Supporting Information for "Molecular Dynamics Computational Study of the ^{199}Hg–^{199}Hg NMR Spin–Spin Coupling Constants of $[Hg–Hg–Hg]^{2+}$ in SO_2 solution"

Jochen Autschbach* and Mariusz Sterzel †

Department of Chemistry,

State University of New York at Buffalo,

Buffalo, NY 14260-3000, USA

email: jochena@buffalo.edu

June 26, 2007

Complete Reference 31: Baerends, E. J.; Autschbach, J.; Bérces, A.; Bickelhaupt, F. M.; Bo, C.; Boerrigter, P. M.; Cavallo, L.; Chong, D. P.; Deng, L.; Dickson, R. M.; Ellis, D. E.; van Faassen, M.; Fan, L.; Fischer, T. H.; Fonseca Guerra, C.; van Gisbergen, S. J. A.; Groeneveld, J. A.; Gritsenko, O. V.; Grüning, M.; Harris, F. E.; van den Hoek, P.; Jacob, C. R.; Jacobsen, H.; Jensen, L.; van Kessel, G.; Kootstra, F.; van Lenthe, E.; McCormack, D. A.; Michalak, A.; Neugebauer, J.; Osinga,

†New address: Academic Computer Centre CYFRONET

Cracow, Poland

V. P.; Patchkovskii, S.; Philipsen, P. H. T.; Post, D.; Pye, C. C.; Ravenek, W.; Ros, P.; Schipper, P. R. T.; Schreckenbach, G.; Snijders, J. G.; Solà, M.; Swart, M.; Swerhone, D.; te Velde, G.; Vernooijs, P.; Versluis, L.; Visscher, L.; Visser, O.; Wang, F.; Wesolowski, T. A.; van Wezenbeek, E.; Wiesenekker, G.; Wolff, S.; Woo, T.; Yakovlev, A.; Ziegler, T., 'ADF2006.01', Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, URL http://www.scm.com.

Animation of the molecular dynamics An AVI file (Windows Media Player compatible) is available that shows the production phase of the molecular dynamics of $[Hg–Hg–Hg]^{2+}$ with nine SO_2 molecules. The close–contact solvent–solute interactions are visualized as "weak bonds" in the animation.