Supplementary Information

A simple methodology for constructing ferromagnetically coupled Cr(III) compounds

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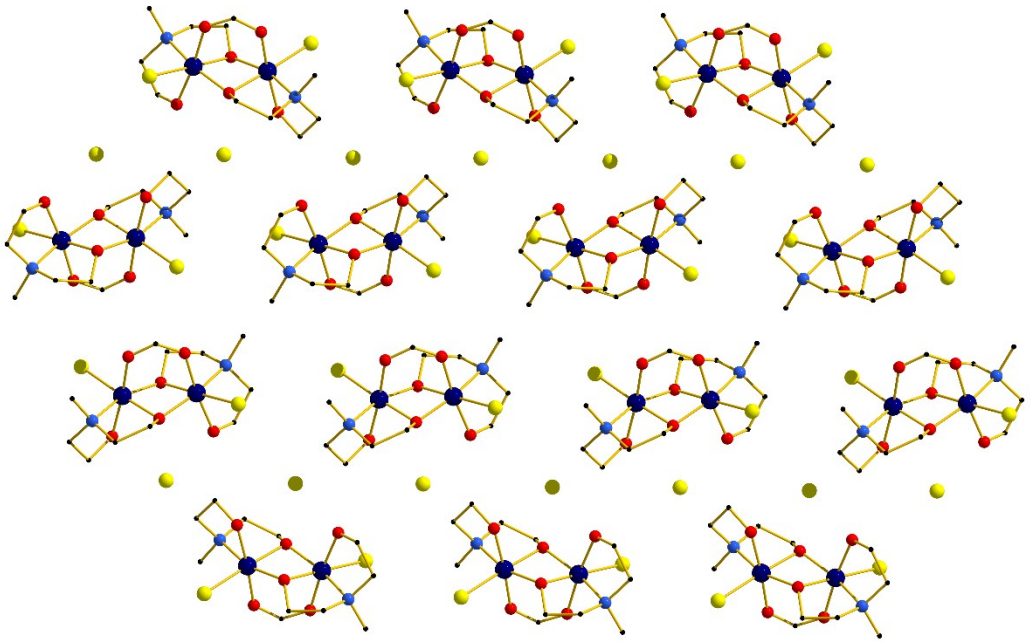

Figure S1. Packing diagram for compound **1** viewed along the *a*-axis.

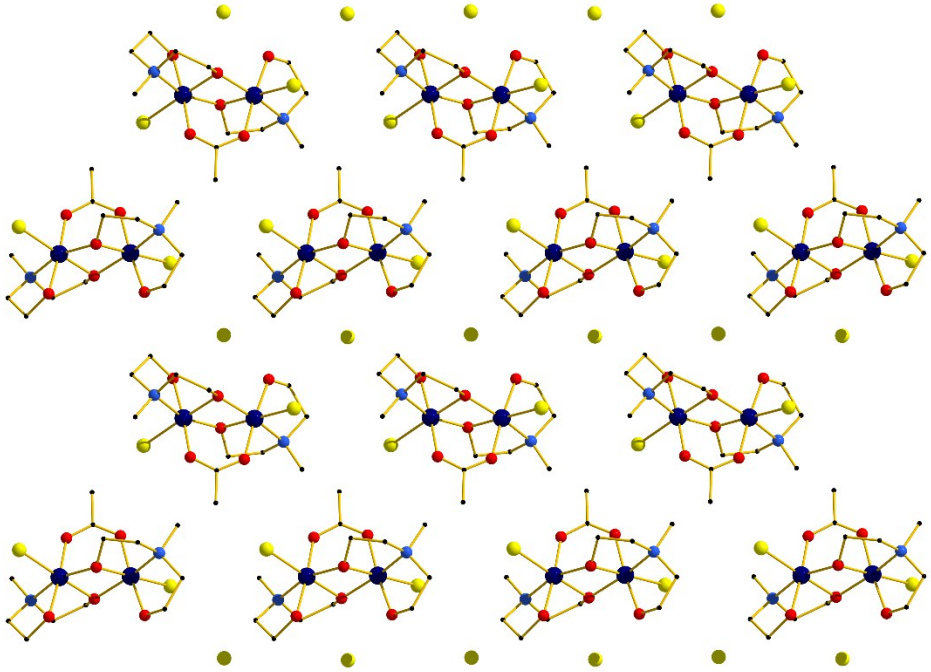

Figure S2. Packing diagram for compound **2** viewed along the *a*-axis.

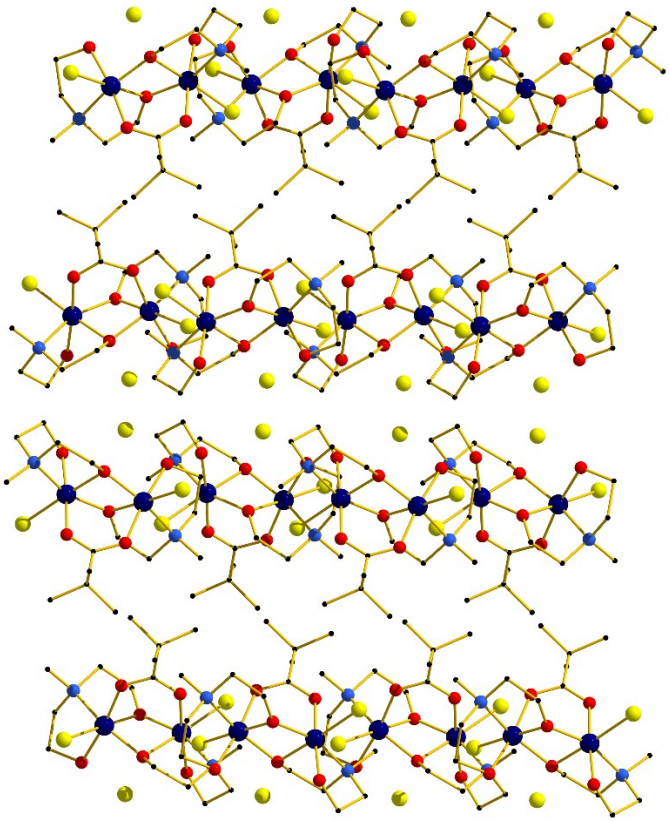

Figure S3. Packing diagram for compound **3** viewed along the *a*-axis.

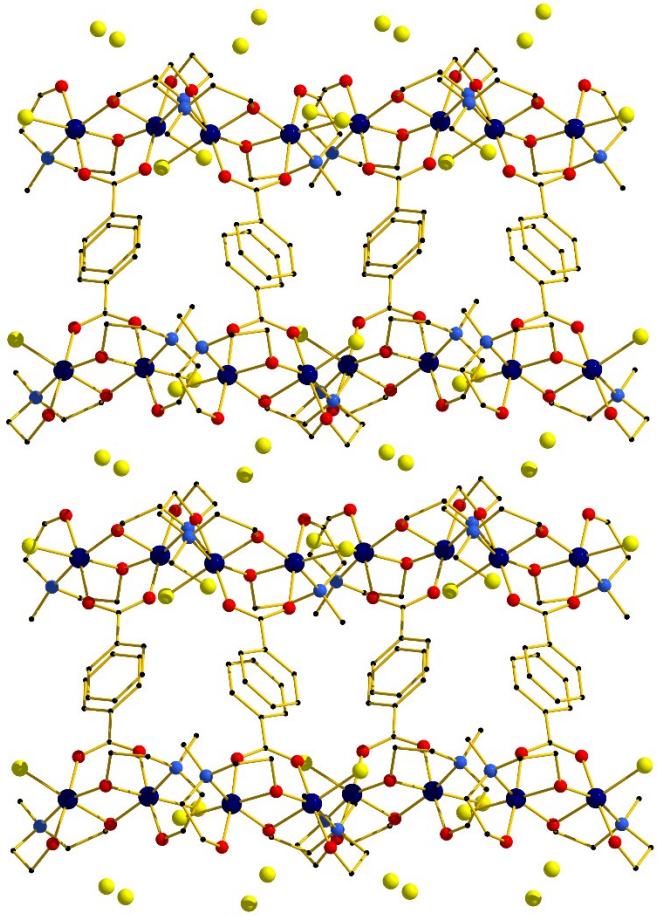

Figure S4. Packing diagram for compound **4** viewed along the *c*-axis.

