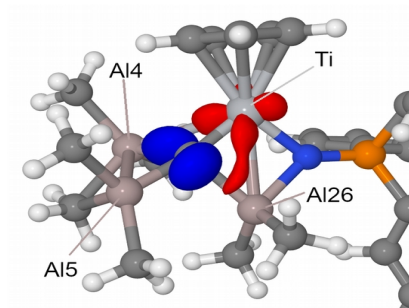
NOCV pair 1



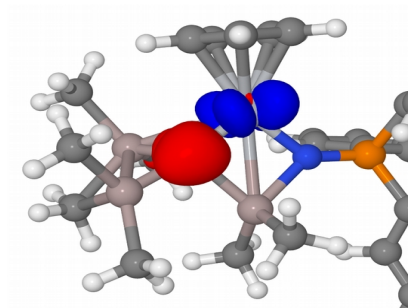
NOCV pair 495



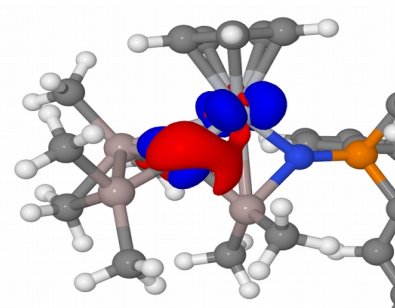
NOCV pair 1,495



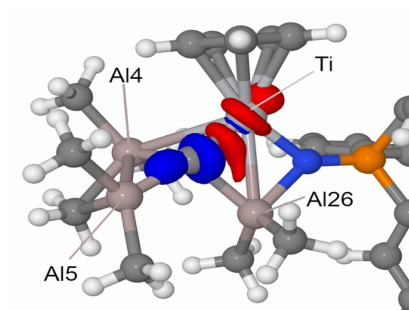
NOCV pair 2



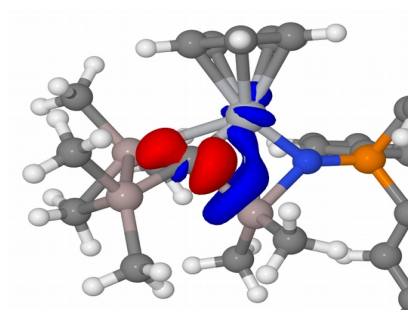
NOCV pair 496



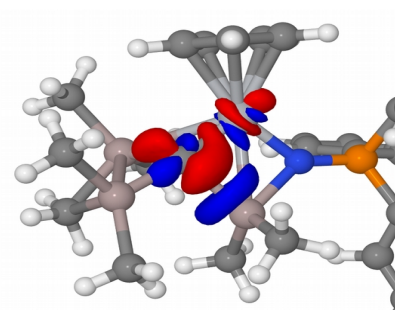
NOCV pair 2,496



NOCV pair 3



NOCV pair 497



NOCV pair 3,497

----- Pair and NOCV orbital information -----

There are totally 988 NOCV pairs and 1976 NOCV orbitals

NOCV orbitals with absolute eigenvalues smaller than 5.0E-02 are not shown

Note: All energies are given in kcal/mol

----- Alpha NOCV orbitals -----

Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1	-49.55	1	0.52800	-102.70	988	-0.52800	-8.86
2	-37.00	2	0.42800	-103.03	987	-0.42800	-16.57
3	-43.28	3	0.40667	-103.04	986	-0.40667	3.39
4	-3.74	4	0.11505	-105.32	985	-0.11505	-72.85
5	-3.49	5	0.10704	-98.32	984	-0.10704	-65.70
6	-1.04	6	0.06685	-111.59	983	-0.06685	-96.03
7	-0.99	7	0.05648	-54.06	982	-0.05648	-36.46

----- Beta NOCV orbitals -----

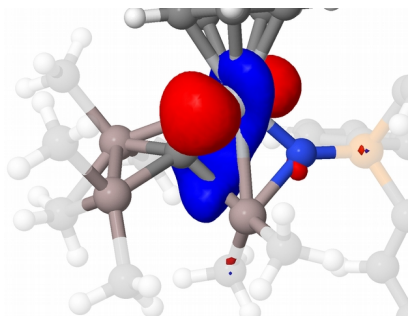
Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
495	-121.65	989	0.98796	-155.20	1976	-0.98796	-32.07
496	-81.28	990	0.78648	-130.89	1975	-0.78648	-27.54
497	-110.55	991	0.59360	-105.46	1974	-0.59360	80.77
498	-2.55	992	0.08915	-121.43	1973	-0.08915	-92.85
499	-1.13	993	0.07697	-94.11	1972	-0.07697	-79.39
500	-0.97	994	0.05341	-36.82	1971	-0.05341	-18.69

Sum of NOCV eigenvalues: Alpha= 0.00001 Beta= 0.00001

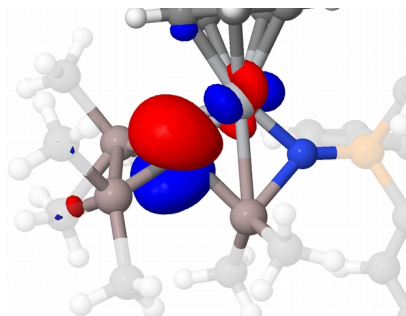
Sum of pair energies: Alpha= -139.10 Beta= -318.13 Total= -457.22

NOVC orbitals

NOVC pair 1:

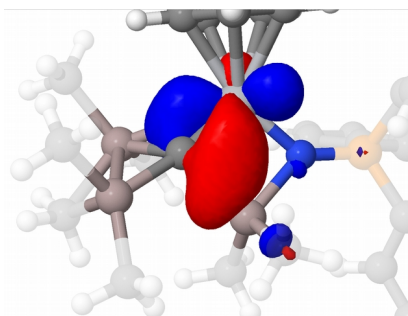


NOVC orbital 1

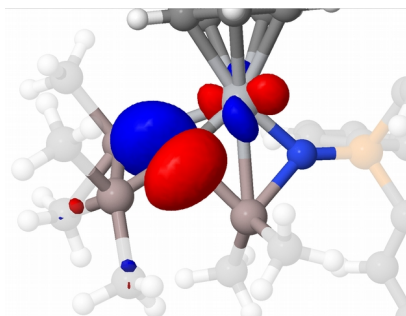


NOVC orbital 988

NOVC pair 2:

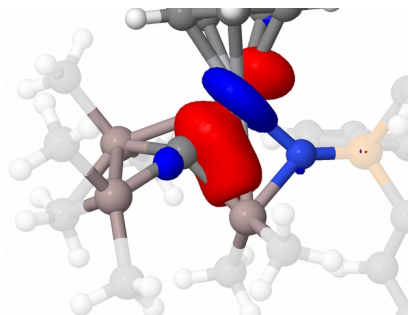


NOVC orbital 2

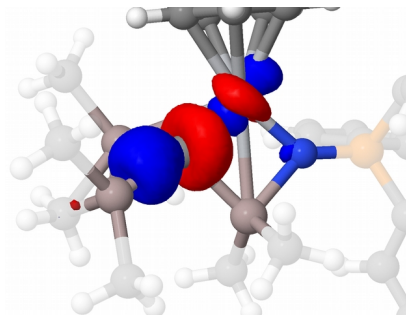


NOVC orbital 987

NOVC pair 3:

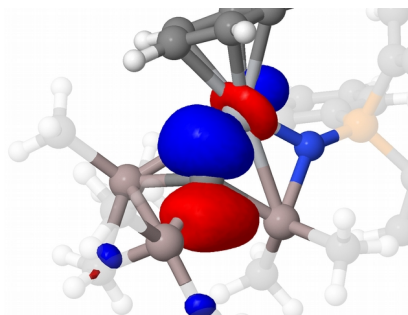


NOVC orbital 3

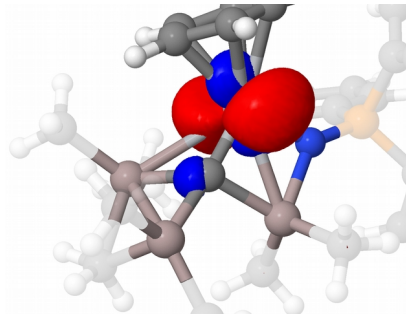


NOVC orbital 986

NOVC pair 495:

