# Indirect Nuclear Spin-Spin Coupling Constants $^1J(^{17}O,^{13}C)$ in Derivatives of Carbon Dioxide and Carbon Monoxide – Density Functional Theory (DFT) Calculations

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Calculations of spin-spin coupling constants $^1J(^{17}O,^{13}C)$ in carbon dioxide (**1**) carbon monoxide (**2**) and several derivatives using density functional theory (DFT) have been carried out. This coupling constant possesses a positive sign [reduced coupling constant $^1K(^{17}O,^{13}C) < 0$] except for the parent acylium cation $[H\text{-}CO]^+$ (**4a**). It is shown that the Fermi contact term (FC) is positive [$< 0$ for $^1K(^{17}O,^{13}C)$] and that there are significant contributions from spin-dipole (SD) and paramagnetic spin-orbital (PSO) interactions.

*Key words:* Carbon Dioxide, Carbon Monoxide, NMR, Coupling Signs, MO Calculations