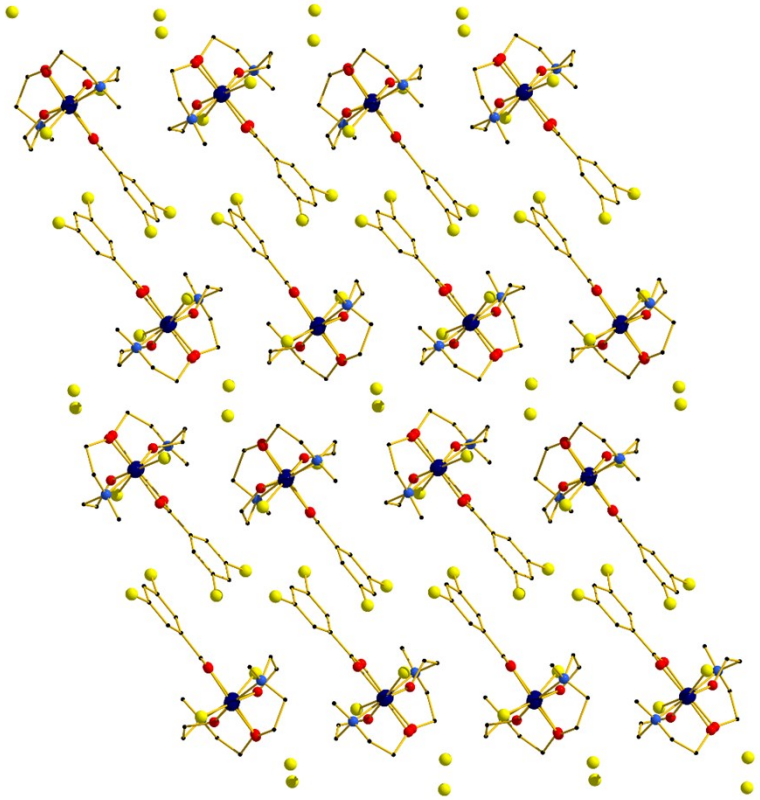

Figure S5. Packing diagram for compound **5** viewed along the *a*-axis.

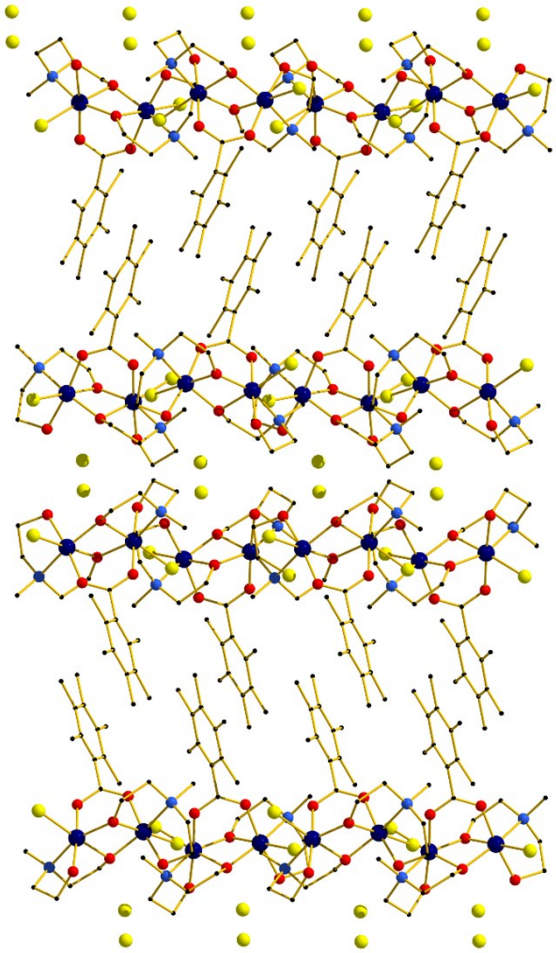

Figure S6. Packing diagram for compound **6** viewed along the *a*-axis.

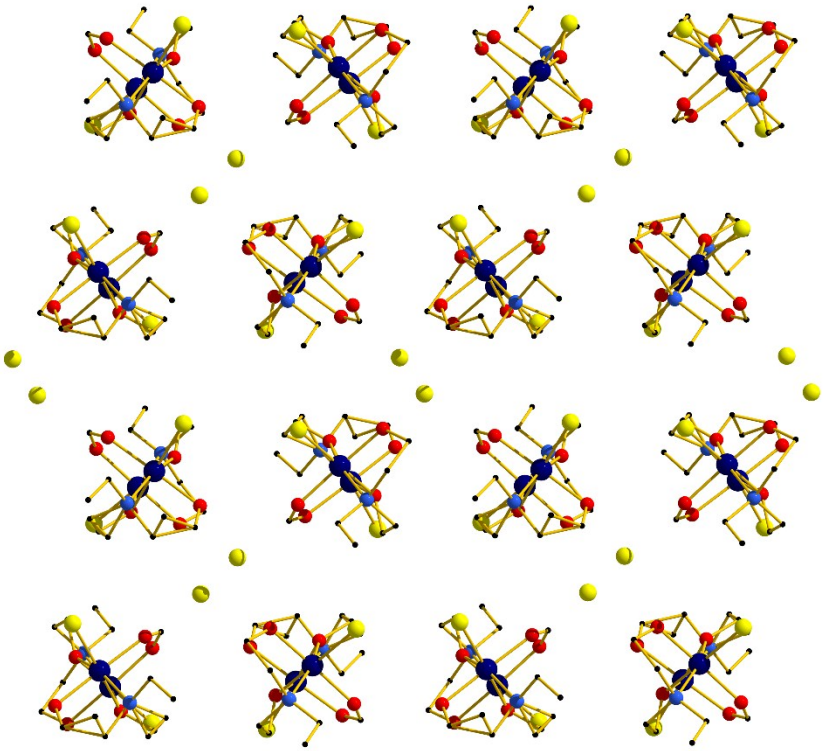

Figure S7. Packing diagram for compound **7** viewed along the *a*-axis.

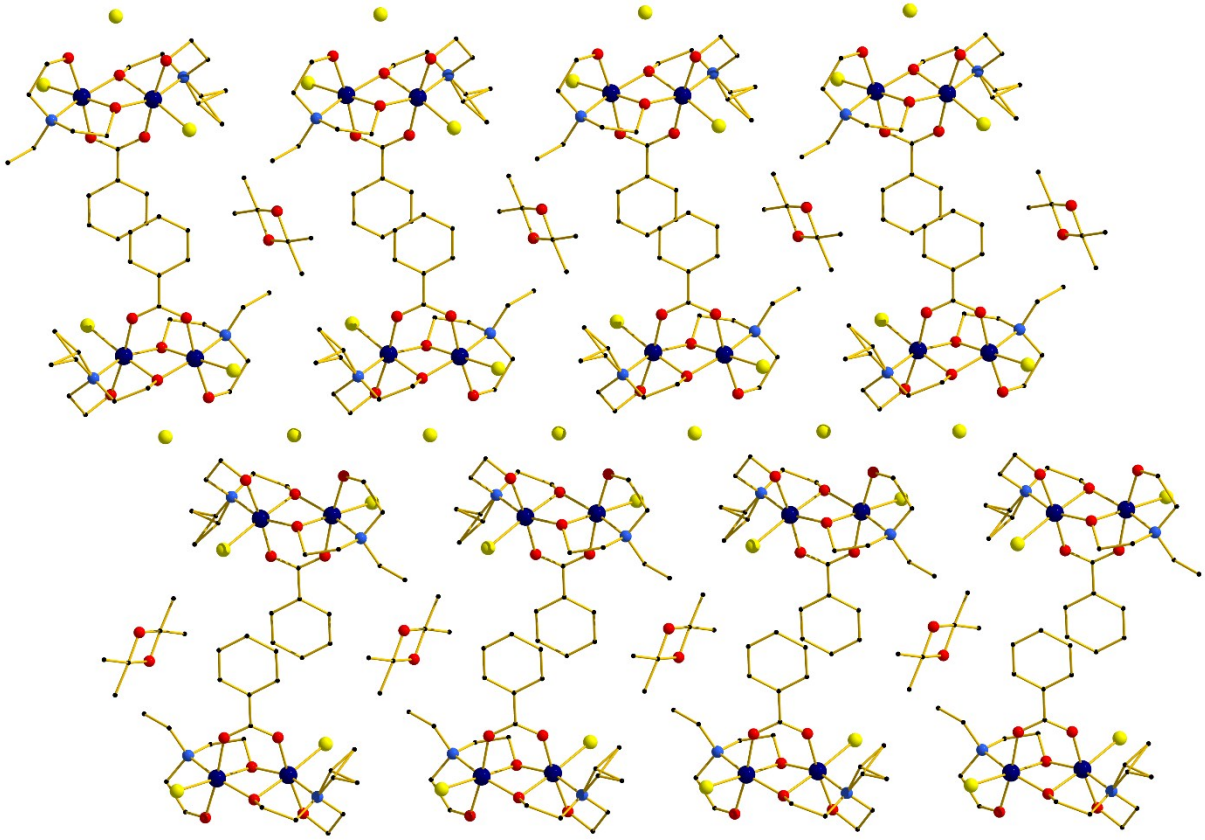

Figure S8. Packing diagram for compound **8** viewed along the *a*-axis.