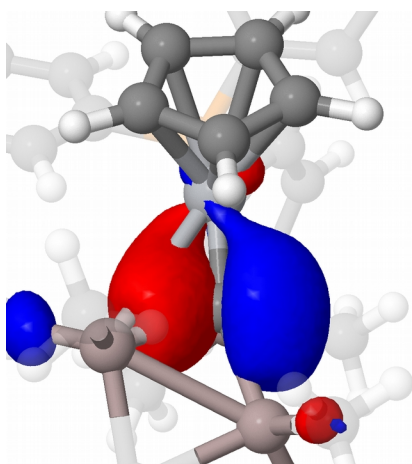


NOVC orbital 989

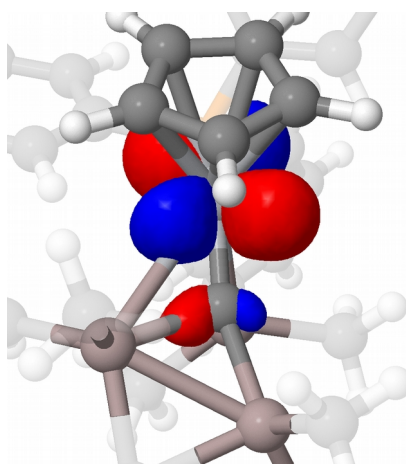


NOVC orbital 1976

NOVC pair 496:

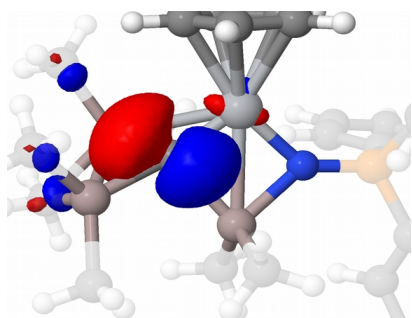


NOVC orbital 990

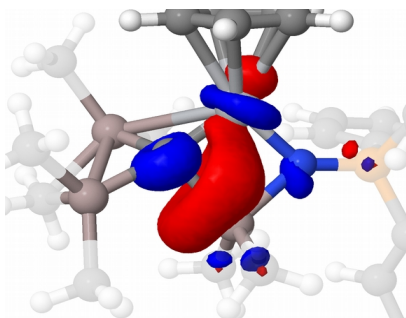


NOVC orbital 1975

NOVC pair 497:



NOVC orbital 991

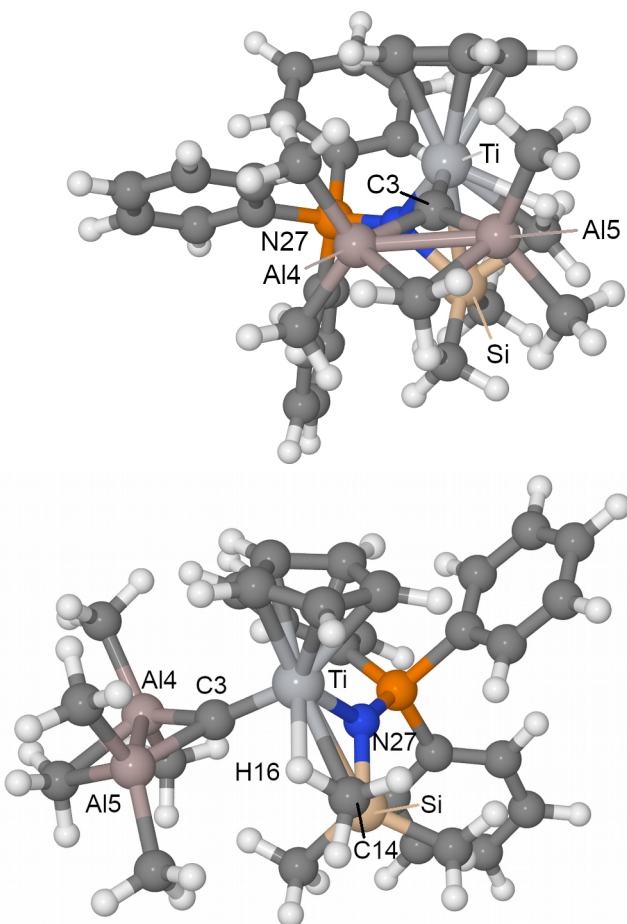


NOVC orbital 1974

Results of 4

Cartesian coordinates of 4 in Å

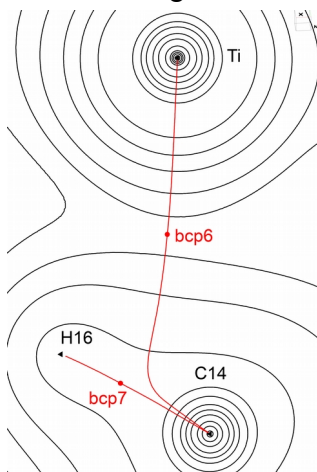
Al	-2.781113	1.170626	1.911893
C	-2.530138	0.348993	0.110090
Ti	-1.508293	-0.793642	-0.749521
N	0.386912	0.154046	-0.708043
Si	-0.118352	1.329646	-1.911172
C	1.210227	1.601102	-3.218332
H	1.597819	0.665904	-3.632467
H	2.051836	2.169194	-2.813258
H	0.786904	2.182235	-4.044568
C	-0.652732	2.980549	-1.238525
H	-1.285335	2.826819	-0.364203
H	-1.225805	3.530331	-1.991510
H	0.213429	3.589476	-0.963602
C	-1.505994	0.441689	-2.903275
H	-1.129263	-0.283616	-3.629240
H	-2.433237	0.070053	-2.419083
H	-1.930247	1.281028	-3.466363
P	1.779840	-0.096255	0.011838
C	1.668316	-0.169649	1.817049
C	0.455027	-0.457970	2.437264
H	-0.446309	-0.595405	1.846603
C	0.381510	-0.515210	3.823171
H	-0.574942	-0.708415	4.295046
C	1.517686	-0.292953	4.590484
H	1.454707	-0.330650	5.672956
C	2.731190	-0.000658	3.975796
H	3.614974	0.190504	4.575126
C	2.808943	0.067946	2.591998
H	3.749494	0.327272	2.115256
C	2.974071	1.225156	-0.324978
C	4.097851	1.020401	-1.123210
H	4.317608	0.030650	-1.509018
C	4.929637	2.090237	-1.433099
H	5.801169	1.930524	-2.058646
C	4.641044	3.359367	-0.946865
H	5.288969	4.193789	-1.194100
C	3.527043	3.563164	-0.137275
H	3.306343	4.552245	0.249280
C	2.694021	2.499534	0.178950
H	1.825972	2.656738	0.813169
C	2.559824	-1.646028	-0.535528
C	2.389827	-2.013835	-1.871443
H	1.774453	-1.398427	-2.518937
C	2.980224	-3.172575	-2.355773
H	2.842341	-3.456531	-3.393731
C	3.734195	-3.975035	-1.505760
H	4.186800	-4.886360	-1.882048
C	3.897885	-3.616989	-0.172777



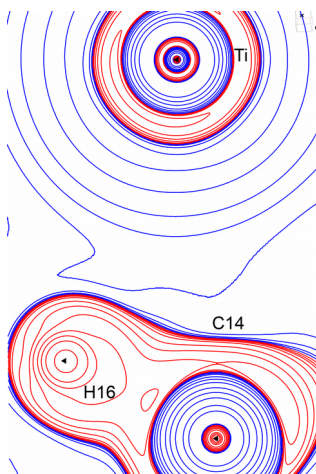
H	4.474999	-4.249030	0.493599
C	3.314138	-2.453937	0.315176
H	3.432238	-2.186480	1.359746
C	-2.889651	-2.663271	-0.447440
C	-2.292587	-2.838463	-1.719125
C	-0.906468	-3.053291	-1.537120
C	-0.642869	-2.984368	-0.153530
H	0.326486	-3.104564	0.311589
C	-1.867363	-2.746545	0.522617
H	-2.008165	-2.644481	1.589144
H	-0.174892	-3.218759	-2.315061
H	-2.813573	-2.821401	-2.668115
H	-3.933387	-2.468913	-0.249715
Al	-4.384190	1.072506	-0.171398
C	-4.442553	2.444347	-1.605602
H	-3.594959	3.135285	-1.536634
H	-5.358671	3.046621	-1.558630
H	-4.418579	1.991959	-2.605828
C	-5.829082	-0.284484	-0.126875
H	-5.741409	-0.935324	0.752186
H	-5.788583	-0.932114	-1.012956
H	-6.834007	0.155862	-0.105421
C	-4.608079	2.331178	1.617001
H	-5.675572	2.164727	1.411904
H	-4.368779	3.351964	1.303868
H	-4.584469	2.321116	2.717106
C	-3.251944	-0.191252	3.287474
H	-4.239929	-0.620732	3.079513
H	-3.283656	0.215071	4.307041
H	-2.549473	-1.034084	3.295207
C	-1.468595	2.576598	2.429599
H	-1.599973	3.505256	1.861954
H	-0.437683	2.238528	2.267023
H	-1.557146	2.833425	3.492816

