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Supporting Information: Soft experimental constraints for soft interactions: A spectroscopic benchmark data set for weak and strong hydrogen bonds

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Table S1: Gaussian keywords employed in the different calculations. For all complexes containing OO, charge and spin multiplicity were specified as 0 3 instead of the typically used 0 1, invoking UHF treatment of the open-shell system.

Level of approximation	Employed keywords
all	int=superfine, Def2QZVP, fopt=verytight, freq=raman, output=pickett
...-D3(BJ)/...	empiricaldispersion=gd3bj
B3LYP-...	b3lyp
PBE0-...	PBE1PBE
M06-2X/...	M062X