Supporting Information

What are the physical contents of Hubbard and Heisenberg Hamiltonian interactions extracted from broken symmetry DFT calculations in magnetic compounds?

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Table S1: Values in cm^{-1} of the extracted parameters of the HDvV model and contributions to the magnetic couplings. The values have been rounded up to the next higher integer value except for the K_{ab} value of compound 4. The experimental (when available) or theoretical values of the magnetic couplings are $\simeq -2000$ cm^{-1} for 1,[51] -2420 cm^{-1} for 2[52–56], -286 cm^{-1} for 3[57], 2 cm^{-1} for 4[58], <-800cm^{-1} for 5[6], -75 cm^{-1} for 6[59] and between 0 and -40 cm^{-1} for 7[1].

		PBE PBE	PBE VWN5	TPSS TPSS	TPSS VWN5	B3LYP_ 20%	B3LYP_ 30%	B3LYP_ 50%	BH&H LYP	ωB97XD
1	K_{ab}	126	117	143	131	115	110	99	101	76
	ΔJ_{KE}	-4419	-4327	-4228	-4144	-3170	-2580	-1738	-1813	-2252
	ΔJ_{SP}	-26	-23	-4	3	-218	-340	-517	-477	-397
2	K_{ab}	167	153	195	172	180	181	177	188	175
	ΔJ_{KE}	-3504	-3525	-3149	-3024	-2684	-2278	-1686	-1808	-2345
	ΔJ_{SP}	-103	-84	-156	-107	-206	-284	-547	-524	-388
3	K_{ab}	27	26	26	24	24	19	9	10	19
	ΔJ_{KE}	-923	-935	-800	-809	-372	-243	-102	-108	-263
	ΔJ_{SP}	-35	-8	-24	-16	-29	-29	-22	-26	-30
4	K_{ab}	13	12	12	10	2	1	0.40	0.45	1
	ΔJ_{KE}	-10	-9	-7	-6	-3	-2	-1	-1	-2
	ΔJ_{SP}	1	1	1	1	2	3	9	9	2
5	K_{ab}	-	-	-	-	149	95	35	36	81
	ΔJ_{KE}	-	-	-	-	-1984	-1222	-484	-502	-1207
	ΔJ_{SP}	-	-	-	-	-108	-123	-92	-89	-144
6	K_{ab}	-	-	-	-	24	15	6	6	13
	ΔJ_{KE}	-	-	-	-	-213	-128	-48	-52	-128
	ΔJ_{SP}	-	-	-	-	6	5	-16	-16	1
7	K_{ab}	-	-	-	-	61	53	33	35	49
	ΔJ_{KE}	-	-	-	-	-186	-139	-70	-73	-136
	ΔJ_{SP}	-	-	-	-	15	19	25	26	21

Table S2: Values in cm^{-1} of the extracted parameters of the Hubbard model and contributions to the magnetic couplings. The values have been rounded up to the next higher integer value except for the K_{ab} value of compound 4. The experimental (when available) or theoretical values of the magnetic couplings are $\simeq -2000$ cm^{-1} for 1,[51] -2420 cm^{-1} for 2[52–56], -286 cm^{-1} for 3[57], 2 cm^{-1} for 4[58], <-800cm^{-1} for 5[6], -75 cm^{-1} for 6[59] and between 0 and -40 cm^{-1} for 7[1].

