

Cyclic Boron Clusters Containing Planar Hypercoordinate Cobalt, Iron and Nickel

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Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

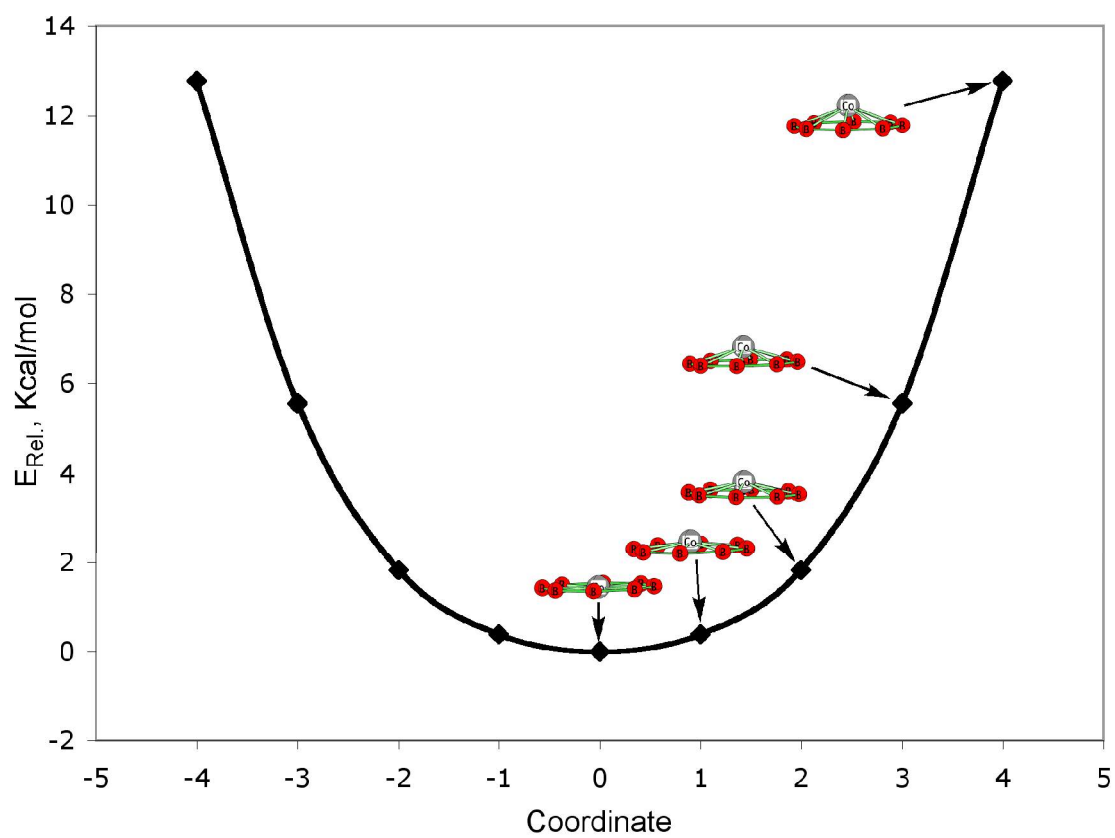


Figure 1S. IRC computation of **1** along the lowest vibrational frequency at BP86/TZVPP level.