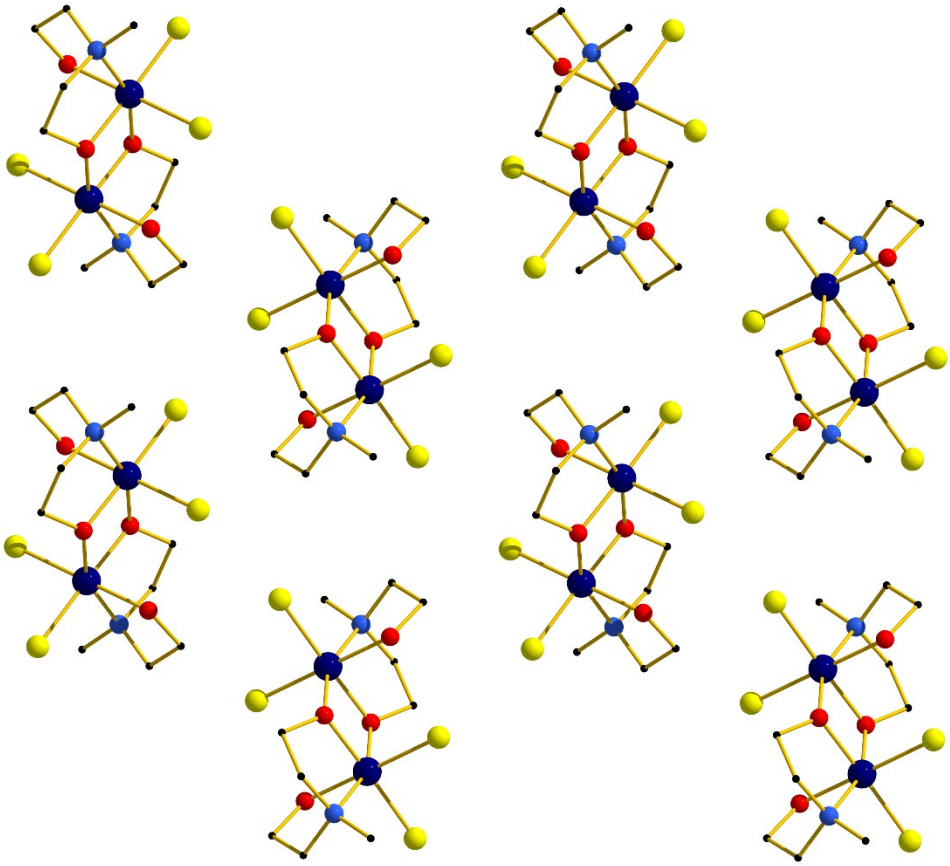

Figure S9. Packing diagram for compound **9** viewed along the *a*-axis.

Table S1. Crystallographic information for compounds **1**-**6**.

Compound	**1**	**2**	**3**	**4**	**5**	**6**
Formula	$C_{11}H_{25}Cl_3Cr_2N_2O_6$	$C_{12}H_{27}Cl_3Cr_2N_2O_6$	$C_{15}H_{33}Cl_3Cr_2N_2O_6$	$C_{17}H_{29}Cl_3Cr_2N_2O_6$	$C_{17}H_{27}Cl_5Cr_2N_2O_6$	$C_{22}H_{39}Cl_3Cr_2N_2O_6$
$D_{calc.}$/ g cm^{-3}	1.721	1.703	1.594	1.618	1.660	1.494
μ/mm^{-1}	1.596	1.538	1.335	1.311	12.174	1.087
Formula Weight	491.68	505.70	547.78	567.77	636.65	637.90
Colour	dark green	dark green	pale green	dark purple	dark purple	pale green
Shape	block	block	plate	block	plate	plate
Size/mm^3	0.41×0.14×0.07	0.39×0.33×0.25	0.53×0.37×0.03	0.47×0.28×0.19	0.32×0.07×0.03	0.45×0.32×0.02
T/K	120.0	120.0	120.0	120.0	120.0	120.0
Crystal System	monoclinic	monoclinic	orthorhombic	monoclinic	triclinic	orthorhombic
Flack/Hooft Parameters	-	0.005(10)/-0.003(9)	-	-	-	-
Space Group	$P2_1/c$	$P2_1$	Pbca	$P2_1/c$	P-1	Pbca
a/Å	7.1130(3)	7.10996(16)	14.0747(4)	16.1908(3)	10.2393(2)	14.0888(6)
b/Å	10.2464(5)	10.2978(2)	10.3531(2)	10.41623(19)	14.2193(3)	10.2661(4)
c/Å	26.0466(13)	13.8317(3)	31.3324(10)	14.1087(3)	18.1746(4)	39.2028(19)
α/°	90	90	90	90	76.834(2)	90
β/°	91.273(4)	103.201(2)	90	101.560(2)	81.3824(19)	90
γ/°	90	90	90	90	89.2989(19)	90
V/Å^3	1897.88(15)	985.95(4)	4565.6(2)	2331.11(8)	2546.84(10)	5670.2(4)
Z (Z')	4 (1)	2 (1)	8 (1)	4 (1)	4 (2)	8 (1)
Wavelength/Å	0.71073	0.71073	0.71073	0.71073	1.54184	0.71073
Radiation type	MoK_α	MoK_α	MoK_α	MoK_α	CuK_α	MoK_α
Θ_{min}/° - Θ_{max}/°	3.076 - 28.753	2.943 – 31.252	2.767 - 31.223	2.970 – 31.306	3.193 – 76.399	2.892 – 25.350
Measured Refl.	111506	31889	48743	48698	51940	41273
Independent Refl.	5954	5981	6888	7156	10528	5174
Reflections Used	5411	5674	5507	6488	9114	3810
R_{int}	0.0863	0.0503	0.0806	0.0417	0.0909	0.1282
Parameters	226	237	264	281	593	329
Restraints	2	1	2	0	4	2
Largest Peak	0.552	0.347	0.520	0.516	1.591	0.490
Deepest Hole	-0.587	-0.487	-0.559	-0.469	-1.041	-0.388
GooF	1.117	1.057	1.110	1.040	1.040	0.933
wR_2 (all data) (wR_2)	0.0984 (0.0970)	0.0582 (0.0564)	0.0990 (0.0915)	0.0696 (0.0671)	0.1546 (0.1471)	0.1536 (0.1334)
R_1 (all data) (R_1)	0.0483 (0.0419)	0.0302 (0.0274)	0.0720 (0.0506)	0.0334 (0.0286)	0.0632 (0.0560)	0.0823 (0.0522)

Table S2. Crystallographic information for compounds **7**-**9**.

Compound	**7**	**8**	**9**
Formula	$C_{13}H_{29}Cl_3Cr_2N_2O_6$	$C_{42}H_{76}Cl_6Cr_4N_4O_{13}$	$C_{10}H_{24}Cl_4Cr_2N_2O_4$
$D_{calc.}$/ g cm^{-3}	1.646	1.525	1.813
μ/mm^{-1}	1.449	1.119	1.851
Formula Weight	519.73	1265.76	482.11
Colour	dark green	dark green	dark purple
Shape	block	block	block
Size/mm^3	0.51×0.24×0.23	0.35×0.09×0.05	0.34×0.12×0.07
T/K	120.0	120.0	120.0
Crystal System	monoclinic	monoclinic	monoclinic
Flack/Hooft Parameters	-	-	-
Space Group	$P2_1/c$	$P2_1/c$	$P2_1/n$
a/Å	11.5711(3)	7.1699(2)	6.8880(2)
b/Å	13.2720(3)	11.0066(3)	9.9275(3)
c/Å	13.6565(3)	34.9817(7)	12.9510(3)
α/°	90	90	90
β/°	90.948(2)	93.103(2)	94.457(3)
γ/°	90	90	90
V/Å^3	2096.96(9)	2756.58(12)	882.91(4)
Z (Z')	4 (1)	2 (0.5)	2 (0.5)
Wavelength/Å	0.71073	0.71073	0.71073
Radiation type	MoK_α	MoK_α	MoK_α
Θ_{min}/° - Θ_{max}/°	3.413 – 29.786	2.845 - 29.773	3.155 – 29.807
Measured Refl.	36587	48300	15425
Independent Refl.	5540	7202	2315
Reflections Used	4952	5556	2149
R_{int}	0.0434	0.0586	0.0378
Parameters	264	365	148
Restraints	43	9	0
Largest Peak	0.813	0.449	0.378
Deepest Hole	-0.495	-0.496	-0.395
GooF	1.079	1.034	1.083
wR_2 (all data) (wR_2)	0.0955 (0.0924)	0.0860 (0.0813)	0.0576 (0.0560)
R_1 (all data) (R_1)	0.0475 (0.0415)	0.0629 (0.0407)	0.0284 (0.0250)

