

Correction to “DFT Calculations of Indirect ^{29}Si – ^1H Spin–Spin Coupling Constants in Organoalkoxysilanes” [*The Journal of Physical Chemistry A* **2010**, *114*, 5279–5286. DOI: 10.1021/jp911327a]. Jyothirmai Ambati, and Stephen E. Rankin*

The chemical shifts reported in Table 1 calculated using the cc-PVTZ and 6-31G basis sets should be $\delta = -42.9$ and -8.6 ppm, respectively. This indicates that 6-311+G(2d,p) and cc-PVTZ are both appropriate basis sets for calculating nuclear shielding tensors, but that the prediction of the 6-31G basis set ($\sim 20\%$ of the experimental value) is unacceptable.

DOI: 10.1021/jp200582p

Published on Web 02/8/2011