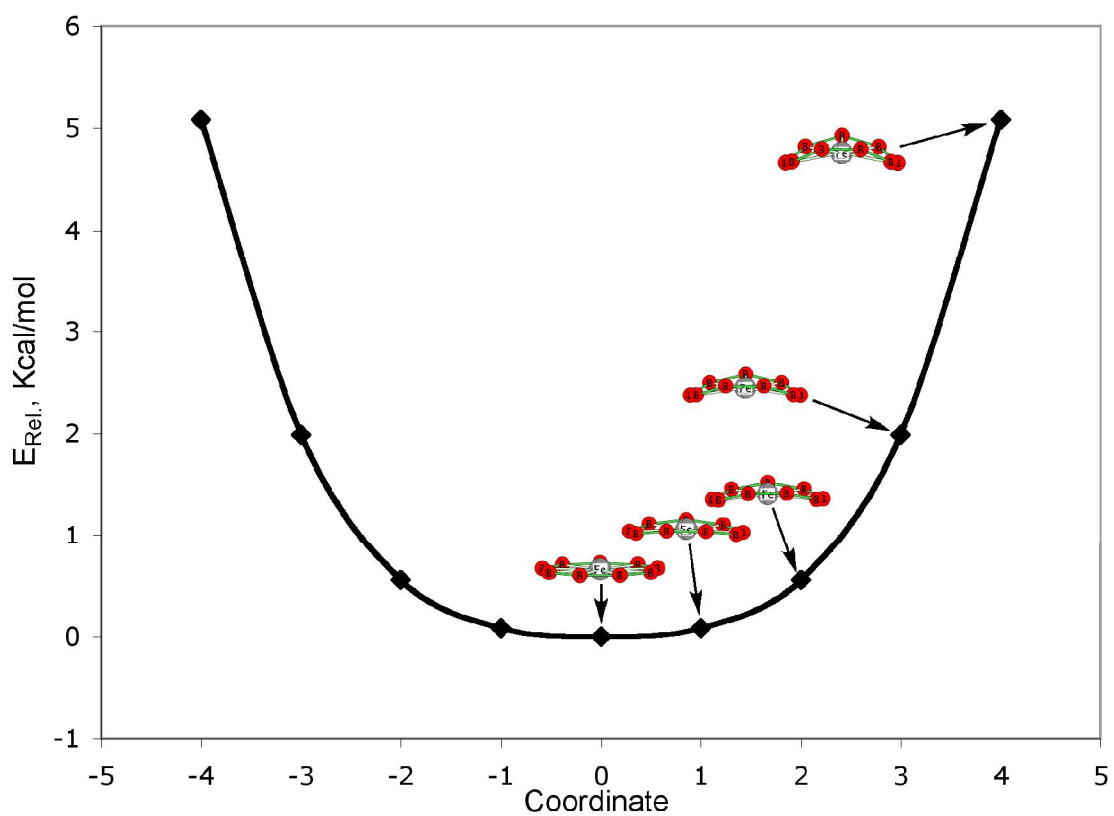


Figure 2S. IRC computation of **2** along the lowest vibrational frequency at BP86/TZVPP level.

