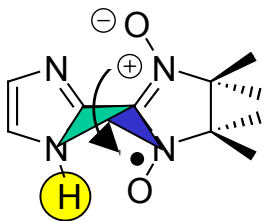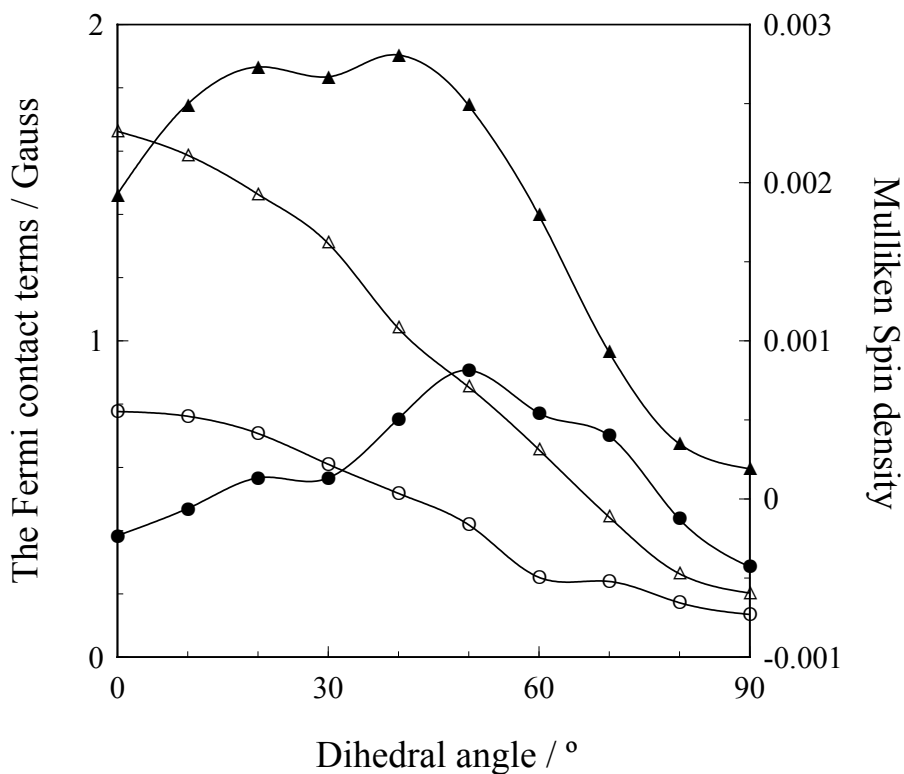Supporting information for

An ideal one-dimensional antiferromagnetic spin system observed in hydrogen-bonded naphth[2,3-*d*]imidazol-2-yl nitronyl nitroxide crystal: the role of hydrogen bond

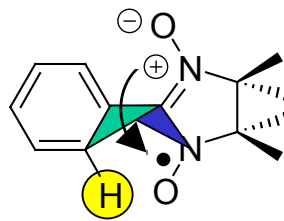Hideaki Nagashima, Hidenari Inoue, and Naoki Yoshioka*

Figure 1S. Variation of the Fermi contact terms and the Mulliken spin densities of the hydrogen atoms with changing the dihedral angles between the aryl rings and the ONCNO moieties (UB3LYP/6-31G*//AM1).

Figure 2S. Angular dependence of calculated *J* values (O: UB3LYP/4-31G; ●: UBLYP/4-31G).

Figure 3S. Angular dependence of calculated *J* values (O: UB3LYP/4-31G; ●: UBLYP/4-31G).