Bader:

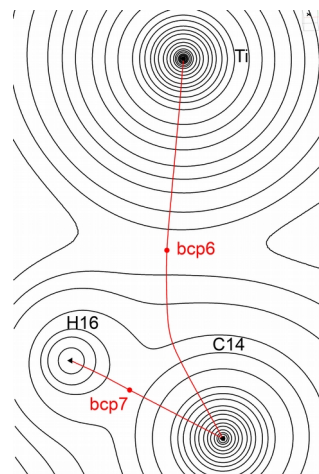
Plane through Ti-C14-H16:



Electron density

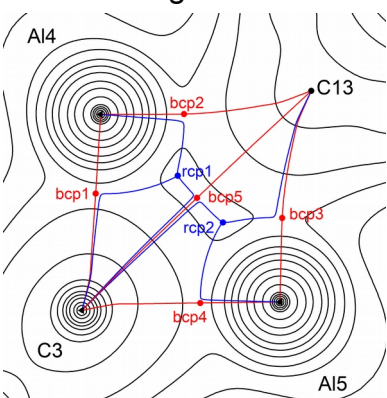


Laplacian

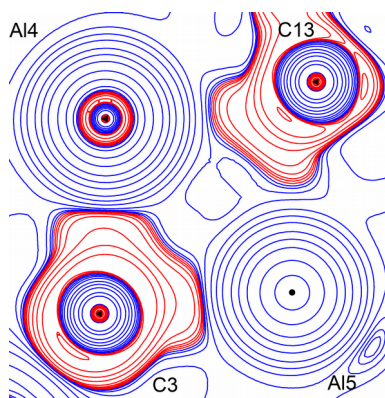


Virial

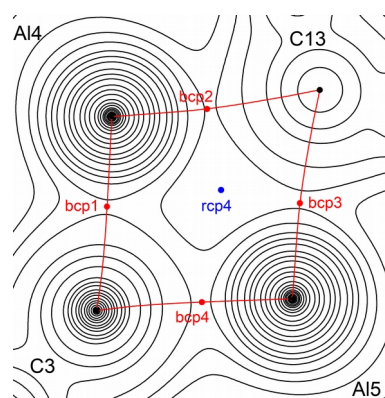
Plane through Ti-C3-Al26:



Electron density



Laplacian

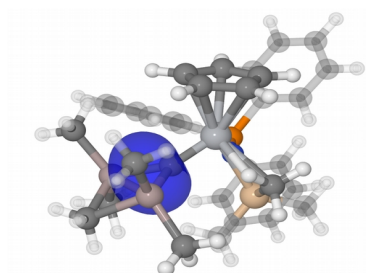


Virial

	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$
bcp1	0.06491	-0.06743
bcp2	0.06721	-0.07085
bcp3	0.04627	-0.04168
bcp4	0.04472	-0.03930
bcp5	0.03812	-0.00203
bcp6	0.03384	-0.03838
bcp7	0.25565	0.19904
rcp1	0.03751	-0.00802
rcp2	0.03715	-0.00855
rcp4	0.03979	-0.00255

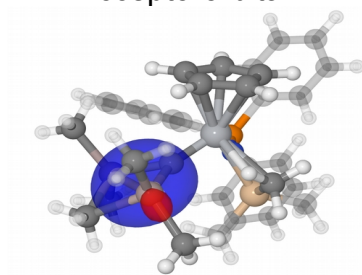
NBO:

Donororbital



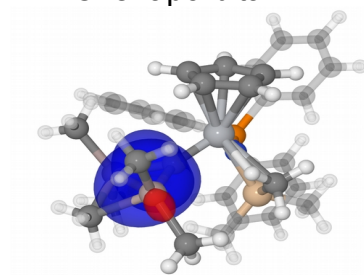
BD Al 1 (15.56%) $sp^{3.44}d^{0.07}$ –
C 2 (84.44%) $sp^{0.86}$

Acceptororbital

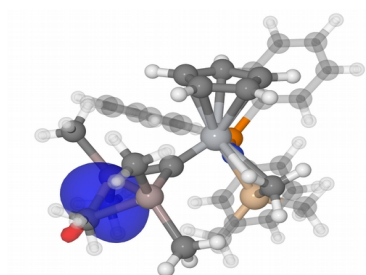


LV Al 62 $sp^{3.78}d^{0.06}$

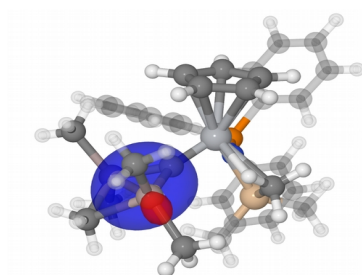
Overlaporbital



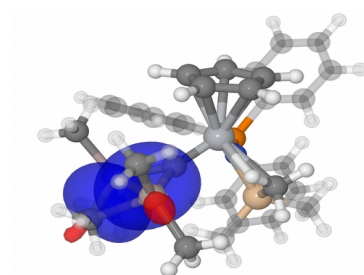
$E(2P) = 109.77 \text{ kcal/mol}$



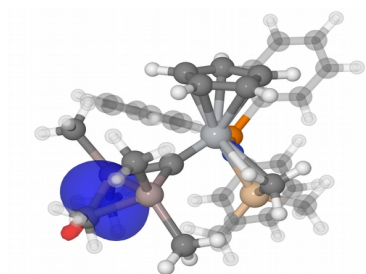
BD Al 1 (11.05%) $sp^{6.16}d^{0.15}$ –
C 71 (88.95%) $sp^{2.15}$



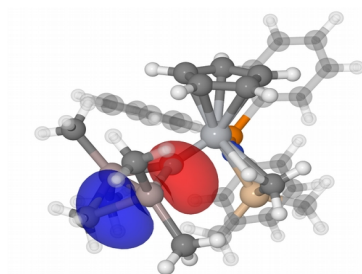
LV Al 62 $sp^{3.78}d^{0.06}$



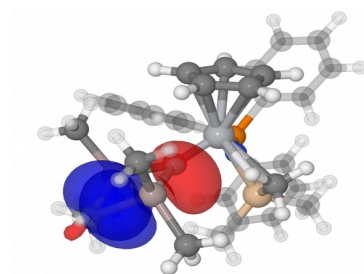
$E(2P) = 44.56 \text{ kcal/mol}$



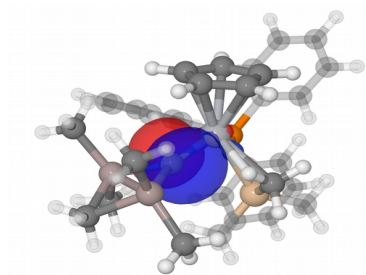
BD Al 1 (11.05%) $sp^{6.16}d^{0.15}$ –
C 71 (88.95%) $sp^{2.15}$



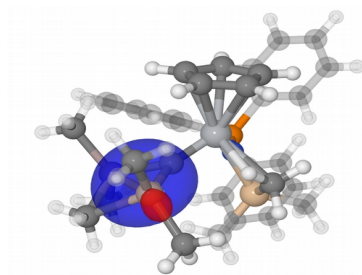
LV Al 62 $sp^{99.99}d^{3.15}$



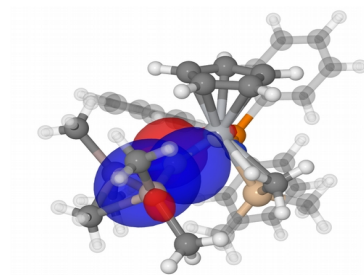
$E(2P) = 39.08 \text{ kcal/mol}$



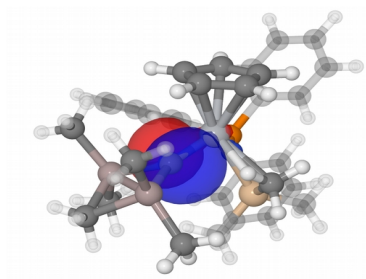
BD C 2 (70.90%) $sp^{85.57}$ –
Ti 3 (29.10%) $sp^{1.72}d^{99.99}$