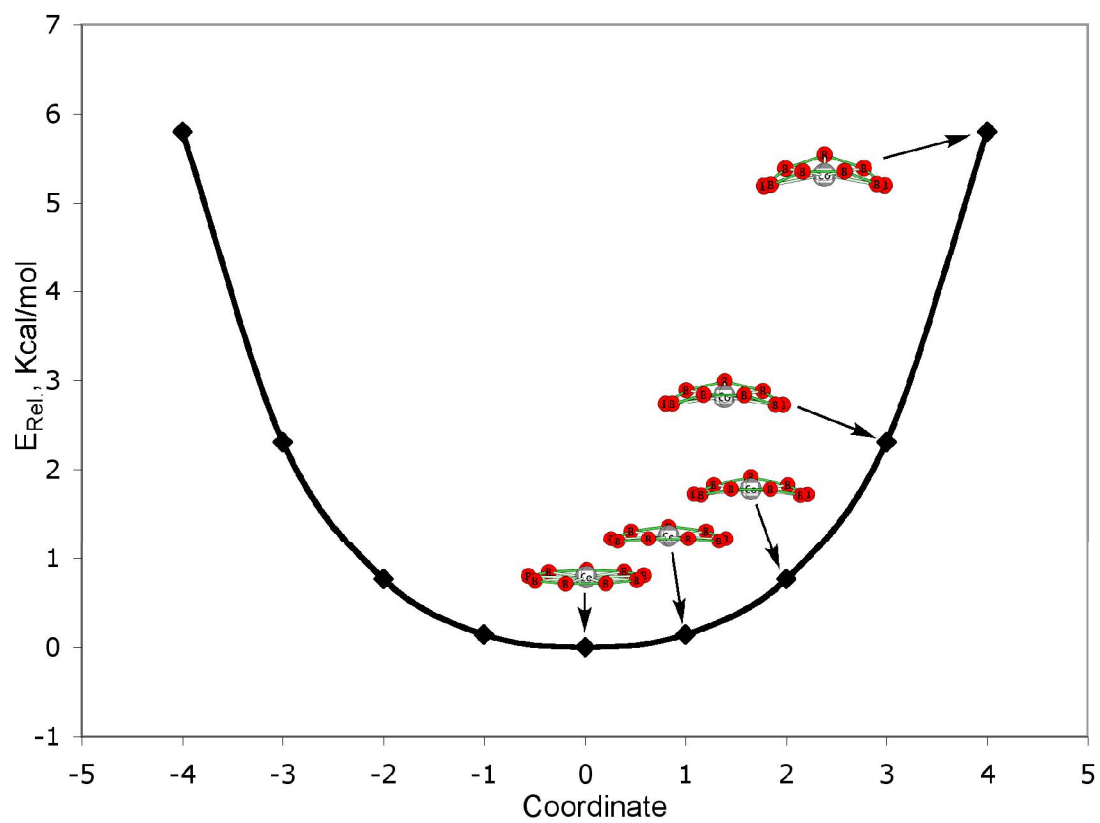


Figure 3S. IRC computation of **3** along the lowest vibrational frequency at BP86/TZVPP level.

