

SUPPORTING INFORMATION

Title: Magnetic Coupling and Anisotropy in a Series of Mixed Chain Charge-Transfer Salts $[M(\text{Cp}^*)_2][M'(\text{tds})_2]$ ($M = \text{Fe, Mn, Cr}$; $M' = \text{Ni, Pt}$)

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The MM' intrachain distances, $D_{MM'}$, the angles between the stacking axis and the Cp rings, ξ_D , and the acceptors plane, ξ_A , as well as the dihedral angle between the Cp rings and the acceptors planes, ζ , are summarized in Table 1SP for compounds **1–6**.

Table S1. Summary of the interatomic separations and angles in the mixed stacks of compounds **1–6**.

	M–M' (Å) ^[a]	ξ_D (°) ^[b]	ξ_A (°) ^[c]	ζ (°) ^[d]	M'–C (Å); q ^[e]	M'–<C> (Å); q ^[f]	Se–C(Å); q ^[g]
1 ^[h]	5.566	81.3	80.5	2.2	3.844; 1.04	3.891; 1.05	3.846; 1.07
2 ^[h]	5.569	81.0	80.3	3.1	3.826; 0.98	3.891; 1.00	3.878; 1.08
3	5.590	81.5	80.7	2.5	3.803; 1.02	3.870; 1.05	3.833; 1.06
4	5.611	81.0	80.4	2.2	3.813; 0.98	3.883; 1.00	3.866; 1.07
5	5.659	81.8	80.7	2.3	3.810; 1.03	3.854; 1.04	3.827; 1.06
6	5.677	81.0	81.6	0.5	3.781; 0.97	3.906; 1.00	3.914; 1.09

[a] M–M' distance within the chain; [b] angle between the average plane of the Cp rings and the stacking axis; [c] angle between the average plane of the acceptors and the stacking axis; [d] dihedral angle between the average planes of the Cp rings and the acceptors; [e] shorter M'–C contact; [f] distance between M' and the Cp centroid; [g] closest separation between a Se atom from the acceptor and a C atom from the Cp ring; [h] from ref. [8]. Table 2. Summary of the interatomic separations and angles in the mixed stacks of compounds **1–6**.

The interchain separation, the closest M–M (M'–M'), M–M' and Se–Se distances are summarized in Table 2SP for compounds **1–6**.

Table S2. Summary of the interchain distances and selected interchain interatomic separations in compounds **1–6**.

	1 ^[a]	2 ^[a]	3	4	5	6
d^{I-II} (Å) ^[b]	8.338	8.388	8.342	8.403	8.352	8.382
d^{I-III} (Å) ^[b]	10.898	11.002	10.875	10.983	10.859	10.842
d^{I-IV} (Å) ^[b]	9.953	9.958	9.936	9.957	9.935	9.868
MM^{I-II} (Å) ^[c]	8.059	8.606	8.582	8.614	8.580	8.568
MM^{I-II} (Å) ^[d]	9.059	9.148	9.077	9.189	9.135	9.282
MM^{I-III} (Å) ^[c]	12.097	12.218	12.107	12.249	12.165	12.311
MM^{I-III} (Å) ^[d]	10.902	11.005	10.879	10.985	10.862	10.842
MM^{I-IV} (Å) ^[c]	10.464	10.521	10.471	10.559	10.541	12.322
MM^{I-IV} (Å) ^[d]	10.225	10.194	10.195	10.175	10.163	10.026
c^{I-II} (Å); q ^[e]	4.582; 1.15	4.349; 1.09	4.574; 1.14	4.331; 1.08	4.568; 1.14	4.234; 1.06

[a] from ref. [8]; [b] interchain distance; [c] closest distance between the identical metallic elements in neighboring chains; [d] closest distance between the distinct metallic elements in neighboring chains; [e] shorter Se–Se contact in neighbouring chain (pair I-II).