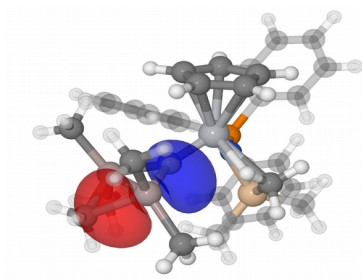
LV Al 62 $sp^{3.78}d^{0.06}$



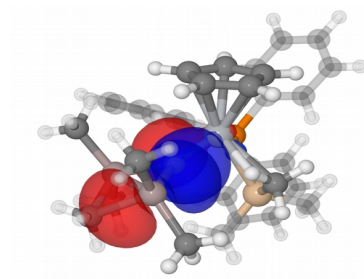
$E(2P) = 24.31 \text{ kcal/mol}$



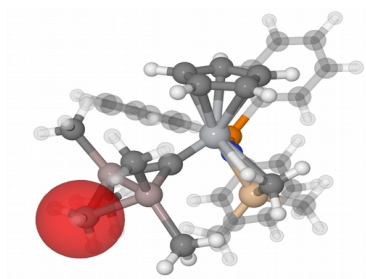
*BD C 2 (70.90%) $sp^{85.57}$ –
Ti 3 (29.10%) $sp^{1.72}d^{99.99}$*



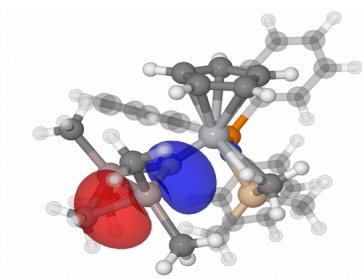
LV Al 62 $sp^{99.99}d^{3.15}$



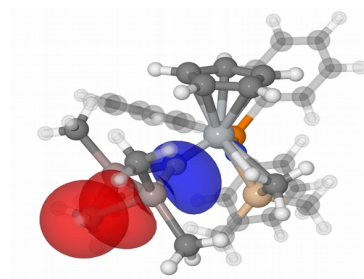
$E(2P) = 14.79 \text{ kcal/mol}$



*BD C 71 (63.66%) $sp^{3.07}$ –
H 72 (36.34%) s*

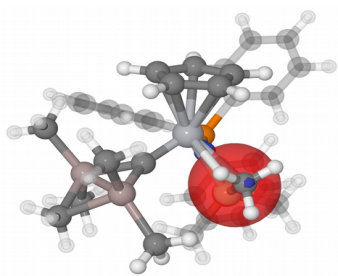


LV Al 62 $sp^{99.99}d^{3.15}$

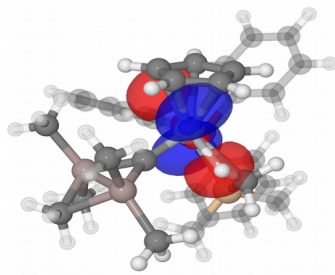


$E(2P) = 13.34 \text{ kcal/mol}$

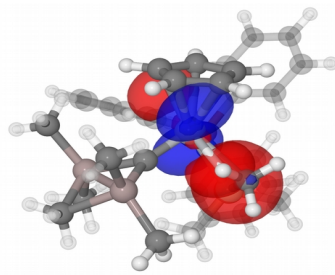
NBO agostic interactions



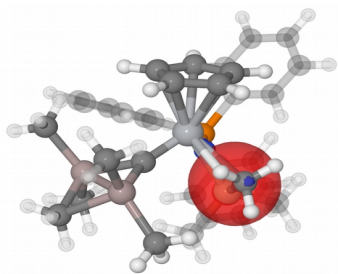
BD Si 5 (24.44%) $sp^{3.34}d^{0.09}$ –
C 14 (75.56%) $sp^{2.23}$



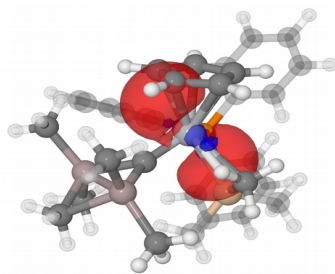
LV Ti 3 $sp^{0.28}d^{99.99}p^{0.19}$



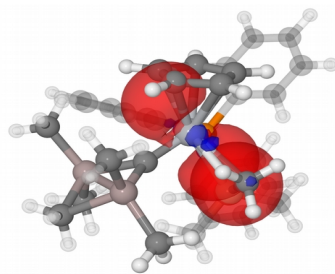
$E(2P) = 16.10$ kcal/mol



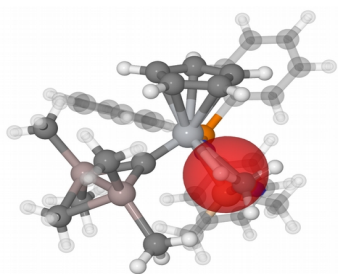
BD Si 5 (24.44%) $sp^{3.34}d^{0.09}$ –
C 14 (75.56%) $sp^{2.23}$



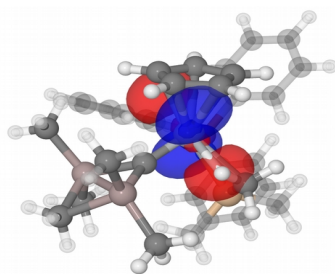
LV Ti 3 $sd^{4.33}$



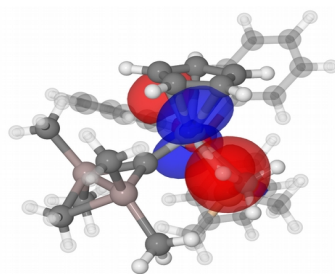
$E(2P) = 24.98$ kcal/mol



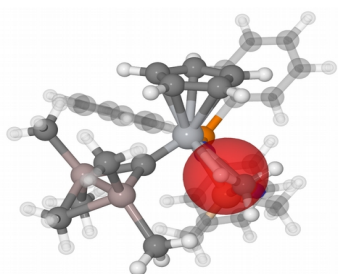
BD C 14 (62.62%) $sp^{3.12}$ –
H 16 (37.38%) s



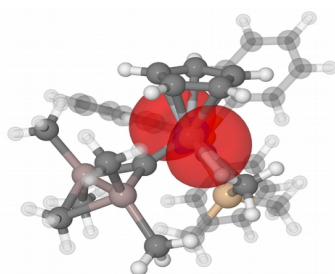
LV Ti 3 $sp^{0.28}d^{99.99}p^{0.19}$



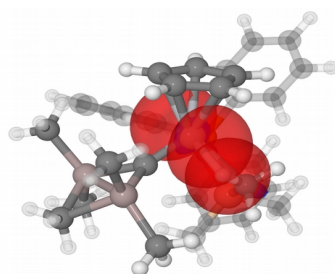
$E(2P) = 18.73$ kcal/mol



BD C 14 (62.62%) $sp^{3.12}$ –
H 16 (37.38%) s

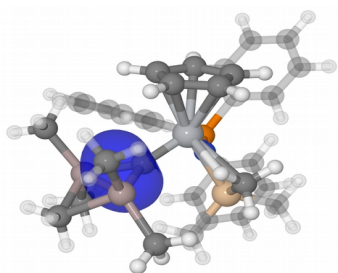


LV Ti 3 $sd^{0.32}$

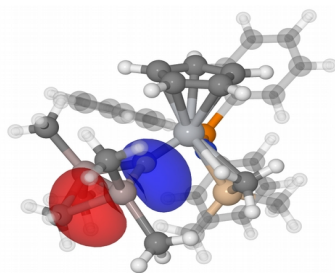


$E(2P) = 13.07$ kcal/mol

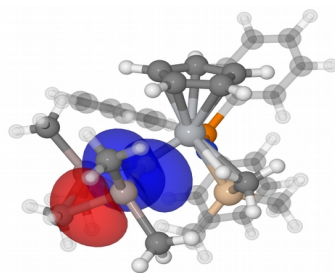
NBO with less than 10 kcal/mol



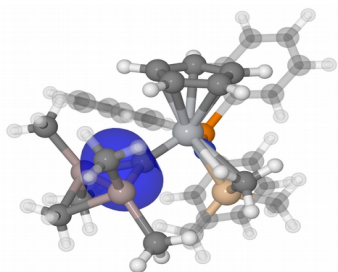
BD Al 1 (15.56%) $sp^{3.44}d^{0.07}$ –
C 2 (84.44%) $sp^{0.86}$