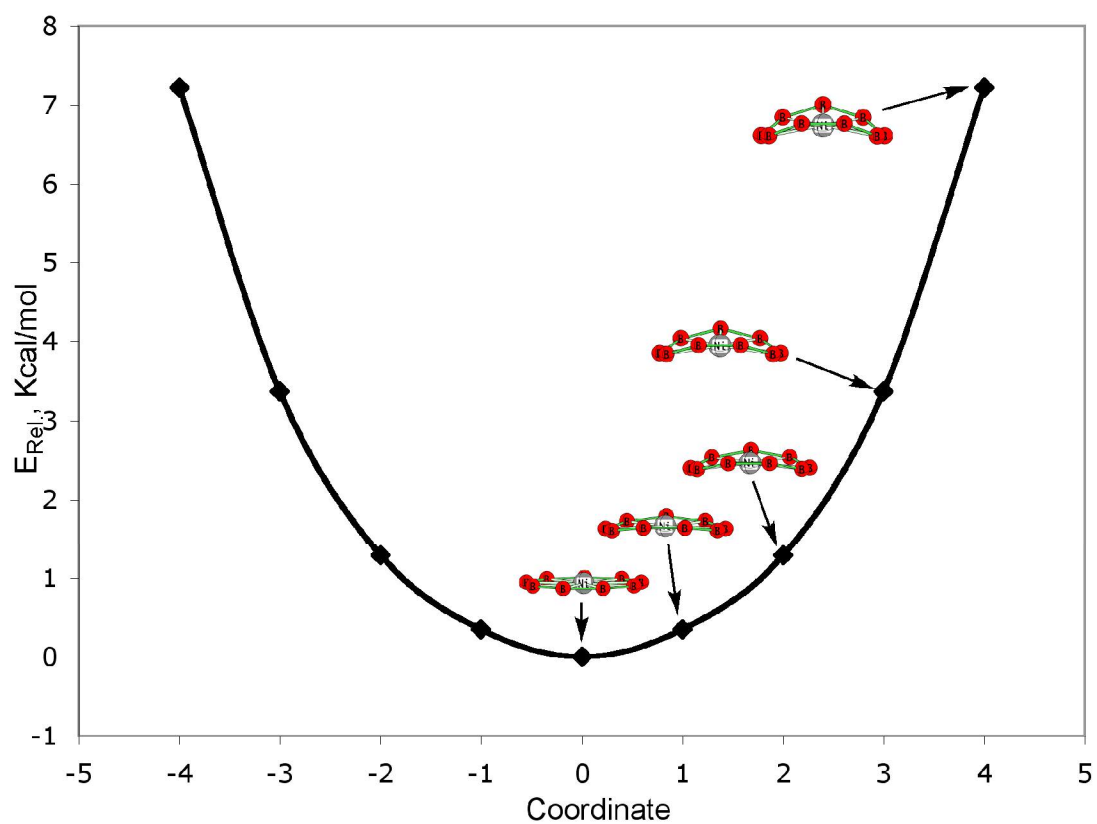


Figure 4S. IRC computation of **4** along the lowest vibrational frequency at BP86/TZVPP level.

