Hf_3 Cluster is Triply (σ-, π-, and δ-) Aromatic in the D_{3h}, $^1A_1$' State.

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Supporting Information

Complete reference 14.

Gaussian 03 (revision D.01). Frisch, M. J.; Trucks, G. M.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, 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.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; 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,.; 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. G.; Chen, W.; Wang, M. W.; Gonzales, C. ; and Pople, J. A., Gaussian, Inc., Wallington, CT, 2003.

Table 1S. Total and Relative energies of the eight lowest Hf_3 structures at the B3LYP/Stuttgart+2f1g level of theory.

Structure	Electronic Configuration	Energy, Hartree	ΔE, kcal/mol
I	$^3A_2'$, $1a_1'^2 1a_2''^2 1e''^4 2a_1'^2 1e''^2$	-143.80400	0.0
II	$^3A_2$, $1a_1^2 1b_2^2 2a_1^2 1b_1^2 3a_1^2 1a_2^1 4a_1^1$	-143.79853	3.4
III	$^3B_1$, $1a_1^2 2a_1^2 1b_2^2 1b_1^2 3a_1^2 2b_1^1 4a_1^1$	-143.79817	3.7
IV	$^3B_1$, $1a_1^2 1b_2^2 2a_1^2 1b_1^2 3a_1^2 1a_2^1 2b_2^1$	-143.79147	7.9
V	$^1A_1'$, $1a_1'^2 2a_1'^2 1e''^4 1a_2''^2 3a_1'^2$	-143.78938	9.2
VI	$^1A_1$, $1a_1^2 1b_2^2 2a_1^2 1b_1^2 3a_1^2 1a_2^2$	-143.78552	11.6
VII	$^3A_2'$, $1a_1'^2 1e''^4 1a_2''^2 2a_1'^2 2e'^2$	-143.77834	16.1
VIII	$^3B_2$, $1a_1^2 1b_2^2 2a_1^2 1b_1^2 1a_2^2 3a_1^1 2b_2^1$	-143.76498	24.5

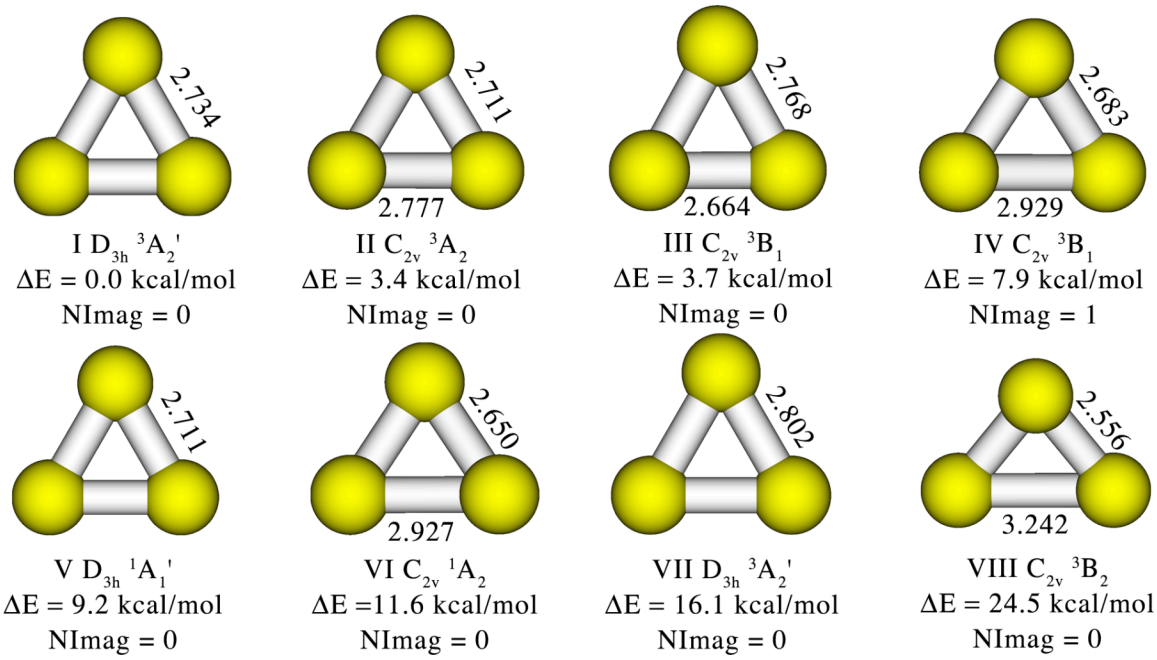

Figure 1S. Geometries and relative energies for eight lowest Hf_3 structures at the B3LYP/Stuttgart+2f1g level of theory.

CASSCF calculations:

For the D_{3h} ($^1A_1$') singlet state the leading coefficient of the Hartree-Fock configuration is 0.842 out of 2,005,003 configurations and for the D_{3h} ($^3A_2$') triplet state the leading coefficient of the Hartree-Fock configuration 0.867 out of 3,006,003 configurations (both at the CASSCF(10,14)/Stuttgart+2f1g level of theory).