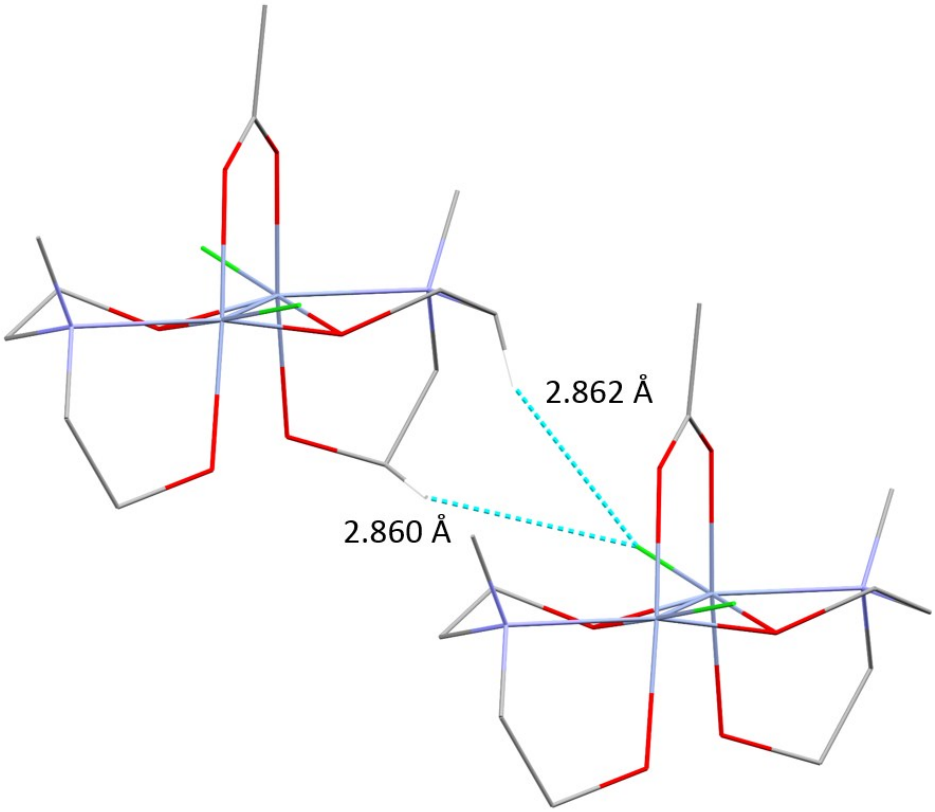

Figure S10. Representative diagrammatic example of $d_{H(Me)\text{-}Cl}$ closest interactions between two dimers in compound **2**. Non-relevant hydrogens and anions have been omitted for clarity.

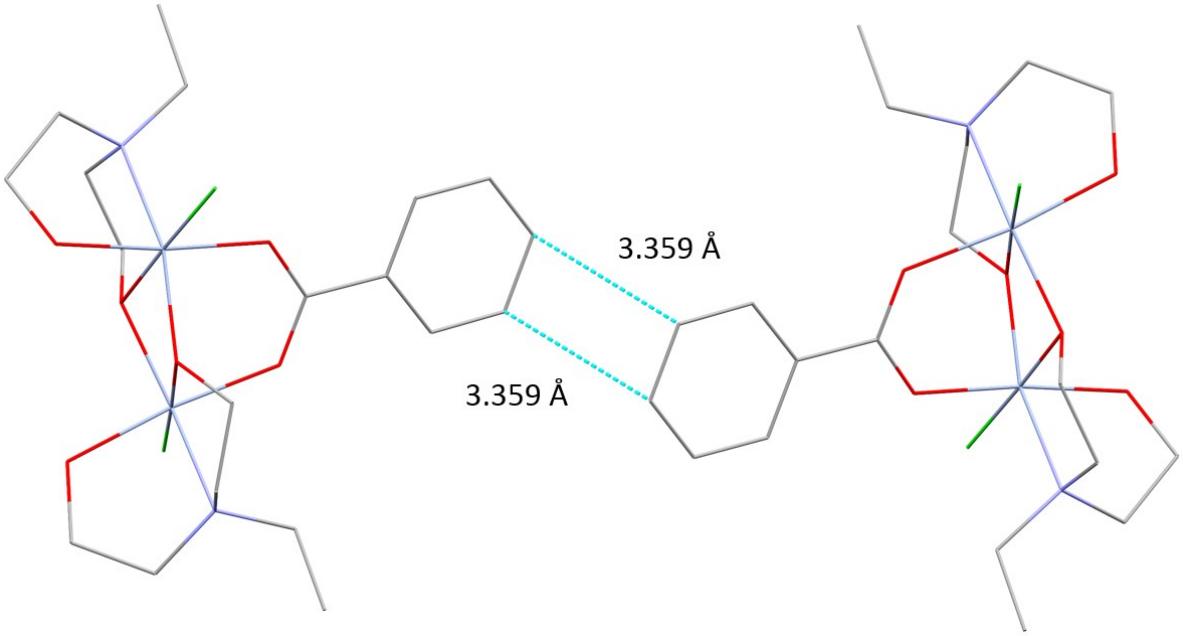

Figure S11. Representative diagrammatic example of $d_{\pi\text{-}\pi}$ closest interactions between two dimers in compound **8**. Hydrogens and anions have been omitted for clarity.

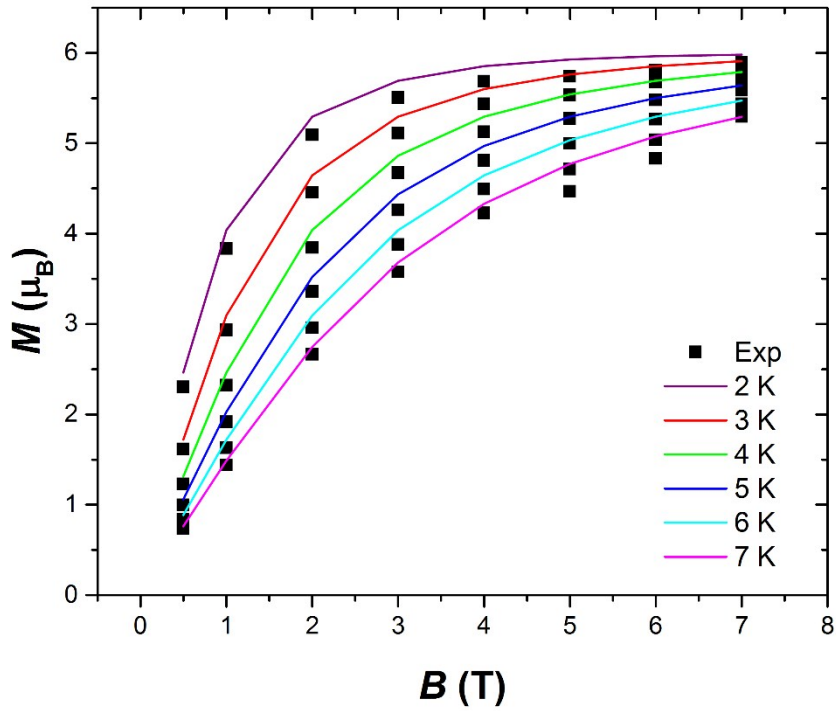

Figure S12. Plot of the magnetization (*M*) versus field (*B*) for compound **1** in the indicated field and temperature ranges. The solid black lines are a fit of the experimental data. See text for full details.

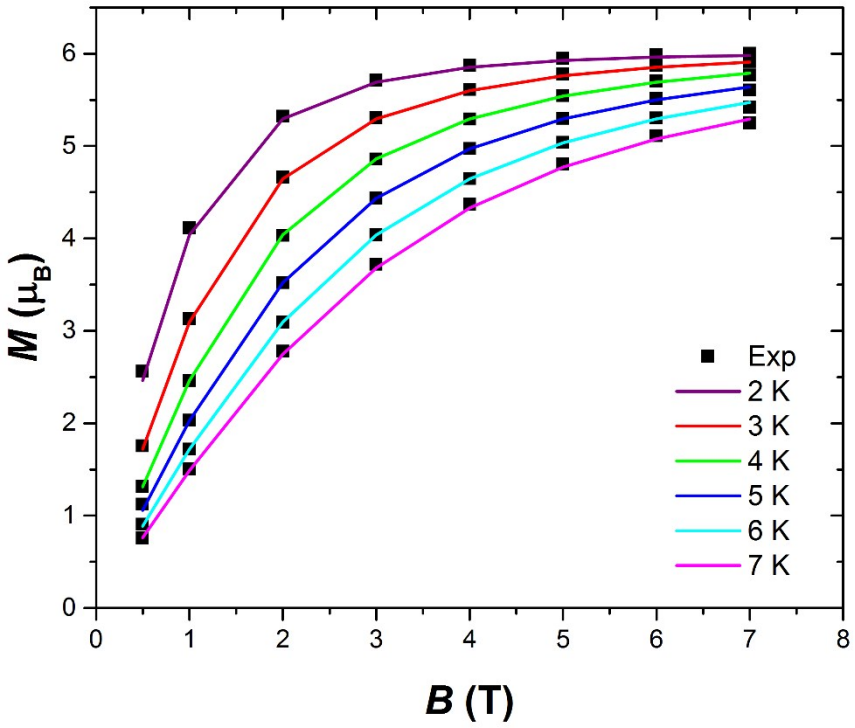

Figure S13. Plot of the magnetization (*M*) versus field (*B*) for compound **2** in the indicated field and temperature ranges. The solid black lines are a fit of the experimental data. See text for full details.