		PBE PBE	PBE VWN5	TPSS TPSS	TPSS VWN5	B3LYP_ 20%	B3LYP_ 30%	B3LYP_ 50%	BH&H LYP	ωB97XD
1	*K*	113	106	141	133	6	-60	-160	-138	-123
	t	-4396	-4292	-4435	-4333	-4662	-4718	-4708	-4777	-4958
	U	10391	9958	12650	12222	23844	31747	49220	48470	41303
2	*K*	116	111	117	119	77	39	-97	-74	-19
	t	-4632	-4509	-4688	-4479	-4687	-4691	-4646	-4749	-4934
	U	20416	18900	24416	23164	29865	36248	49499	48029	39062
3	*K*	10	22	14	16	10	5	-2	-3	4
	t	-1681	-1666	-1724	-1710	-1855	-1809	-1529	-1558	-1802
	U	11255	10862	14007	13600	36615	53574	91377	89789	49101
4	*K*	14	13	13	11	3	3	5	5	2
	t	-157	-147	-153	-142	-163	-156	-128	-136	-162
	U	10246	9889	13054	12677	36338	53933	94314	93327	56482
5	*K*	-	-	-	-	95	34	-11	-9	9
	t	-	-	-	-	-4386	-4135	-3413	-3450	-4250
	U	-	-	-	-	36715	54710	95883	94234	58614
6	*K*	-	-	-	-	27	18	-2	-2	14
	t	-	-	-	-	-1383	-1315	-1081	-1111	-1383
	U	-	-	-	-	35738	53989	96336	94773	59549
7	*K*	-	-	-	-	69	63	46	48	60
	t	-	-	-	-	-1220	-1285	-1223	-1237	-1268
	U	-	-	-	-	31882	47502	85813	84345	47262

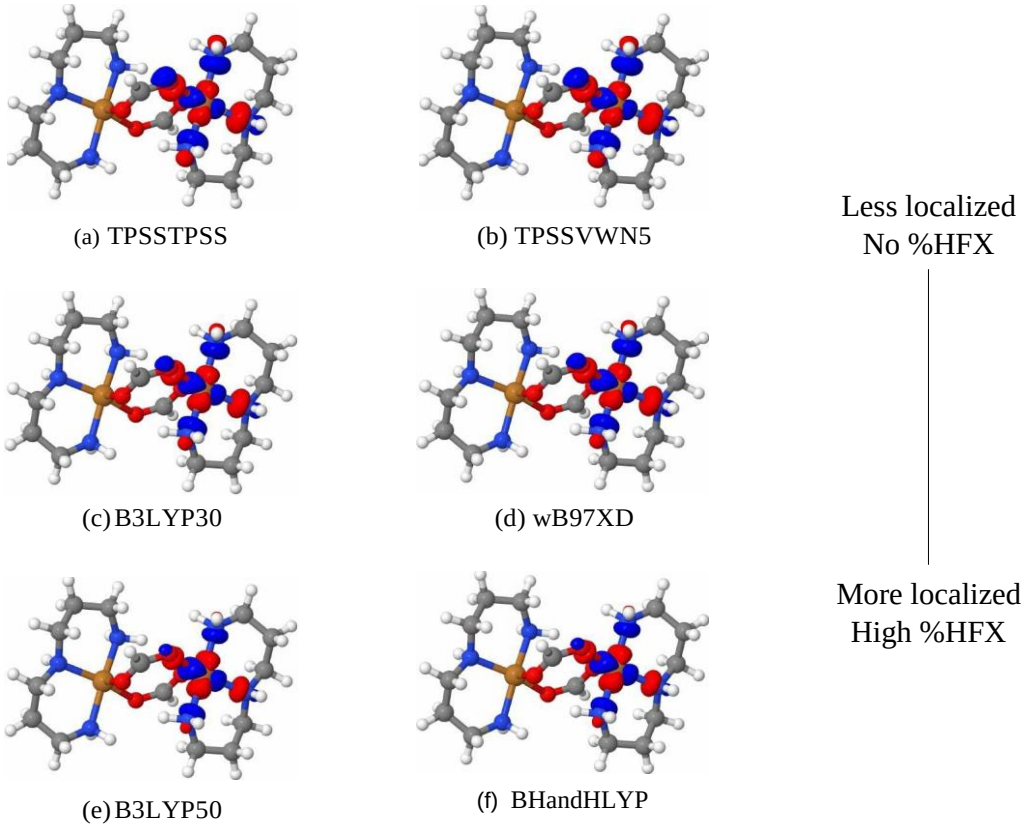

Figure S1: Magnetic orbitals *a* of compound **4** optimized using different functionals and amount of **HFX.**