Supplementary Material (ESI) for Chemical Communications

Supporting Information for

Syntheses and Structures of Mononuclear Lutetium Imido Complexes with Very Short Lu-N Bonds

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Contents:

Details of the Electronic Structure Calculation on [(η^8-C_8H_8)Lu(NIm^{Me})] (3)

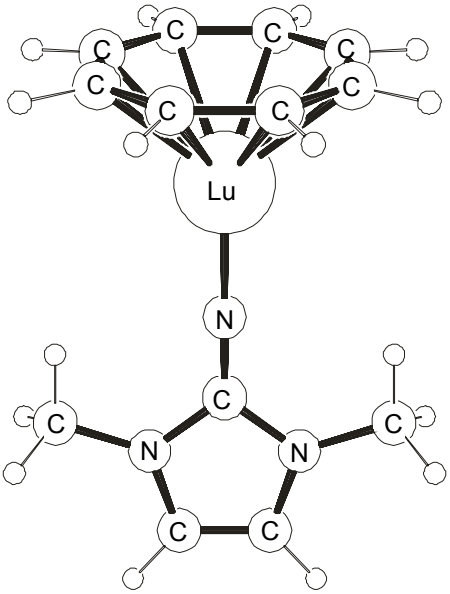
($Im^{Me}N$ = 1,3-dimethylimidazolin-2-imide)

All computations were performed using the hybrid density functional method B3PW91 implemented in the *Gaussian03* program.[1] For all main-group elements (C, H, N) the all-electron triple-ζ basis set (6-311G**) was used, whereas for the Lu atom the *Stuttgart RSC ANO/ECP* basis set was employed.[2,3]

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, T. Ishida, M. 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 C.02, Gaussian, Inc., Wallingford, CT, 2004.

2 X. Cao and M. Dolg, *J. Chem. Phys.*, 2001, **115**, 7348.

3 Basis sets were obtained from the Extensible Computational Chemistry Environment Basis Set Database, Version 02/25/04 (http://www.emsl.pnl.gov/forms/basisform.html), 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, WA 99352, and funded by the U.S. Department of Energy. The Pacific Northwest Laboratory is a multiprogram laboratory operated by Battelle Memorial Institute for the U.S. Department of Energy under Contract No. DE-AC06-76RLO 1830. Contact David Feller or Karen Schuchardt for further information.



Structure of 3 (atom, x-, y-, z-positions in Å):

Lu	0.000000	0.000000	-0.768982
N	0.000000	0.000000	1.270806
N	0.000000	1.094386	3.412326
N	0.000000	-1.094386	3.412326
C	0.000000	0.000000	2.547863
C	0.000000	0.674393	4.732123
C	0.000000	-0.674393	4.732123
C	0.000000	2.459666	2.957687
C	0.000000	-2.459666	2.957687
C	1.707019	-0.707133	-2.432604
C	1.707019	0.707133	-2.432604
C	0.707232	1.707512	-2.432602
C	-0.707232	1.707512	-2.432602
C	-1.707019	0.707133	-2.432604
C	-1.707019	-0.707133	-2.432604
C	-0.707232	-1.707512	-2.432602
C	0.707232	-1.707512	-2.432602
H	0.000000	1.369574	5.555071
H	0.000000	-1.369574	5.555071
H	2.706256	-1.120628	-2.336790
H	2.706256	1.120628	-2.336790
H	1.121520	2.706792	-2.340479
H	-1.121520	2.706792	-2.340479
H	-2.706256	1.120628	-2.336790
H	-2.706256	-1.120628	-2.336790
H	-1.121520	-2.706792	-2.340479
H	1.121520	-2.706792	-2.340479
H	0.891905	2.992193	3.302357
H	0.000000	2.433883	1.867468
H	-0.891905	2.992193	3.302357
H	-0.891905	-2.992193	3.302357
H	0.000000	-2.433883	1.867468
H	0.891905	-2.992193	3.302357

Energies for the optimized structure:

Compound	E(0 K)[a] [Ha]	H(298 K)[b] [Ha]	G(298 K)[b] [Ha]
3	-1905.505360	-1905.486898	-1905.553478

[a]DFT energy incl. ZPE.

[b]standard conditions T = 298.15 K and p = 1 atm.