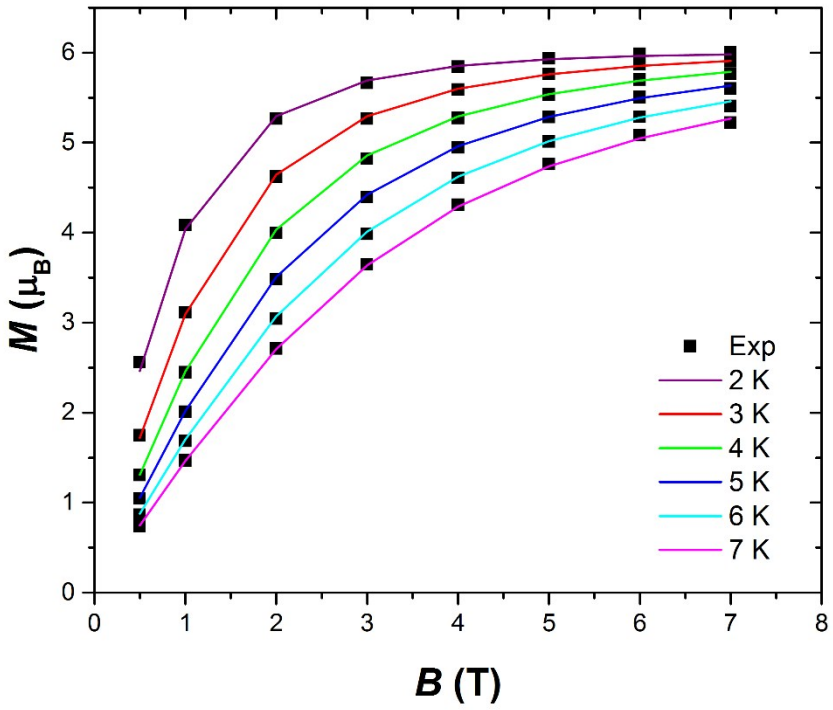

Figure S14. Plot of the magnetization (*M*) versus field (*B*) for compound **3** in the indicated field and temperature ranges. The solid black lines are a fit of the experimental data. See text for full details.

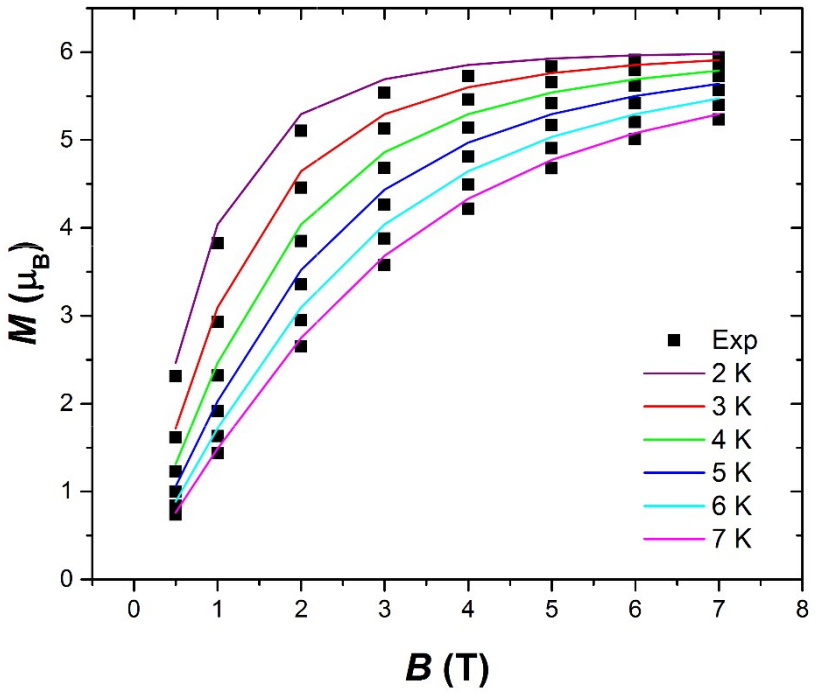

Figure S15. Plot of the magnetization (*M*) versus field (*B*) for compound **4** in the indicated field and temperature ranges. The solid black lines are a fit of the experimental data. See text for full details.

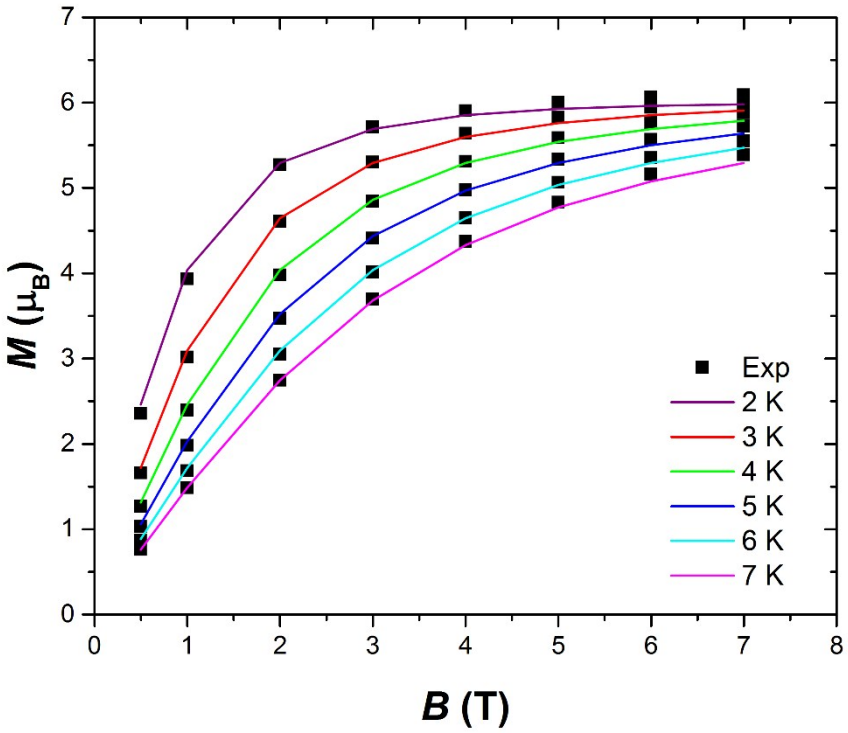

Figure S16. Plot of the magnetization (*M*) versus field (*B*) for compound **5** in the indicated field and temperature ranges. The solid black lines are a fit of the experimental data. See text for full details.

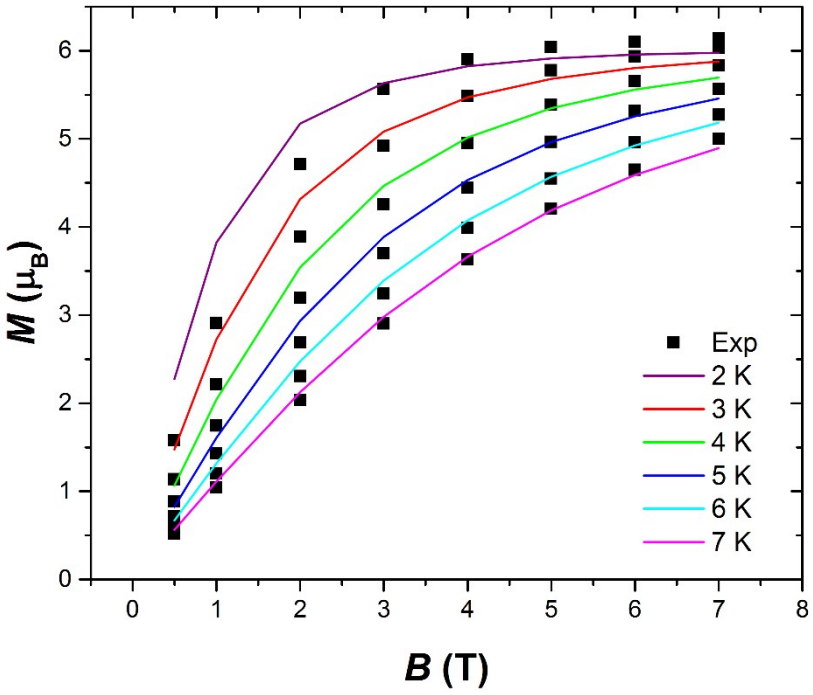

Figure S17. Plot of the magnetization (*M*) versus field (*B*) for compound **6** in the indicated field and temperature ranges. The solid black lines are a fit of the experimental data. See text for full details.

