

Supplementary Materials

Quantum-Chemical Characterization of Nuclear Spin-Spin Couplings Across Hydrogen Bonds

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Theoretical values of the trans-hydrogen-bond J coupling ${}^3J_{\text{NC}}$ and the isotropic chemical shift $\delta(\text{H}^{\text{N}})$ of the hydrogen atom involved in the hydrogen bond obtained from deMon-NMR DFT calculations for the NMA-NMA dimer.

Table 1: ${}^3J_{\text{NC}}$ coupling in Hz

r_{NO}/θ	140	150	160	170	180	190	200	210	220
2.6	-1.95	-2.24	-2.45	-2.57	-2.61	-2.56	-2.43	-2.23	-1.94
2.7	-1.43	-1.64	-1.83	-1.94	-1.98	-1.94	-1.82	-1.61	-1.41
2.8	-1.07	-1.23	-1.34	-1.42	-1.44	-1.41	-1.32	-1.21	-1.06
2.9	-0.77	-0.90	-1.02	-1.07	-1.08	-1.06	-1.02	-0.91	-0.81
3.0	-0.60	-0.67	-0.73	-0.79	-0.81	-0.79	-0.73	-0.69	-0.58
3.1	-0.41	-0.49	-0.55	-0.58	-0.59	-0.59	-0.56	-0.50	-0.40
3.2	-0.29	-0.32	-0.38	-0.42	-0.43	-0.42	-0.39	-0.32	-0.29
3.3	-0.25	-0.27	-0.26	-0.29	-0.30	-0.29	-0.27	-0.24	-0.20
3.4	-0.17	-0.22	-0.24	-0.22	-0.21	-0.21	-0.21	-0.17	-0.16

The values of the trans-hydrogen-bond J coupling ${}^3J_{\text{NC}}$ in the NMA-NMA dimer are given as a function of the hydrogen bond length r_{NO} (Å) and the hydrogen bond angle θ (deg). The J-coupling values constitute the two-dimensional surface shown in Figure 1 of the paper.

Table 2: Isotropic chemical shift $\delta(\text{H}^{\text{N}})$ in ppm

r_{NO} / θ	140	150	160	170	180	190	200	210	220
2.6	9.32	10.17	10.84	11.28	11.43	11.28	10.84	10.16	9.32
2.7	8.42	9.12	9.67	10.01	10.14	10.02	9.67	9.11	8.41
2.8	7.74	8.30	8.74	9.03	9.13	9.04	8.74	8.29	7.73
2.9	7.23	7.67	8.03	8.26	8.34	8.26	8.03	7.66	7.22
3.0	6.84	7.19	7.47	7.66	7.73	7.66	7.48	7.18	6.83
3.1	6.54	6.82	7.04	7.19	7.25	7.20	7.05	6.81	6.53
3.2	6.30	6.53	6.71	6.83	6.88	6.84	6.72	6.53	6.31
3.3	6.13	6.31	6.46	6.56	6.60	6.56	6.47	6.31	6.13
3.4	5.99	6.14	6.26	6.34	6.37	6.34	6.26	6.14	5.99

The values of the isotropic chemical shift $\delta(\text{H}^{\text{N}})$ of the hydrogen atom involved in the hydrogen bond in the NMA-NMA dimer are given with respect to TMS (calculated using the same DFT method) as a function of the hydrogen bond length r_{NO} (Å) and the hydrogen bond angle θ (deg). The isotropic shift surface is closely related to the J-coupling surface as illustrated by the correlation given in Figure 2 of the paper.