Prussian Blue Analogue $CsFe[Cr(CN)_6]$ as a Matrix for the Fe(II) Spin-Crossover

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Supporting information

Table S1. Energy differences ($\Delta E = E(^5T_{2g}) - E(^1A_{1g})$, in cm^{-1}) between the HS and LS spin states using different point charges environments. ΔE(HT) and ΔE(LT) refer to the energy differences for the high- and low-temperature structures, respectively.

Point charges		***ΔE***	***ΔE(HT)***	***ΔE(LT)***
-		-16737	-15881	+2313
Formal charges	n = 1	-21057	-16839	+832
	n = 2	-21169	-16836	+830
	n = 3	-21189	-16835	+834
	n = 4	-21197	-16835	+834
	n = 5	-21203	-16838	+830
Mulliken charges	n = 1	+12477	-16378	+1534
	n = 2	+12474	-16379	+1532
	n = 3	+12531	-16374	+1531
	n = 4	+12547	-16376	+1531
	n = 5	+12553	-16378	+1532