Supplementary Information

1,2-Difluoroethane: The angular dependance on $^1J_{CF}$ coupling constants is independant of hyperconjugation †

Matheus P. Freitas,[a] Michael Bühl[b] and David O'Hagan*[b]

[a] *Departamento de Química, Universidade Federal de Lavras, Lavras, Brazil - MG - C.P. 3037, 37200-000, Tel. (35) 3829-1891; Fax. (35) 3829 1271*
[b] *EastChem School of Chemistry*, *University of St Andrews, North Haugh, St Andrews, Fife, KY16 9ST, UK* Fax: 01334 463800; Tel: 01334 467171;
E-mail: do1@st-andrews.ac.uk

Table of Contents

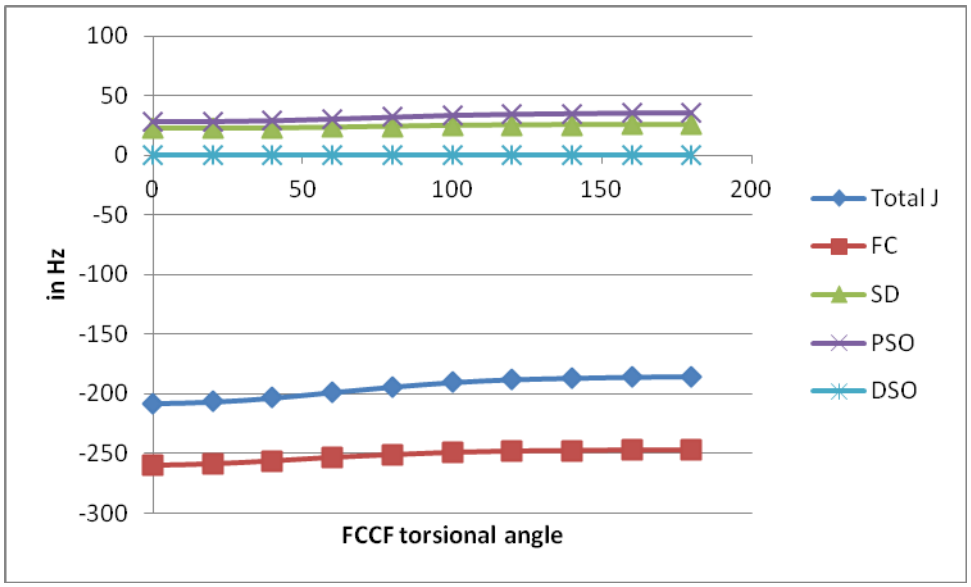

Fig. S1 Dependence of $^{1}J_{C,F}$ and its contributing terms (FC = Fermi contact; SD = spin dipolar; PSO = paramagnetic spin-orbit; DSO = diamagnetic spin-orbit) for 1,2-difluoroethane **1**, as a function of the FCCF torsional angle.