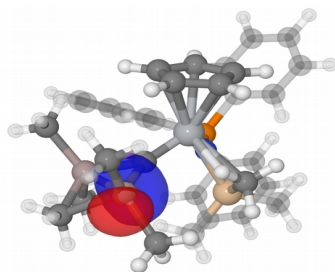
LV Al 62 $sp^{99.99}d^{3.15}$



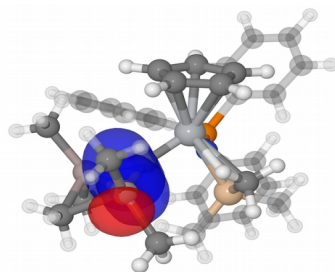
$E(2P) = 7.24$ kcal/mol



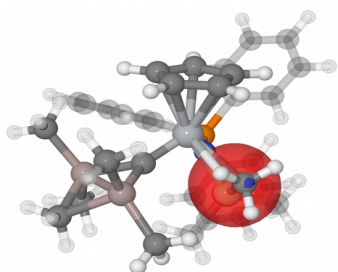
BD Al 1 (15.56%) $sp^{3.44}d^{0.07}$ –
C 2 (84.44%) $sp^{0.86}$



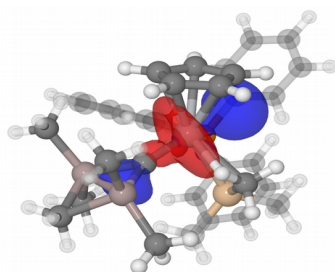
RY Al 62 $sp^{3.38}d^{0.86}$



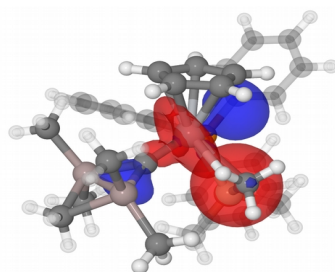
$E(2P) = 5.61$ kcal/mol



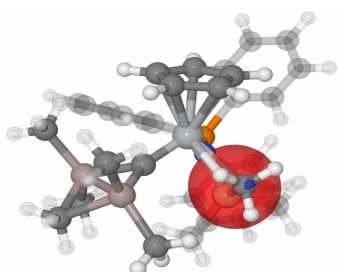
BD Si 5 (24.44%) $sp^{3.34}d^{0.09}$ –
C 14 (75.56%) $sp^{2.23}$



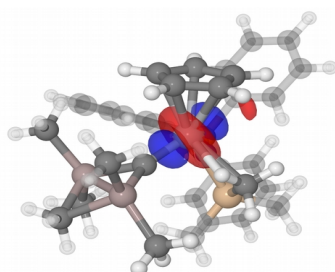
BD* C 2 (33.90%) $sp^{1.32}$ –
Ti 3 (66.10%) $sp^{0.02}d^{21.51}p^{0.01}$



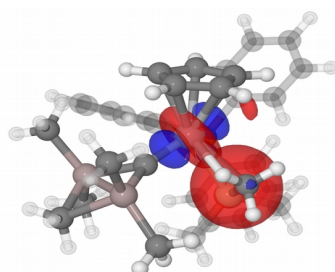
$E(2P) = 3.49$ kcal/mol



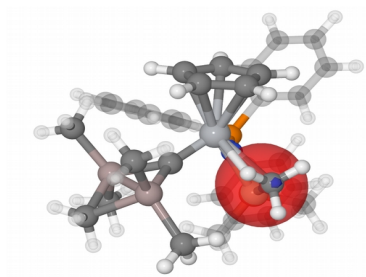
BD Si 5 (24.44%) $sp^{3.34}d^{0.09}$ –
C 14 (75.56%) $sp^{2.23}$



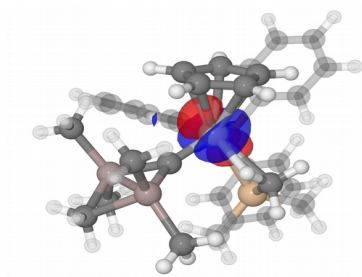
RY Ti 3 $sp^{4.03}d^{99.99}p^{0.37}$



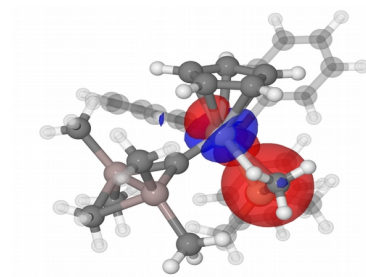
$E(2P) = 4.53$ kcal/mol



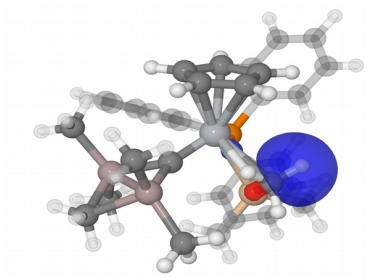
BD Si 5 (24.44%) $sp^{3.34}d^{0.09}$ –
C 14 (75.56%) $sp^{2.23}$



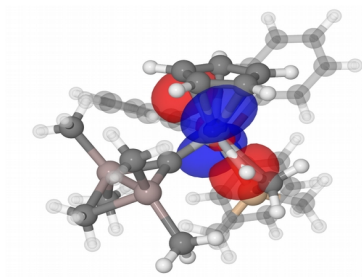
RY Ti 3 $sp^{9.40}d^{69.54}f^{1.29}$



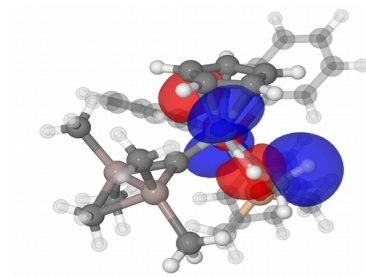
$E(2P) = 7.81 \text{ kcal/mol}$



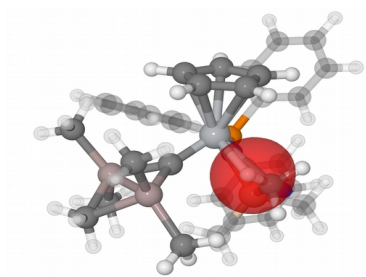
BD C 14 (63.25%) $sp^{3.15}$ –
H 15 (36.75%) s