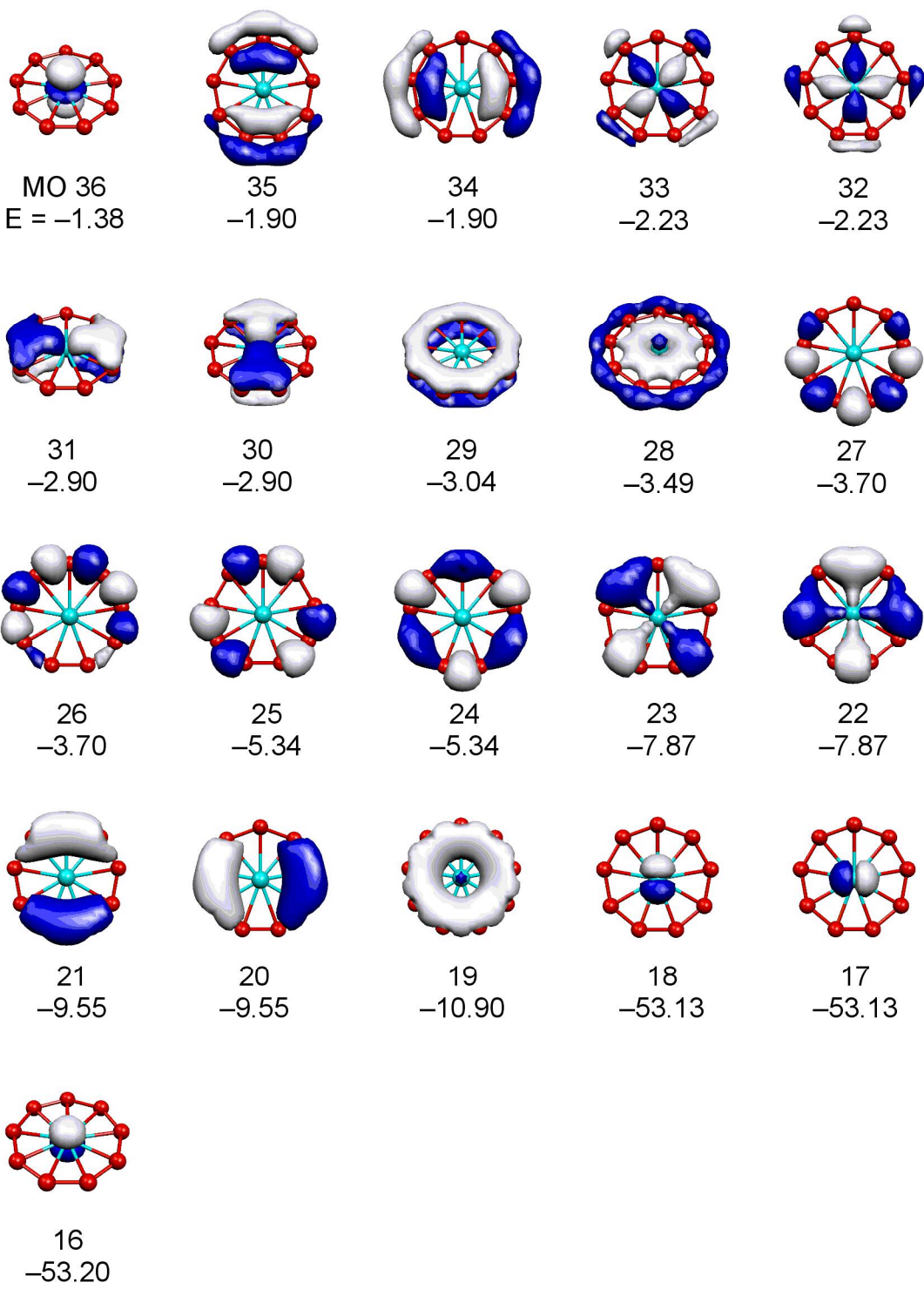


Figure 5S. Valence MO of **2** at BP86/TZVPP. Energies of the MOs are in eV.