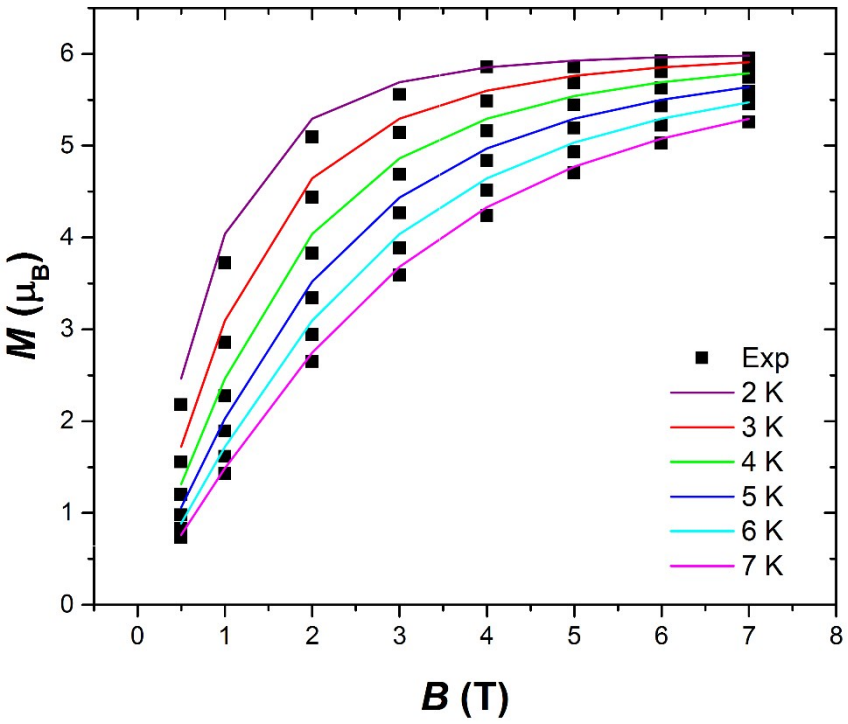

Figure S18. Plot of the magnetization (*M*) versus field (*B*) for compound **7** in the indicated field and temperature ranges. The solid black lines are a fit of the experimental data. See text for full details.

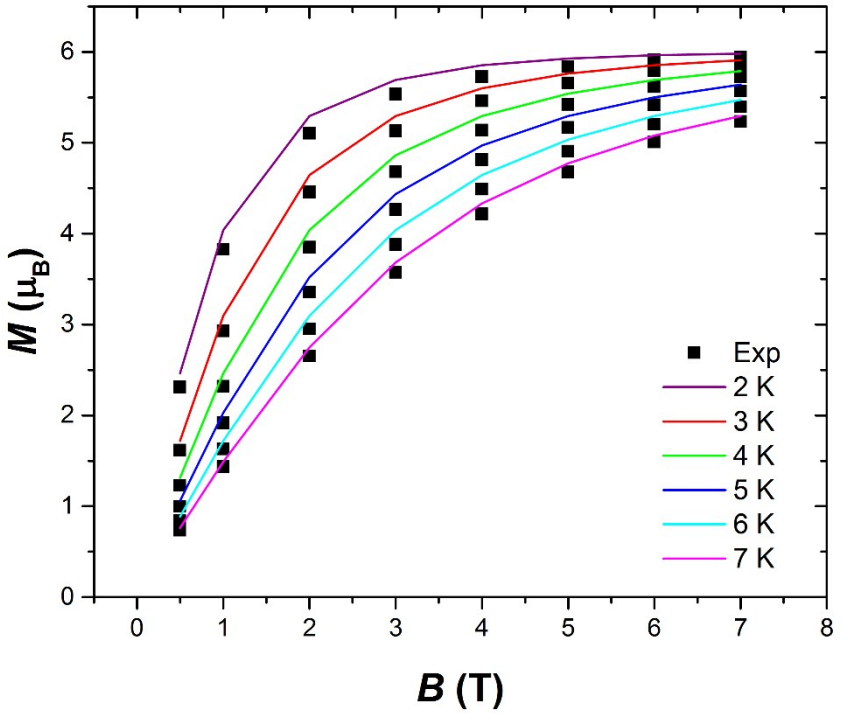

Figure S19. Plot of the magnetization (*M*) versus field (*B*) for compound **8** in the indicated field and temperature ranges. The solid black lines are a fit of the experimental data. See text for full details.

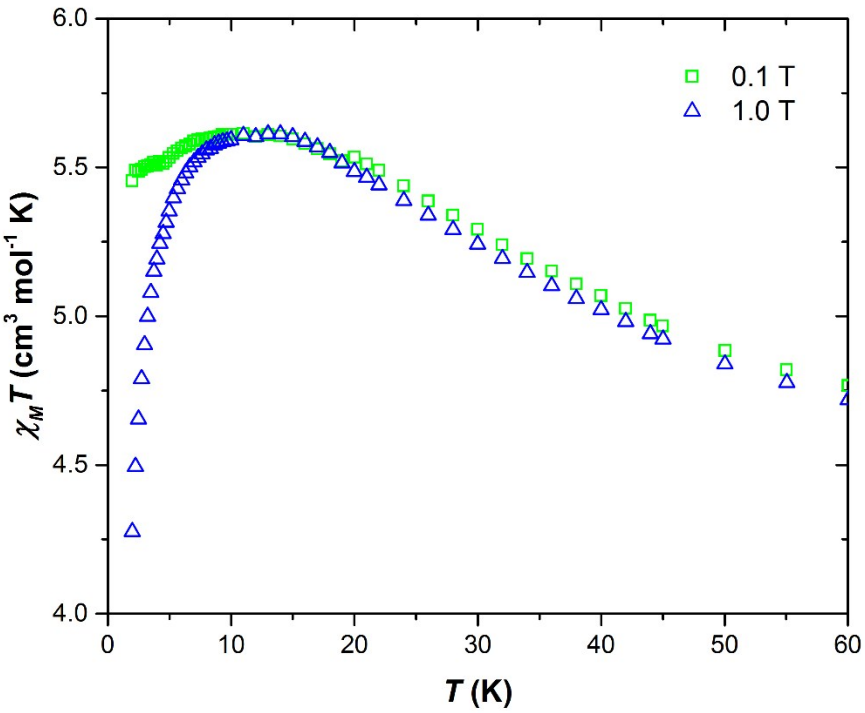

Figure S20. Plot of the $\chi_M T$ product versus T for complex **1** in applied fields of 0.1 T and 1.0 T as shown. The graph shows the field dependence of the intermolecular interactions. See main text for full details.

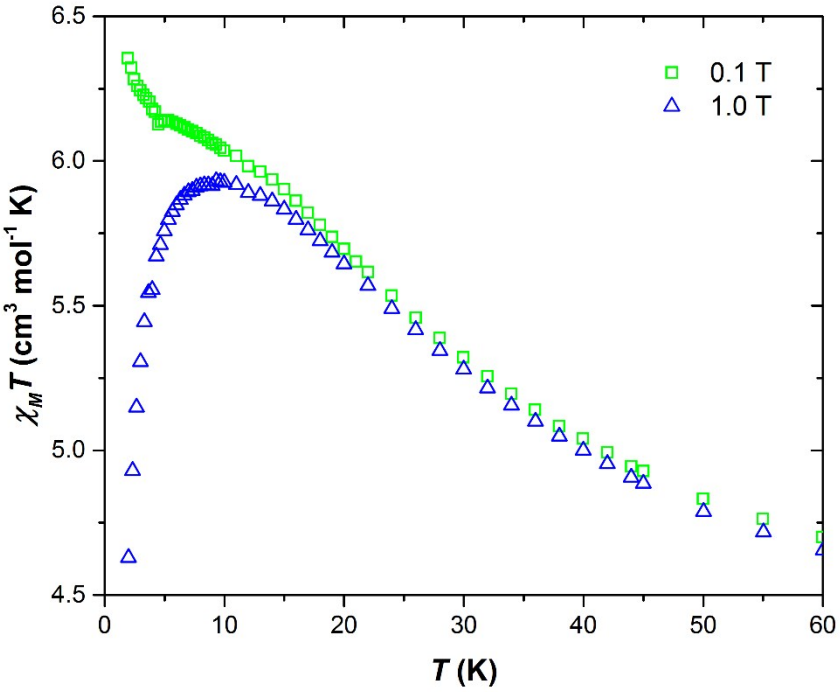

Figure S21. Plot of the $\chi_M T$ product versus T for complex **2** in applied fields of 0.1 T and 1.0 T as shown. The graph shows the field dependence of the intermolecular interactions. See main text for full details.