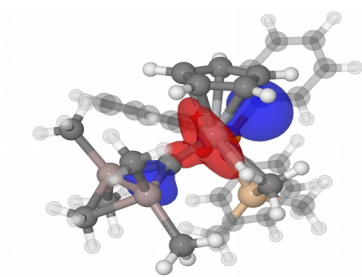
LV Ti 3 $sp^{0.28}d^{99.99}f^{0.19}$



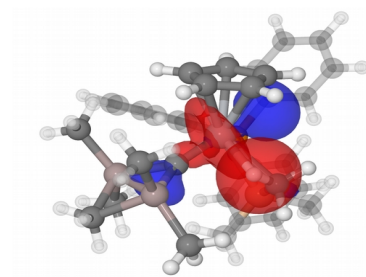
$E(2P) = 3.16 \text{ kcal/mol}$



BD C 14 (62.62%) $sp^{3.12}$ –
H 16 (37.38%) s

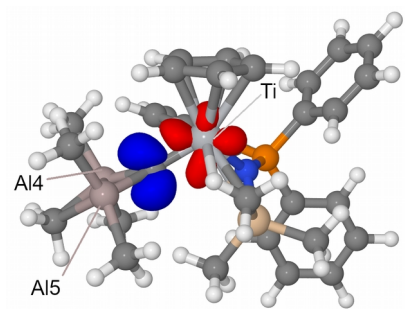


BD* C 2 (33.90%) $sp^{1.32}$ –
Ti 3 (66.10%) $sp^{0.02}d^{21.51}f^{0.01}$

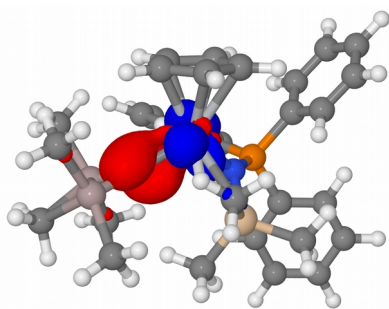


$E(2P) = 3.67 \text{ kcal/mol}$

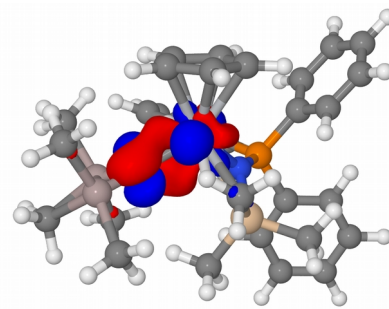
ETS-NOVC



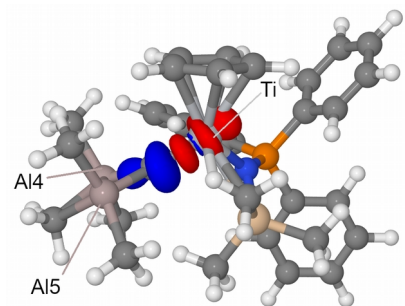
NOVC pair 1



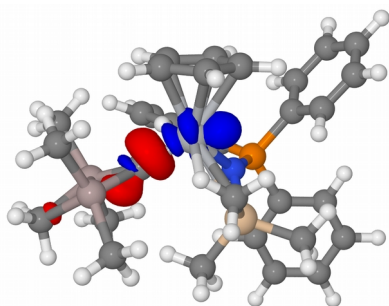
NOVC pair 514



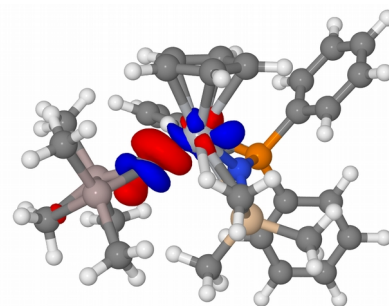
NOVC pair 1,514



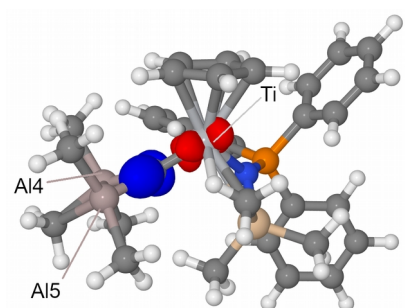
NOVC pair 2



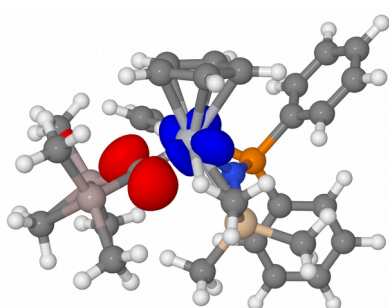
NOVC pair 516



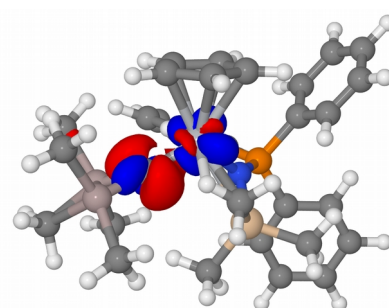
NOVC pair 2,516



NOVC pair 3



NOVC pair 515



NOVC pair 3,515

----- Pair and NOCV orbital information -----

There are totally 1026 NOCV pairs and 2050 NOCV orbitals

NOCV orbitals with absolute eigenvalues smaller than 5.0E-02 are not shown

Note: All energies are given in kcal/mol

----- Alpha NOCV orbitals -----

Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1	-51.46	1	0.57921	-81.98	1025	-0.57921	6.86
2	-47.38	2	0.44254	-87.29	1024	-0.44254	19.78
3	-32.02	3	0.42733	-83.44	1023	-0.42733	-8.51
4	-1.92	4	0.08620	-85.75	1022	-0.08620	-63.48
5	-2.54	5	0.08309	-73.62	1021	-0.08309	-43.09
6	-1.04	6	0.06249	-82.44	1020	-0.06249	-65.72

----- Beta NOCV orbitals -----

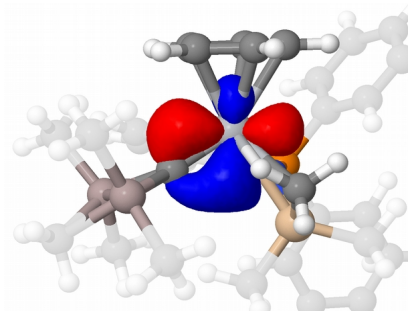
Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
514	-89.83	1026	0.94282	-118.28	2050	-0.94282	-23.00
515	-75.69	1027	0.71583	-102.15	2049	-0.71583	3.59
516	-116.66	1028	0.68025	-98.83	2048	-0.68025	72.66
517	-1.27	1029	0.06855	-70.74	2047	-0.06855	-52.16
518	-1.14	1030	0.06006	-61.74	2046	-0.06006	-42.78
519	-0.75	1031	0.05556	-59.79	2045	-0.05556	-46.30

Sum of NOCV eigenvalues: Alpha= -0.00000 Beta= -0.00000

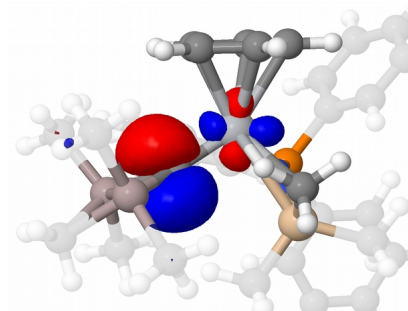
Sum of pair energies: Alpha= -136.36 Beta= -285.34 Total= -421.70

NOVC Orbitals

NOVC pair 1:

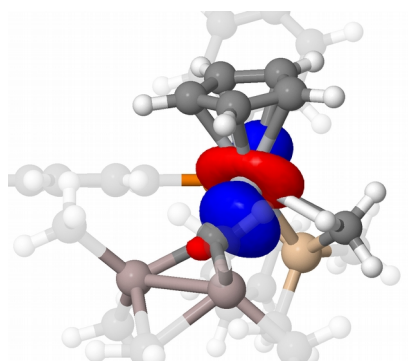


NOVC orbital 1

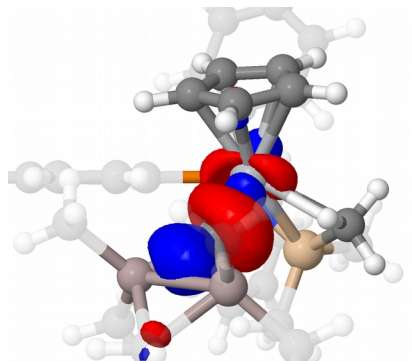


NOVC orbital 1025

NOVC pair 2:

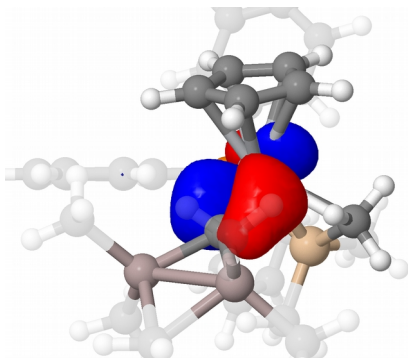


NOVC orbital 2

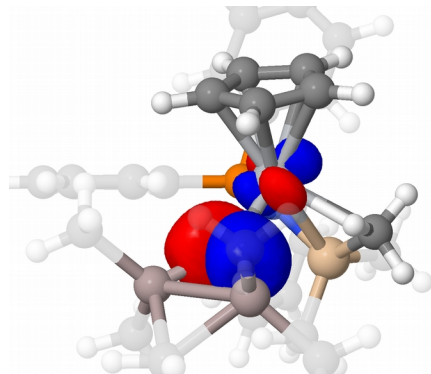


NOVC orbital 1024

NOVC pair 3:

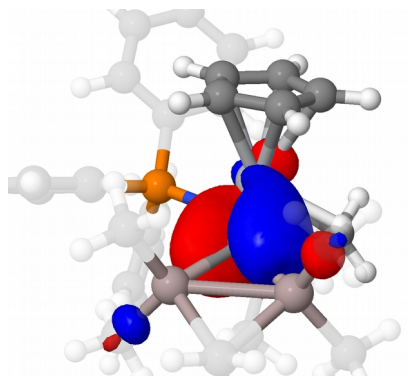


NOVC orbital 3

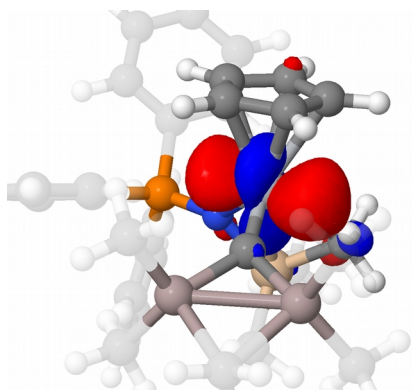


NOVC orbital 1023

NOVC pair 514:

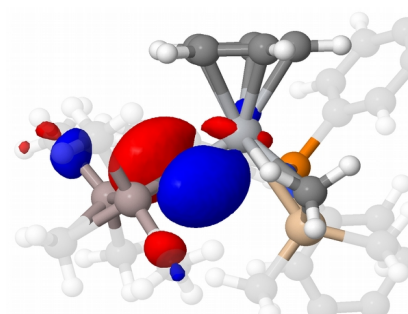


NOVC orbital 1026

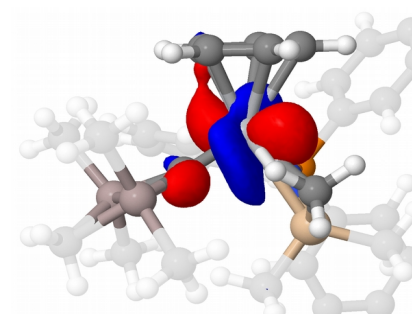


NOVC orbital 2050

NOVC pair 515:

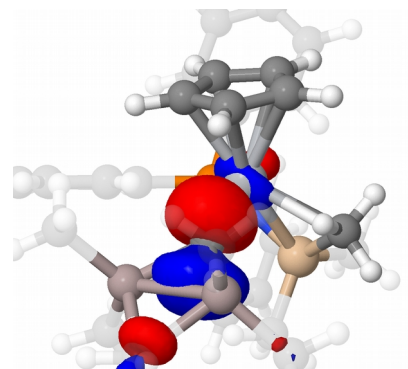


NOVC orbital 1027

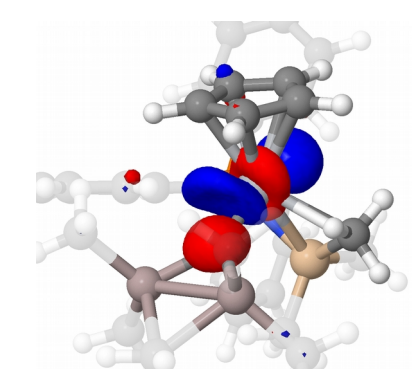


NOVC orbital 2049

NOVC pair 516:



NOVC orbital 1028

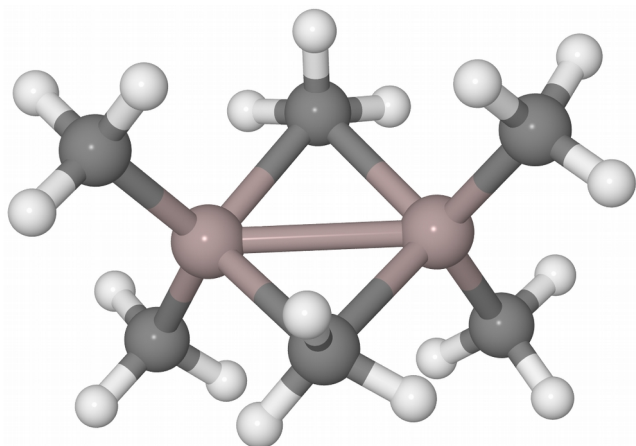


NOVC orbital 2048

Results of Al_2Me_6

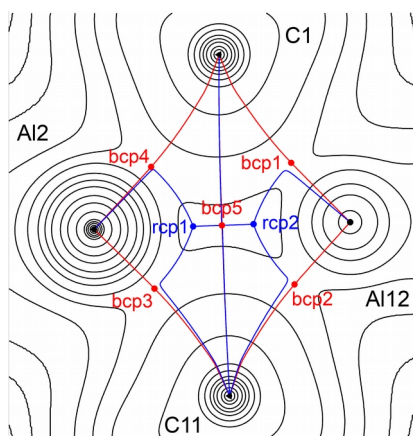
Cartesian coordinates of Al_2Me_6 in Å

C	-0.036894	-0.692379	1.567094
Al	-1.282814	-0.062211	-0.048457
C	-2.463881	1.301016	0.721096
H	-1.902390	2.139546	1.148735
H	-3.142497	1.716460	-0.032943
H	-3.094655	0.893136	1.519773
C	-1.934829	-1.661175	-0.986304
H	-2.468809	-1.407274	-1.909741
H	-2.637900	-2.231837	-0.367542
H	-1.121989	-2.342476	-1.261743
C	0.003134	1.027267	-1.358868
Al	1.292874	0.048734	0.044009
C	2.160650	-1.477987	-0.831690
H	2.892825	-1.148764	-1.578426
H	1.443773	-2.126408	-1.347762
H	2.703321	-2.106531	-0.116019
C	2.250513	1.530332	0.900502
H	2.807472	2.126556	0.168631
H	1.563646	2.212364	1.414550
H	2.976298	1.179483	1.642609
H	-0.043610	2.087688	-1.097399
H	-0.809190	0.830024	-2.075837
H	0.883335	0.887912	-2.006340
H	0.914798	-1.175729	1.839032
H	-0.739393	-1.531435	1.681473
H	-0.240667	0.035711	2.357184

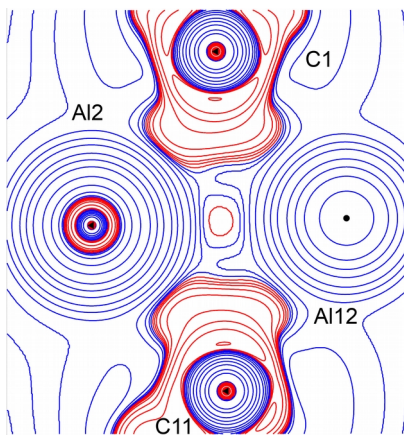


Bader

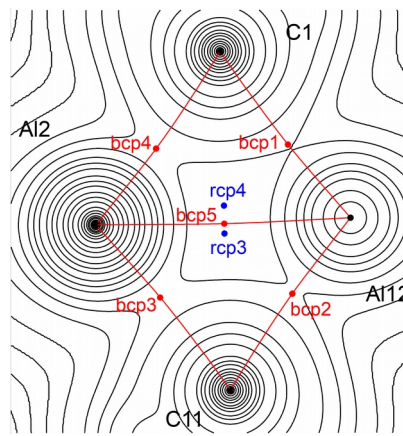
Plane through C11-Al2-C1:



Electron density



Laplacian

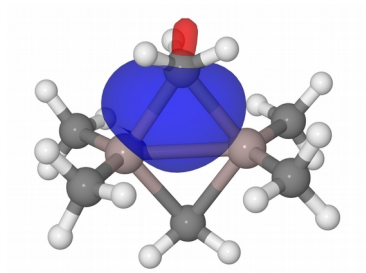


Virial

	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$
bcp1	0.04953	-0.04537
bcp2	0.05035	-0.04676
bcp3	0.05117	-0.04810
bcp4	0.05118	-0.04772
bcp5	0.03798	0.00113
rcp1	0.03715	-0.00750
rcp2	0.03693	-0.00784

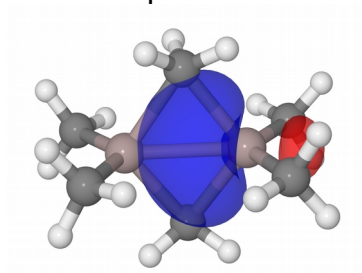
NBO:

Donororbital



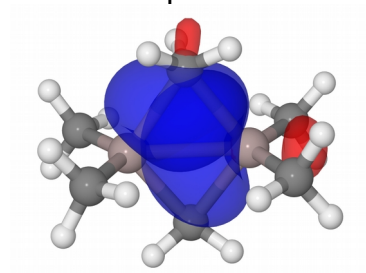
BD C 1 (87.35%) $sp^{2.28}$ –
Al 2 (12.65%) $sp^{5.16}d^{0.16}$