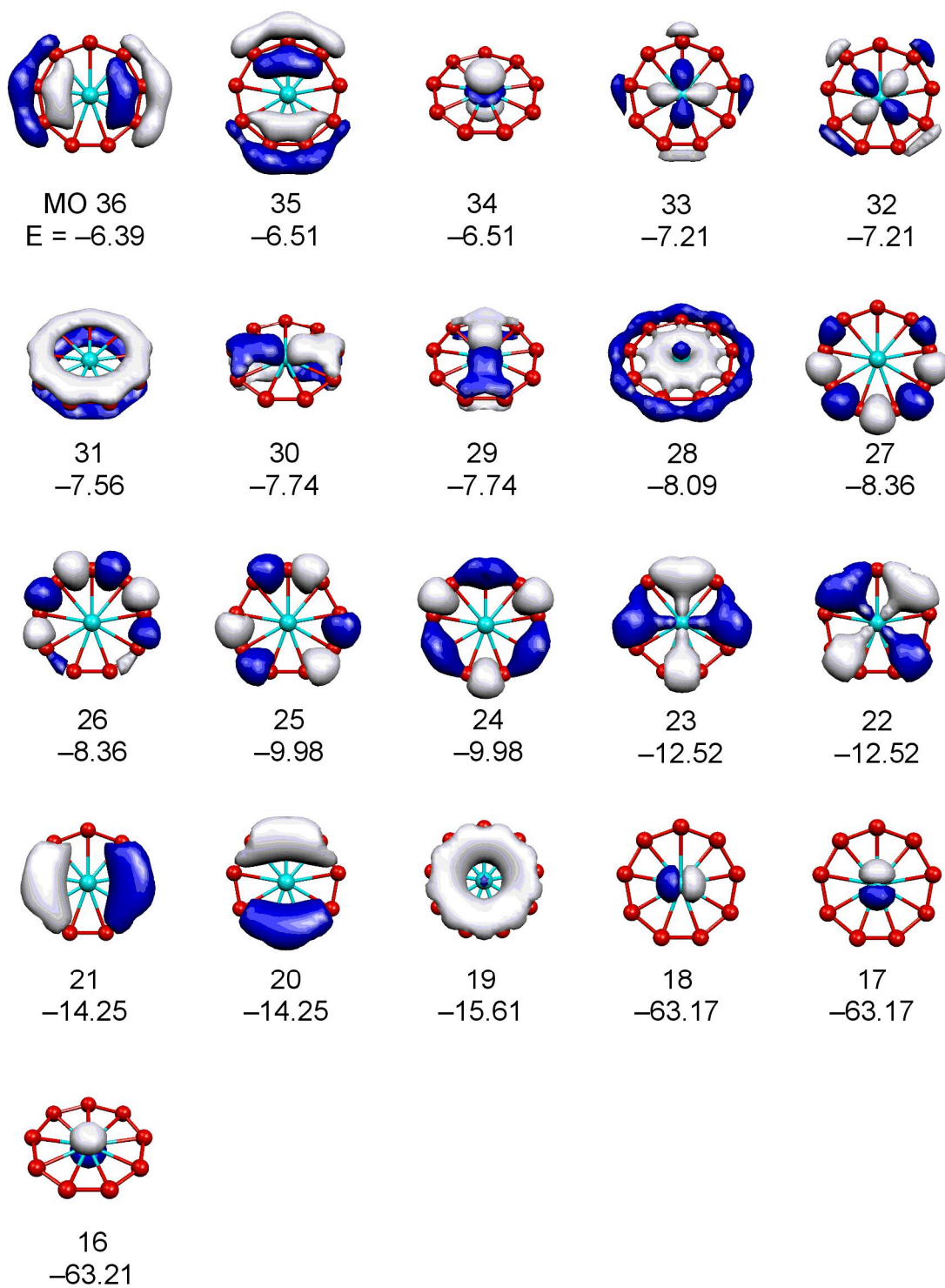


Figure 6S. Valence MO of **3** at BP86/TZVPP. Energies of the MOs are in eV.