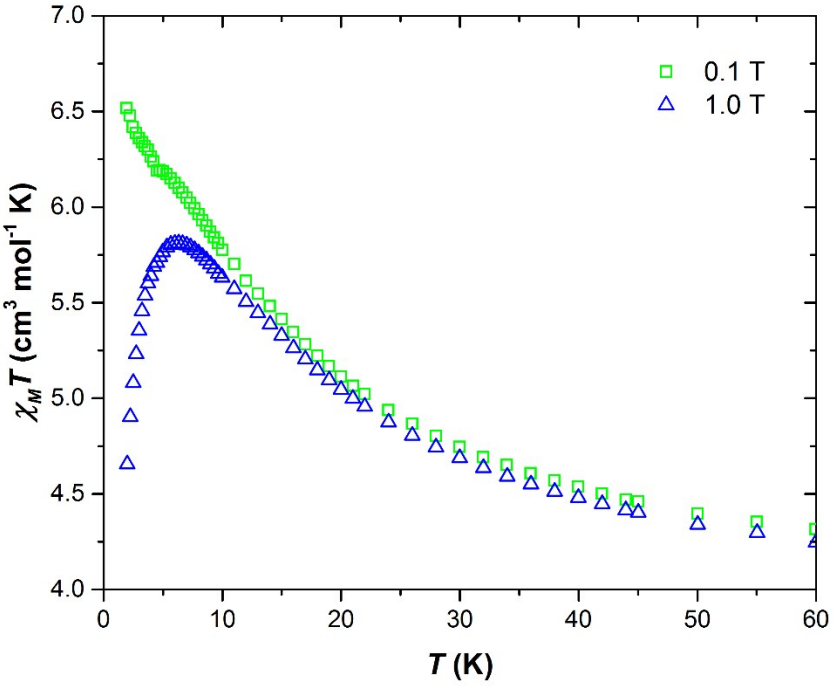

Figure S22. Plot of the $\chi_M T$ product versus T for complex **3** in applied fields of 0.1 T and 1.0 T as shown. The graph shows the field dependence of the intermolecular interactions. See main text for full details.

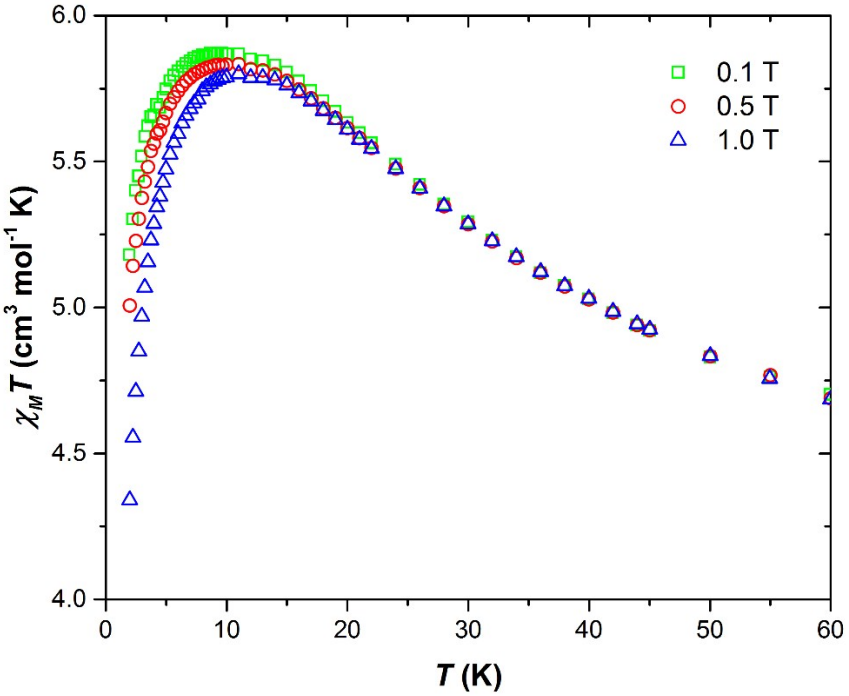

Figure S23. Plot of the $\chi_M T$ product versus T for complex **4** in applied fields of 0.1 T, 0.5 T and 1.0 T as shown. The graph shows the field dependence of the intermolecular interactions. See main text for full details.

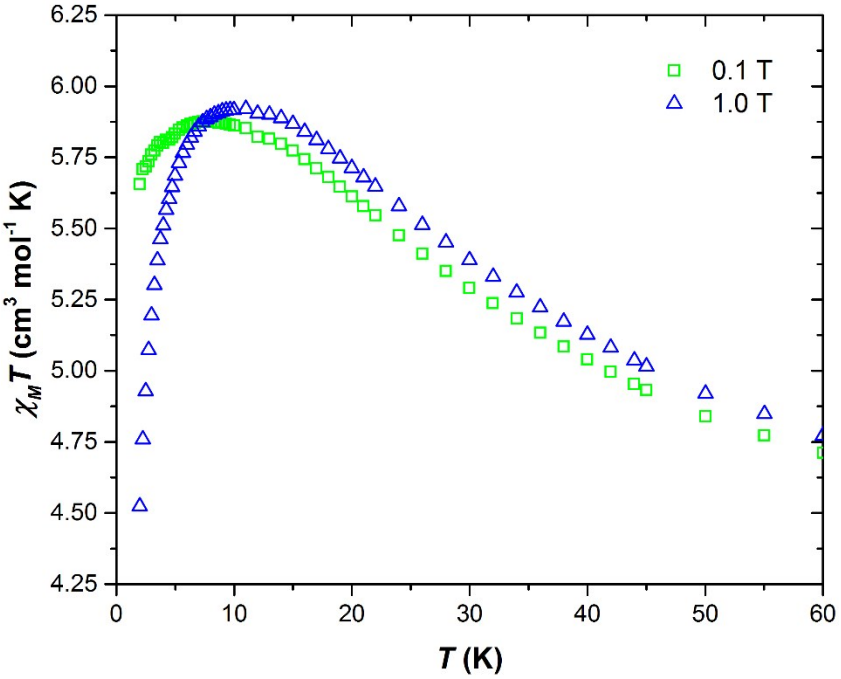

Figure S24. Plot of the $\chi_M T$ product versus T for complex **5** in applied fields of 0.1 T and 1.0 T as shown. The graph shows the field dependence of the intermolecular interactions. See main text for full details.

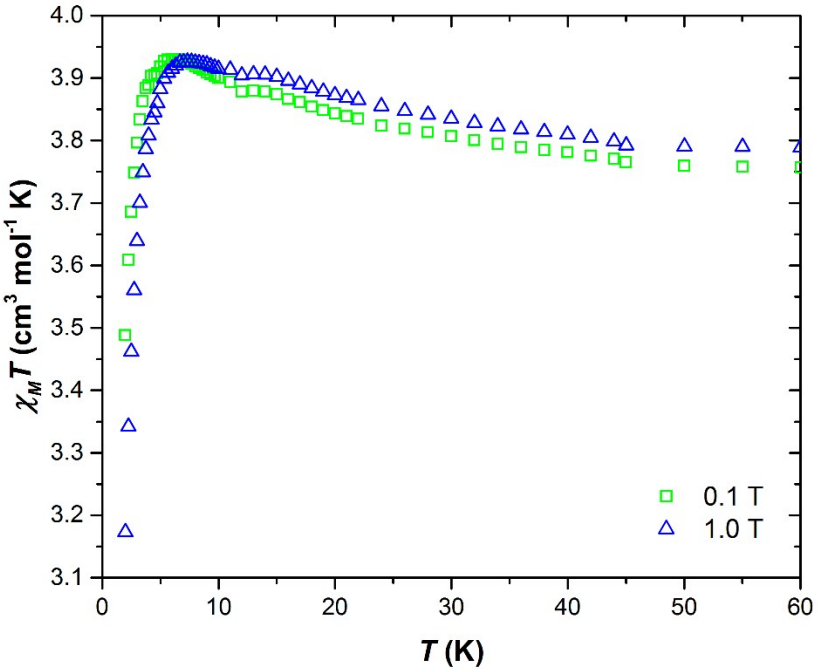

Figure S25. Plot of the $\chi_M T$ product versus T for complex **6** in applied fields of 0.1 T and 1.0 T as shown. The graph shows the field dependence of the intermolecular interactions. See main text for full details.

