Supplementary Material (ESI) for Chemical Communications

An early-late heterobimetallic complex with an unsupported dative bond: synthesis and structure of $[(Cy_3P)_2Pt–ZrCl_4]$

Holger Braunschweig, Krzysztof Radacki and Katrin Schwab

Supplementary Information

Theoretical Calculations

All computations were performed on a cluster of Linux workstations using *Gaussian03, Revision E.01* (Gaussian, Inc., Pittsburgh PA, **2003**).[1] Calculations were performed using DFT methods, applying the three hybrid functional B3LYP using 6-31G(d,p) basis function sets for non-metals and the Stuttgart relativistic, small core ECP basis set for Pt and Zr.[2]

Notes and references

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, M. 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. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, *Gaussian* 03 revision *E01*, Inc., Wallingford CT, **2004**.

2 a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648; b) S. H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* **1980**, *58*, 1200; c) C. Lee, W. Yang, R. G. Parr, *Phys. Rev.* **1988**, *B37*, 785; d) Stuttgart RSC 1997 ECP Basis Set was obtained from the Extensible Computational Chemistry Environment Basis Set Database, Version 02/25/04, as developed and distributed by the Molecular Science Computing Facility,

Environmental and Molecular Sciences Laboratory which is part of the Pacific Northwest Laboratory, P.O. Box 999, Richland, Washington 99352, USA, and funded by the U.S. Department of Energy.