Acceptororbital

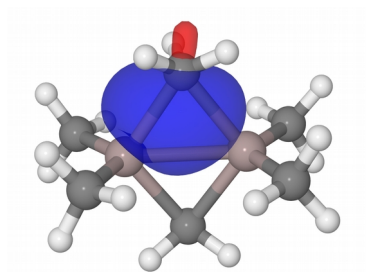


LV Al 12 $sp^{4.54}d^{0.08}$

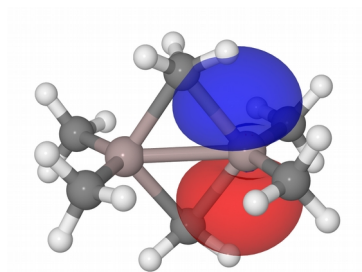
Overlaporbital



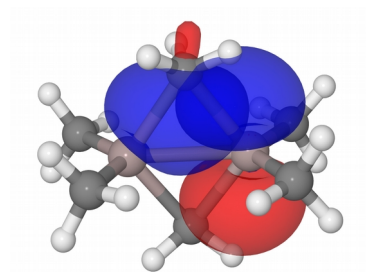
$E(2P) = 78.12 \text{ kcal/mol}$



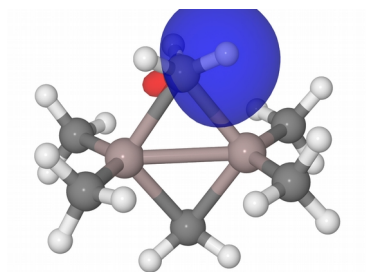
BD C 1 (87.35%) $sp^{2.28}$ –
Al 2 (12.65%) $sp^{5.16}d^{0.16}$



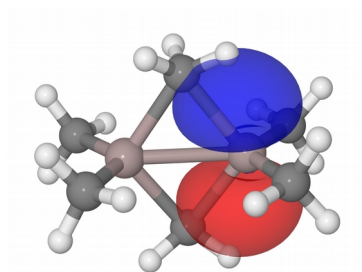
LV Al 12 $p^{1.00}d^{0.01}$



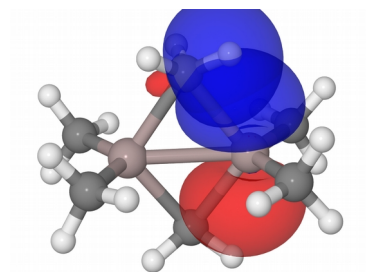
$E(2P) = 22.16 \text{ kcal/mol}$



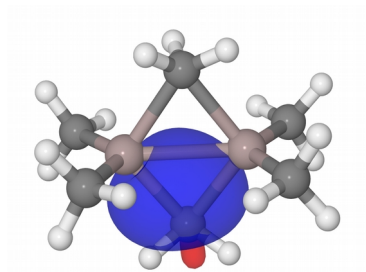
BD C 1 (64.17%) $sp^{2.95}$ –
H 24 s



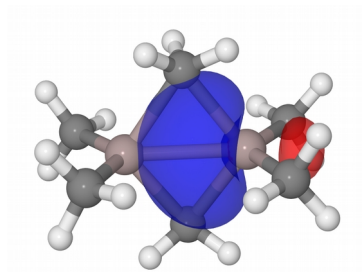
LV Al 12 $p^{1.00}d^{0.01}$



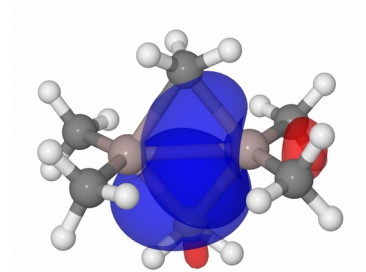
$E(2P) = 17.15 \text{ kcal/mol}$



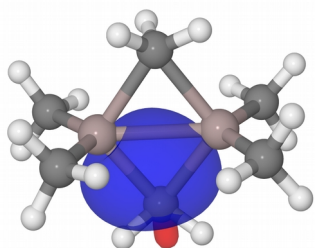
BD Al 2 (12.55%) $sp^{5.17}d^{0.16}$ –
C 11 (87.45%) $sp^{2.29}$



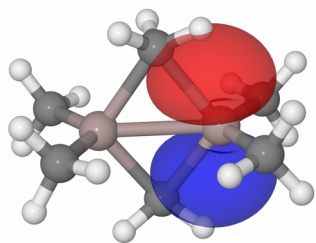
LV Al 12 $sp^{4.54}d^{0.08}$



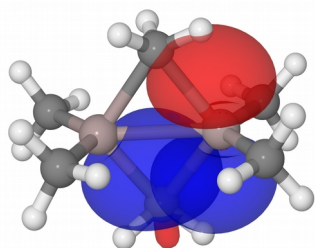
$E(2P) = 79.92 \text{ kcal/mol}$



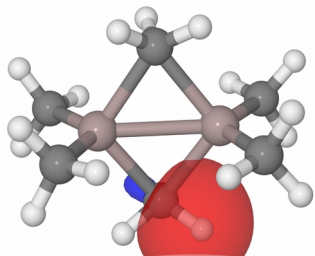
BD Al 2 (12.55%) $sp^{5.17}d^{0.16}$ –
C 11 (87.45%) $sp^{2.29}$



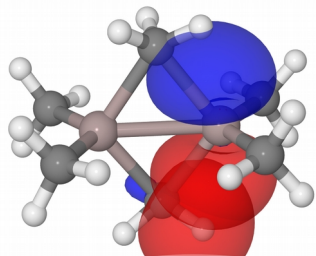
LV Al 12 $p^{1.00}d^{0.01}$



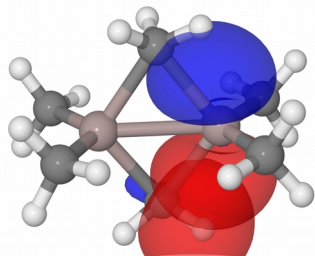
$E(2P) = 23.11 \text{ kcal/mol}$



BD C 11 (64.26%) $sp^{2.95}$ –
H 23 (35.74%) s

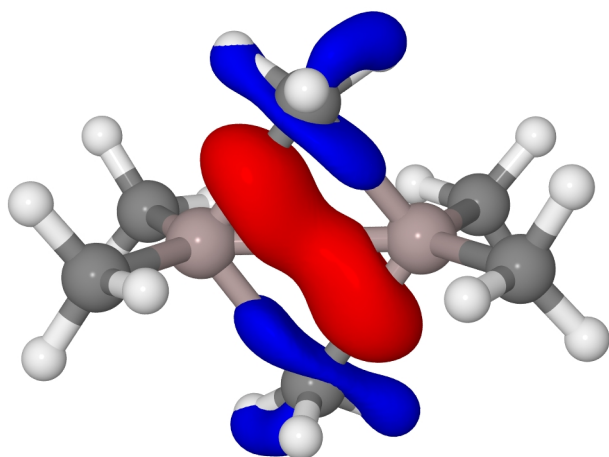


LV Al 12 $p^{1.00}d^{0.01}$

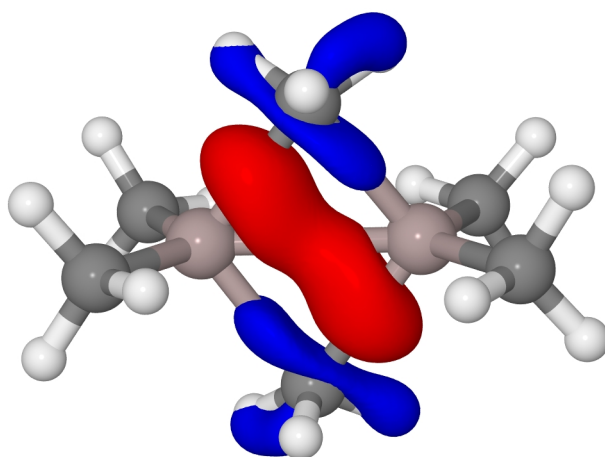


$E(2P) = 15.18 \text{ kcal/mol}$

ETS-NOVC



NOCV pair 1



NOCV pair 2

----- Pair and NOCV orbital information -----

There are totally 138 NOCV pairs and 276 NOCV orbitals

NOCV orbitals with absolute eigenvalues smaller than 5.0E-02 are not shown

Note: All energies are given in kcal/mol

Pair	Energy	Orbital	Eigenvalue	Energy	Orbital	Eigenvalue	Energy
1	-63.38	1	0.62104	-91.44	276	-0.62104	10.62
2	-14.21	2	0.27937	-75.13	275	-0.27938	-24.26
3	-3.22	3	0.13972	-62.34	274	-0.13972	-39.31
4	-3.55	4	0.12840	-63.58	273	-0.12840	-35.93
5	-1.86	5	0.10278	-78.25	272	-0.10278	-60.15
6	-1.52	6	0.08503	-60.34	271	-0.08503	-42.52
7	-1.14	7	0.07326	-62.02	270	-0.07326	-46.43
8	-1.31	8	0.06787	-2.07	269	-0.06787	17.19
9	-0.60	9	0.05278	-9.67	268	-0.05278	1.62

Sum of NOCV eigenvalues: 0.00000

Sum of pair energies: -90.78 kcal/mol