

Supplementary Information for:

Disproportionation and radical formation in the coordination of “Gal” with bis(imino)pyridines.

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EPR spectrum of compound **7** 1 page

Computational details 1 pages

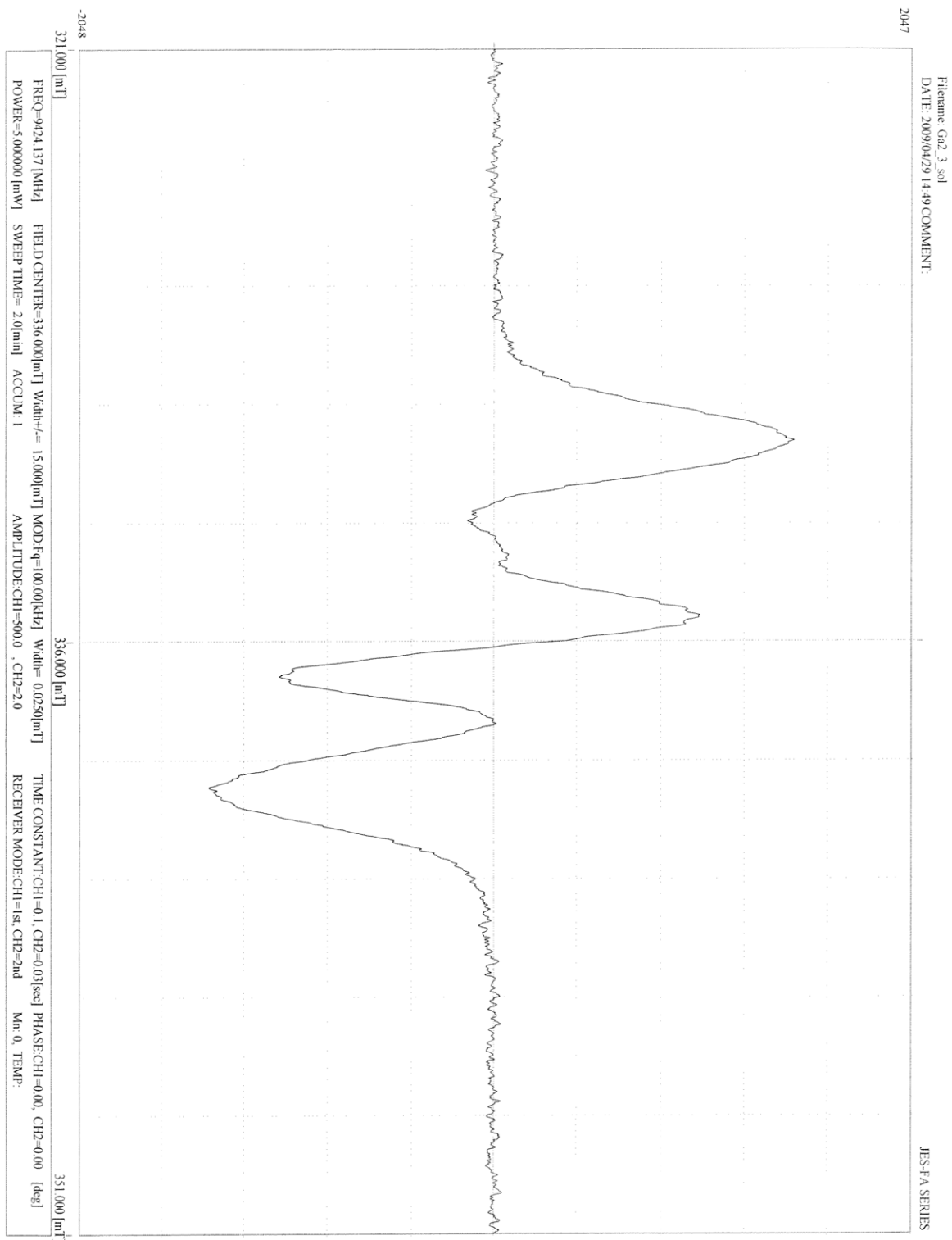


Figure S1. EPR spectrum for compound 7.

Computational Details

Both the thermochemical analysis of the disproportionation reaction of 2,6- $\{\text{DippN}=\text{CPh}\}_2(\text{NC}_5\text{H}_3)\text{GaI}$ in the presence of GaI and the optimization of compound **6** were performed with DFT calculations and the B3LYP functional using the Gaussian 03 (revision D.01) suite of programs.¹ The basis set DGDZVP was employed.

The compounds and atom in equation 1 were optimized and the results presented in Table 1. The enthalpy of atomization for Ga of 276kJ/mol = 0.10518 au/atom was used to calculate the net reaction enthalpy. This data provides a net reaction enthalpy of -0.108552 au = -4.73259×10^{-22} kJ or -28.5003 kJ/mole.

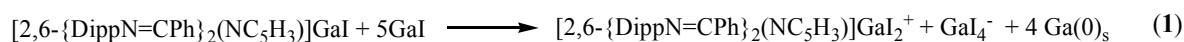


Table 1. Energies of the species in eq. 1 obtained by computation.

Compound	Energy (atomic units)
2,6- $\{\text{DippN}=\text{CPh}\}_2(\text{NC}_5\text{H}_3)\text{GaI}$	-10675.7050987
GaI	-8844.4058746
2,6- $\{\text{DippN}=\text{CPh}\}_2(\text{NC}_5\text{H}_3)]\text{GaI}_2^+$	-17595.430207
GaI_4^-	-29604.2606012
Ga_s	-1924.4328944 - 0.42060

¹ Gaussian 03, Revision D.01, 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, 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, Inc., Wallingford CT, 2004.