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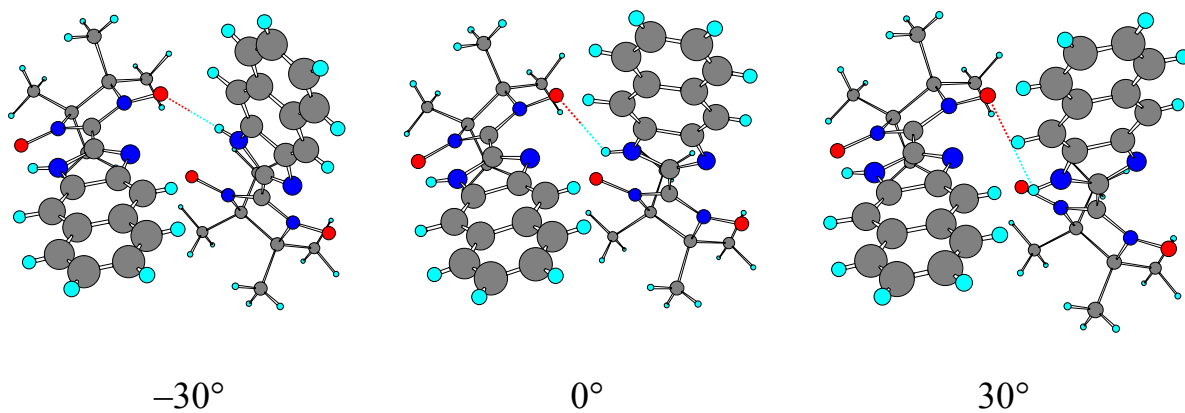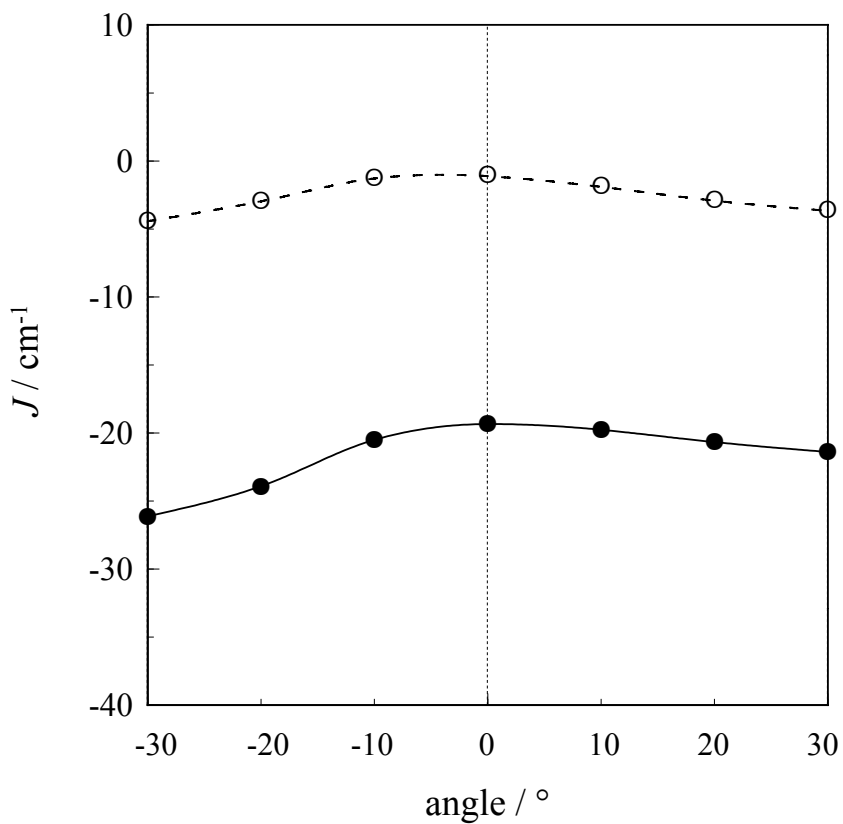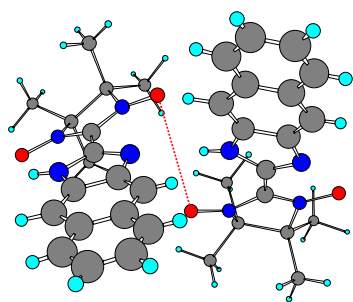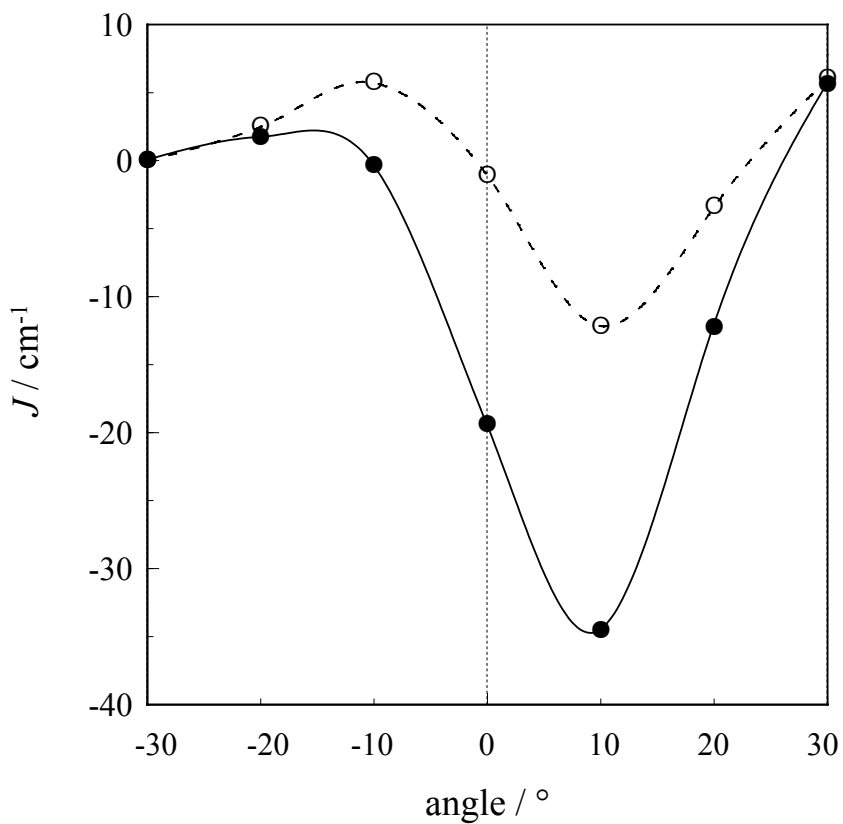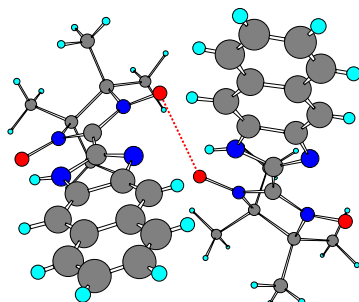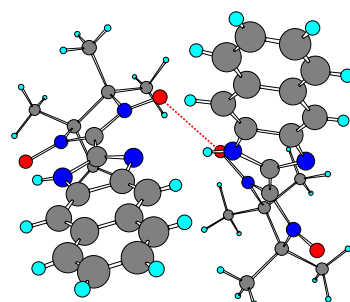
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