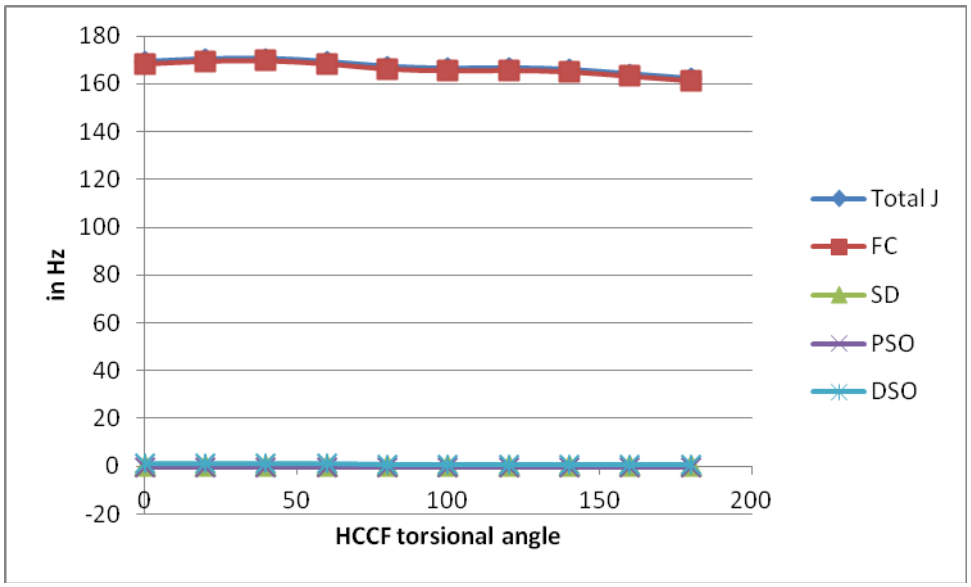

Fig. S2 Dependence of $^{1}J_{C,H}$ and its contributing terms (FC = Fermi contact; SD = spin dipolar; PSO = paramagnetic spin-orbit; DSO = diamagnetic spin-orbit) for 1,2-difluoroethane **1**, as a function of the HCCF torsional angle.

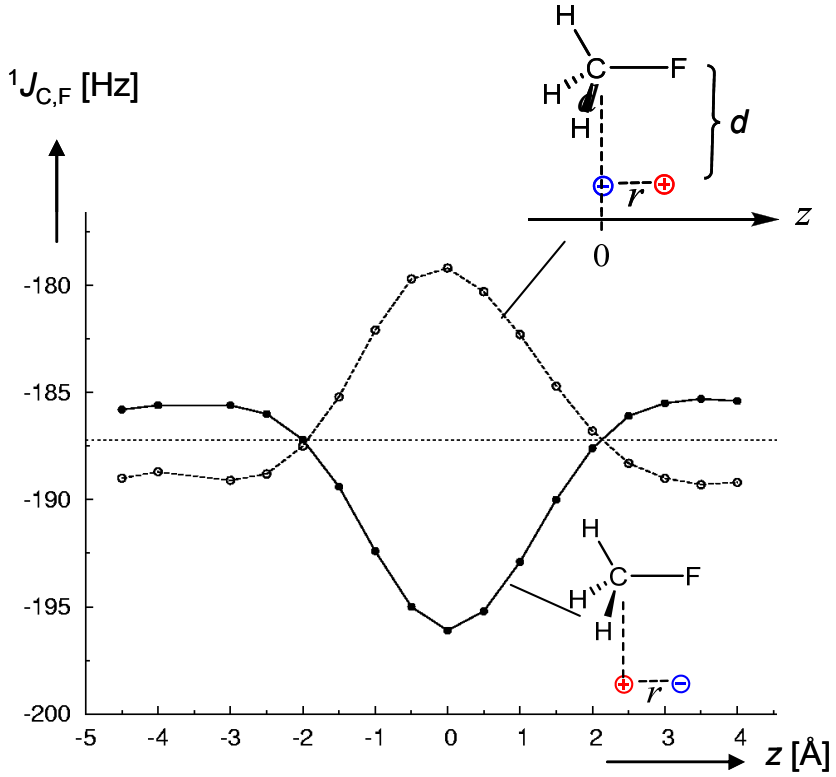

Fig. S3: Changes in the computed $^1J_{CF}$ in **9** (Hz) in the presence of a dipole from two elementary charges (separated by $r = 0.4$ Å, corresponding to $\mu = 2$ D). The dipole is shifted parallel (solid line) or antiparallel to the C-F bond (dashed line) at a distance of $d = 2.7$ Å (horizontal dotted line: dipole of pristine **9**). Note how the effect on $^1J_{CF}$ switches upon reversal of the dipole moment.

