Electronic Supplementary Information for Dalton Transactions

Supplementary Information

Diverse reactions of sterically protected 1,3-diphosphacyclobutane-2,4-diyls with hydride

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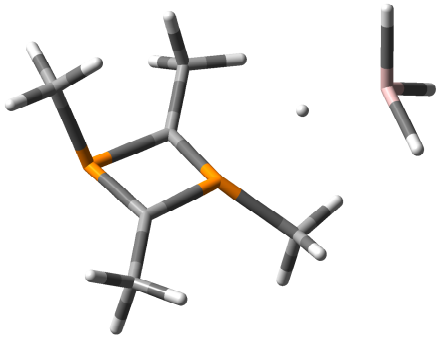
Note:

Quality structural analysis of **1i** was not possible due to perturbation by non-solved disorders and/or a crystalline polymorphism. Data is available from CCDC (No. 746700).

DFT Calculation[1]



Job cpu time: 0 days 6 hours 38 minutes 15.0 seconds.

E(RB+HF-LYP) = -1163.36811125 au
Dipole = 6.9733 Debye

Stoichiometry C6H16AlP2(1-)
Framework group C1[X(C6H16AlP2)]
Deg. of freedom 69
Full point group C1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-3.486157	-0.392717	0.992309
2	1	0	-4.197860	-1.097460	-0.289925
3	1	0	-3.447128	-1.327638	2.315942
4	1	0	-1.840411	-0.168969	0.502708
5	1	0	-4.039535	1.112150	1.265183
6	15	0	-0.287613	0.367621	-0.471196
7	6	0	0.678555	-0.969481	-0.934526
8	6	0	-1.447710	1.246143	-1.599274
9	1	0	-1.970552	2.024554	-1.034658
10	1	0	-2.191821	0.537421	-1.972325
11	1	0	-0.887600	1.684574	-2.429889
12	15	0	2.106789	-0.198508	-0.061844
13	6	0	0.982121	1.201811	0.295218
14	6	0	2.282304	-1.166512	1.547792
15	1	0	2.698120	-2.160502	1.336366
16	1	0	2.977357	-0.645194	2.216672
17	1	0	1.315229	-1.276364	2.049366
18	6	0	0.353224	-2.431173	-1.058990
19	6	0	1.279829	2.654326	0.527539
20	1	0	-0.602183	-2.583023	-1.576472
21	1	0	1.116096	-2.953493	-1.654243
22	1	0	0.278351	-2.966300	-0.094089
23	1	0	1.866454	3.122536	-0.283655
24	1	0	0.349588	3.230529	0.618096
25	1	0	1.838357	2.825129	1.459954

Rotational constants (GHZ): 1.1038616 0.6029953 0.5158709

Reference

1 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery Jr, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, N. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. M. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian 03, Revision D.01, Gaussian Inc., Wallingford CT, 2004.