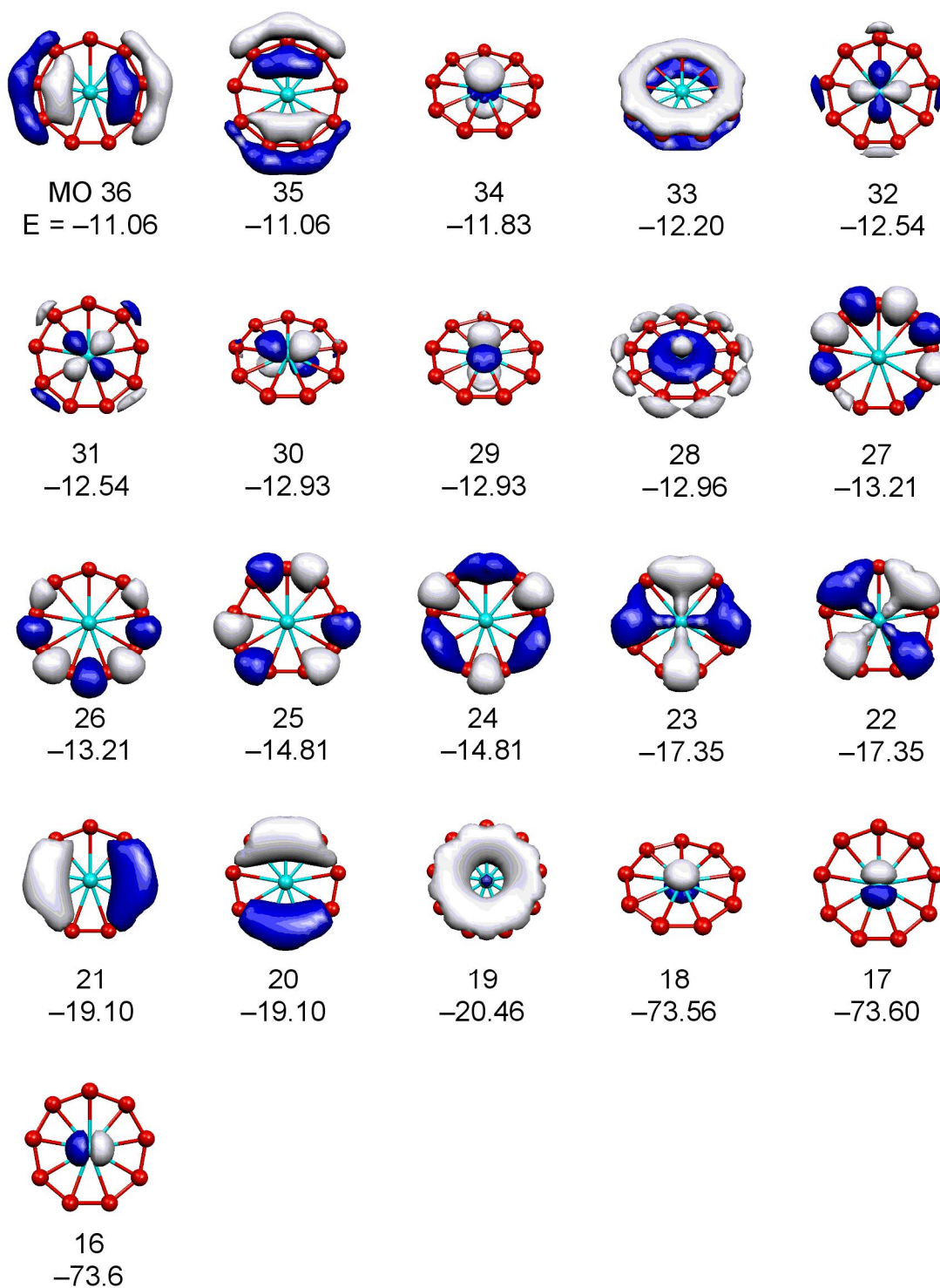


Figure 7S. Valence MO of **4** at BP86/TZVPP. Energies of the MOs are in eV.

Cartesian coordinates of phTM minima at BP86/TZVPP. Total Energies ($E_{\text{Tot.}}$) are in a.u.,
coordonates are in Å.

1 (CoB_8^- , D_{8h})

$$E_{\text{Tot.}} = -1581.80024$$

Co	0.00000	0.00000	0.00000
B	2.04897	0.00000	0.00000
B	0.00000	-2.04897	0.00000
B	0.00000	2.04897	0.00000
B	-2.04897	0.00000	0.00000
B	-1.44884	-1.44884	0.00000
B	1.44884	1.44884	0.00000
B	1.44884	-1.44884	0.00000
B	-1.44884	1.44884	0.00000

2 (FeB_9^- , D_{9h})

$$E_{\text{Tot.}} = -1487.53869$$

Fe	0.00000	0.00000	0.00000
B	2.23439	-0.00000	0.00000
B	-1.11719	1.93504	0.00000
B	-1.11719	-1.93504	0.00000
B	1.71164	-1.43624	0.00000
B	0.38800	2.20044	0.00000
B	-2.09964	-0.76421	0.00000
B	0.38800	-2.20044	0.00000
B	1.71164	1.43624	0.00000
B	-2.09964	0.76421	0.00000

3 (CoB_9 , D_{9h})

$$E_{\text{Tot.}} = -1606.50693$$

Co	0.00000	0.00000	0.00000
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B	0.38904	2.20637	0.00000
B	-2.10529	-0.76626	0.00000
B	1.71625	-1.44011	0.00000
B	1.71625	1.44011	0.00000
B	-2.10529	0.76626	0.00000
B	0.38904	-2.20637	0.00000
B	2.24041	0.00000	0.00000
B	-1.12020	1.94025	0.00000
B	-1.12020	-1.94025	0.00000

4 (NiB_9^+ , D_{9h})

$E_{\text{Tot.}} = -1731.76914$

Ni	0.00000	0.00000	0.00000
B	2.12771	0.77442	0.00000
B	-0.39318	-2.22986	0.00000
B	-1.73452	1.45544	0.00000
B	1.13213	1.96090	0.00000
B	1.13213	-1.96090	0.00000
B	-2.26426	-0.00000	0.00000
B	-0.39318	2.22986	0.00000
B	2.12771	-0.77442	0.00000
B	-1.73452	-1.45544	0.00000