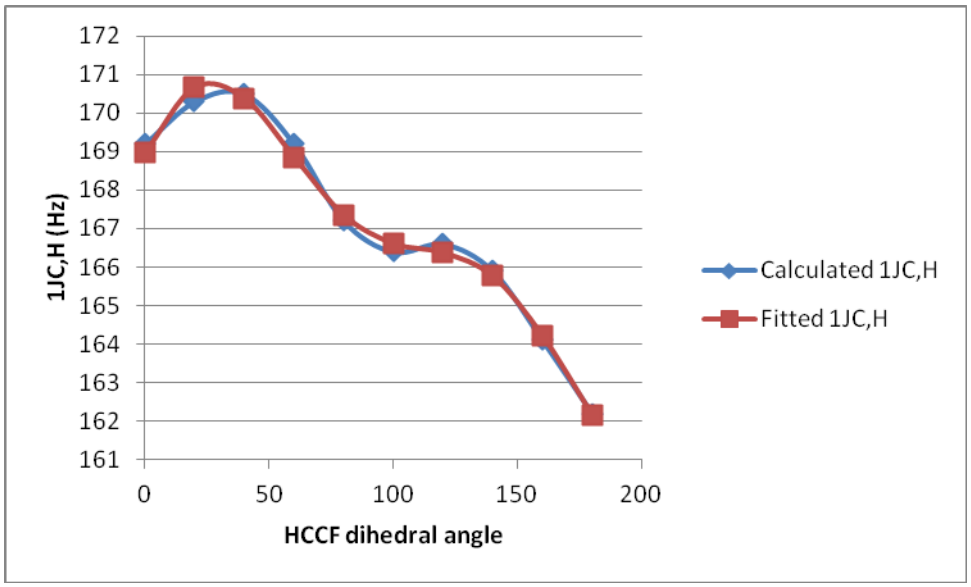

Fig. S4 Angular dependence of $^{1}J_{C,H}$ in 1,2-difluoroethane **1**. Calculated and fitted curves. Fitting: $^{1}J_{C,H}$ = 166 + 1.488×cos(φ×0.02325) + 3.711×sin(φ×0.02325) + 1.484×cos(2φ×0.02325) + 0.9809×sin(2φ×0.02325)

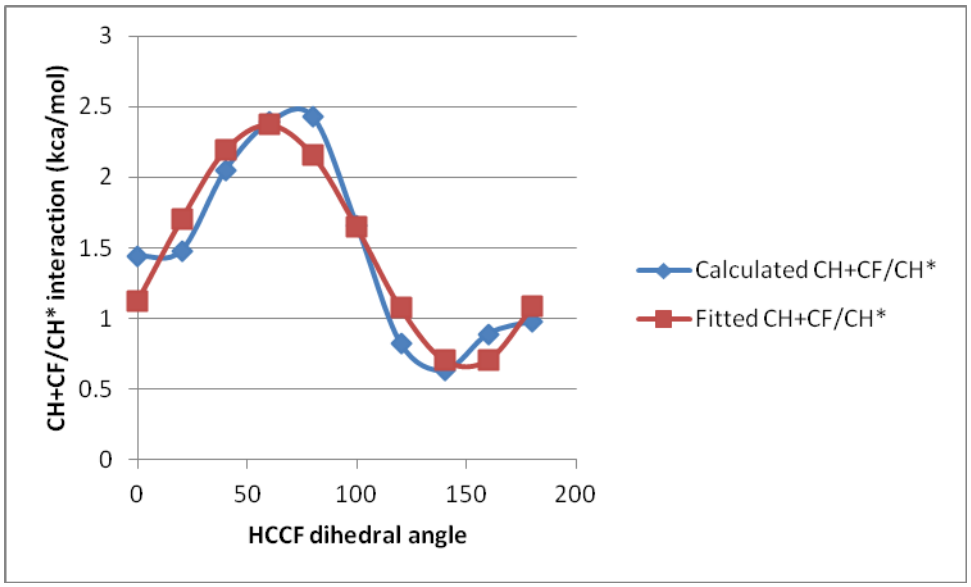

Fig. S5 Angular dependence of $\sigma_{CHb} + \sigma_{CF} \rightarrow \sigma^*_{CHa}$ in 1,2-difluoroethane **1**. Calculated and fitted curves. Fitting: $\sigma_{CHb} + \sigma_{CF} \rightarrow \sigma^*_{CHa} = 1.515 - 0.3917 \times \cos(\varphi \times 0.03461) + 0.7644 \times \sin(\varphi \times 0.03461)$

Full citation of the quantum-chemical program package used (Gaussian 09):

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, 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, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision A.1, Gaussian, Inc., Wallingford CT, 2009.