Supplementary information

The spin magnetic order of Co_n^+ ($n \leq 5$) clusters

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2. Comparison of measured infrared spectra of Co_4^+ and Co_5^+ with calculations of vibrational frequencies
3. XYZ coordinates (in units of Å)

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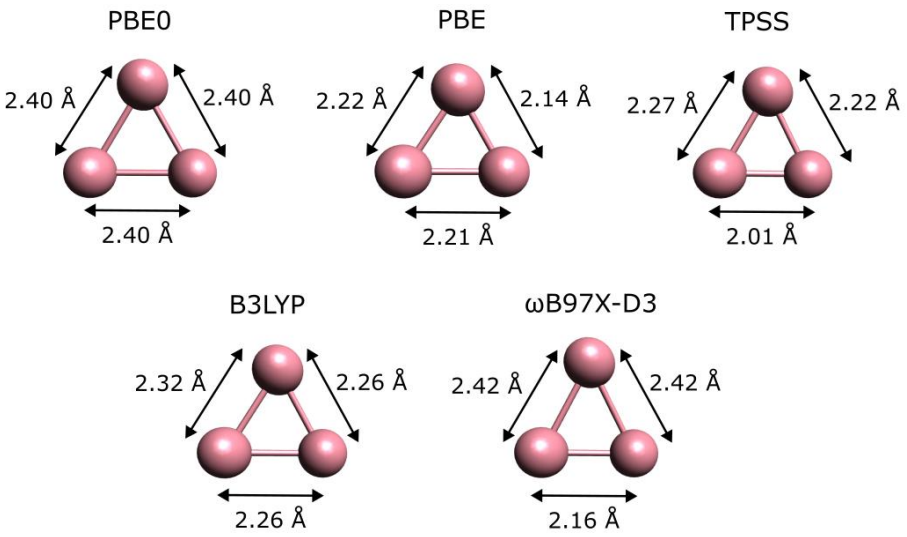

Figure S1. Comparison of the geometries of Co_3^+ (M = 7) optimized with different functionals.

2. Comparison of measured infrared spectra of Co_4^+ and Co_5^+ with calculations of vibrational frequencies

Table S1. Comparison of the vibrational bands measured for Co_4^+ and Co_5^+ (from Ref. [1]) and those calculated with DFT using the PBE0 functional (same level and for the computations presented in the main article).

Cluster	Experiment (cm^{-1})	DFT (cm^{-1})
Co_4^+	181 ± 11	181
	195 ± 8	194
Co_5^+	197 ± 21	204
	220 ± 13	210
	242 ± 11	242

[1] R. Gehrke, P. Gruene, A. Fielicke, G. Meijer and K. Reuter, J. Chem. Phys., 130, 034306, 2009.

3. XYZ coordinates (in units of Å)

All XYZ files can be downloaded from *https://webdav.data.ru.nl/hfml-felix/felix-pub-2022-ferrari-pccp_dsc_499*