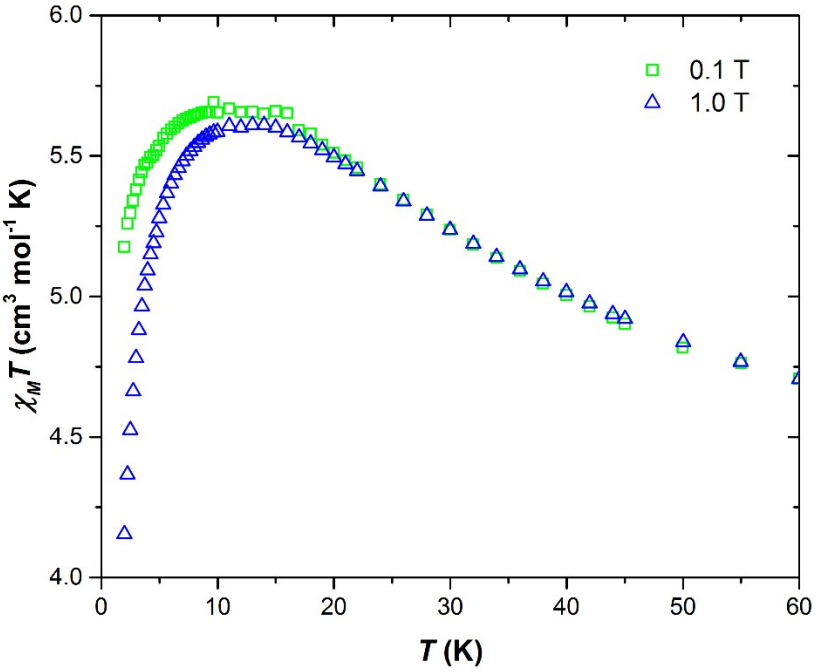

Figure S26. Plot of the $\chi_M T$ product versus *T* for complex **7** in applied fields of 0.1 T and 1.0 T as shown. The graph shows the field dependence of the intermolecular interactions. See main text for full details.

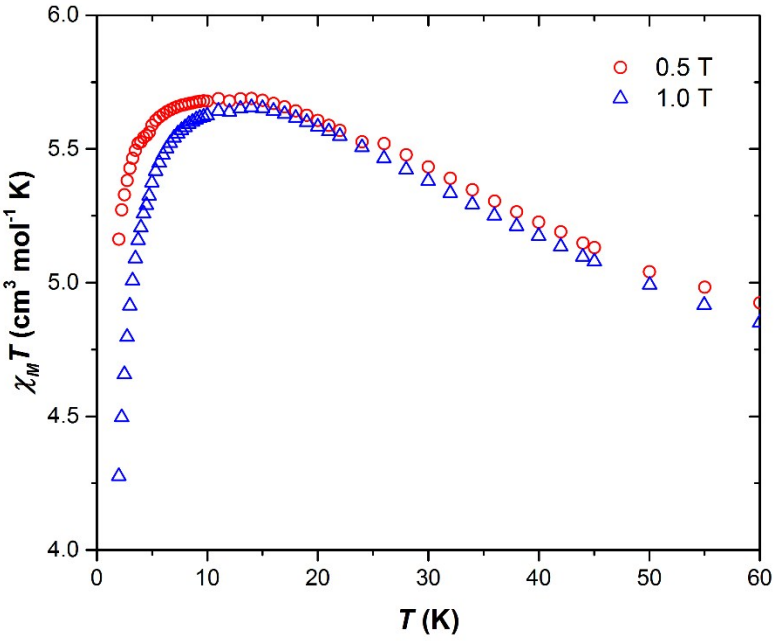

Figure S27. Plot of the $\chi_M T$ product versus *T* for complex **8** in applied fields of 0.5 T and 1.0 T as shown. The graph shows the field dependence of the intermolecular interactions. See main text for full details.

Table S3. *J* values using the GHP model.

Complex	*J* (cm^{-1})
1	0.65
2	-1.34
3	21.38
4	0.42
5	11.87
6	10.60
7	15.86
8	17.30
9	-682.46

Table S4. Overlap integrals for compounds **1**-**9**.

Overlap integral of complex **1**

Beta **Alpha**	$\mathbf{d_{xy}}$	$\mathbf{d_{yz}}$	$\mathbf{d_{xz}}$
$\mathbf{d_{xy}}$	0.137	-0.153	-0.217
$\mathbf{d_{yz}}$	-0.100	-0.21	-0.041
$\mathbf{d_{xz}}$	0.038	-0.006	-0.049

Overlap integral of complex **2**

Beta **Alpha**	$\mathbf{d_{xy}}$	$\mathbf{d_{yz}}$	$\mathbf{d_{xz}}$
$\mathbf{d_{xy}}$	-0.075	0.031	-0.034
$\mathbf{d_{yz}}$	0.024	-0.011	-0.003
$\mathbf{d_{xz}}$	0.097	-0.017	-0.157

Overlap integral of complex **3**

Beta **Alpha**	$\mathbf{d_{xy}}$	$\mathbf{d_{yz}}$	$\mathbf{d_{xz}}$
$\mathbf{d_{xy}}$	-0.080	-0.103	0.004
$\mathbf{d_{yz}}$	0.065	-0.006	0.083
$\mathbf{d_{xz}}$	-0.023	-0.003	0.303

Overlap integral of complex **4**

Beta **Alpha**	$\mathbf{d_{xy}}$	$\mathbf{d_{yz}}$	$\mathbf{d_{xz}}$
$\mathbf{d_{xy}}$	-0.079	0.095	-0.001
$\mathbf{d_{yz}}$	-0.079	-0.130	-0.049
$\mathbf{d_{xz}}$	0.006	-0.068	0.042

Overlap integral of complex **5**

Beta **Alpha**	$\mathbf{d_{xy}}$	$\mathbf{d_{yz}}$	$\mathbf{d_{xz}}$
$\mathbf{d_{xy}}$	0.078	0.162	0.087
$\mathbf{d_{yz}}$	-0.151	-0.246	-0.048
$\mathbf{d_{xz}}$	0.071	-0.063	0.037

Overlap integral of complex **6**

Beta **Alpha**	$\mathbf{d_{xy}}$	$\mathbf{d_{yz}}$	$\mathbf{d_{xz}}$
$\mathbf{d_{xy}}$	0.021	-0.074	0.008
$\mathbf{d_{yz}}$	0.111	0.043	-0.158
$\mathbf{d_{xz}}$	0.012	-0.084	0.064

Overlap integral of complex **7**

Beta **Alpha**	$\mathbf{d_{xy}}$	$\mathbf{d_{yz}}$	$\mathbf{d_{xz}}$
$\mathbf{d_{xy}}$	-0.069	-0.067	0.009
$\mathbf{d_{yz}}$	-0.181	0.016	-0.161
$\mathbf{d_{xz}}$	0.038	-0.068	0.038

Overlap integral of complex **8**

Beta Alpha	d_{xy}	d_{yz}	d_{xz}
d_{xy}	-0.069	-0.067	0.009
d_{yz}	-0.181	0.016	-0.161
d_{xz}	0.038	-0.069	0.038

Overlap integral of complex **9**

Beta Alpha	d_{xy}	d_{yz}	d_{xz}
d_{xy}	-0.115	0.036	-0.079
d_{yz}	0.036	0.047	-0.101
d_{xz}	0.079	0.101	0.150

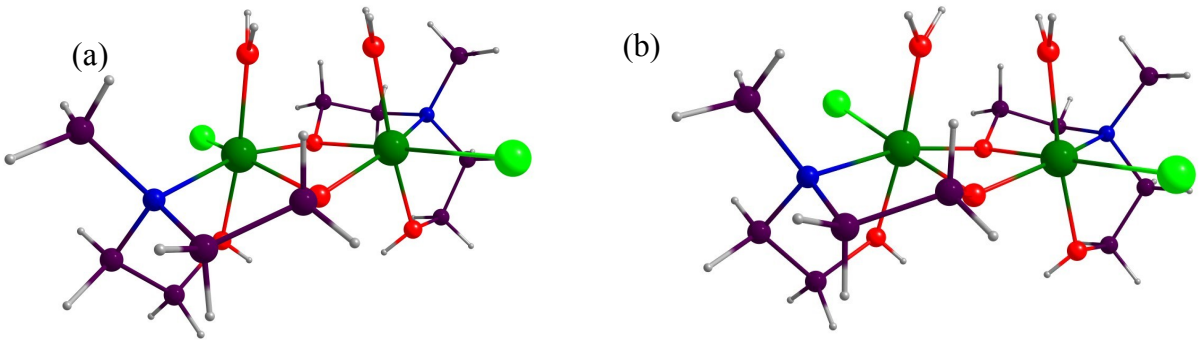

Figure S28. Structure of complexes (a) **1a** and (b) **4a**.

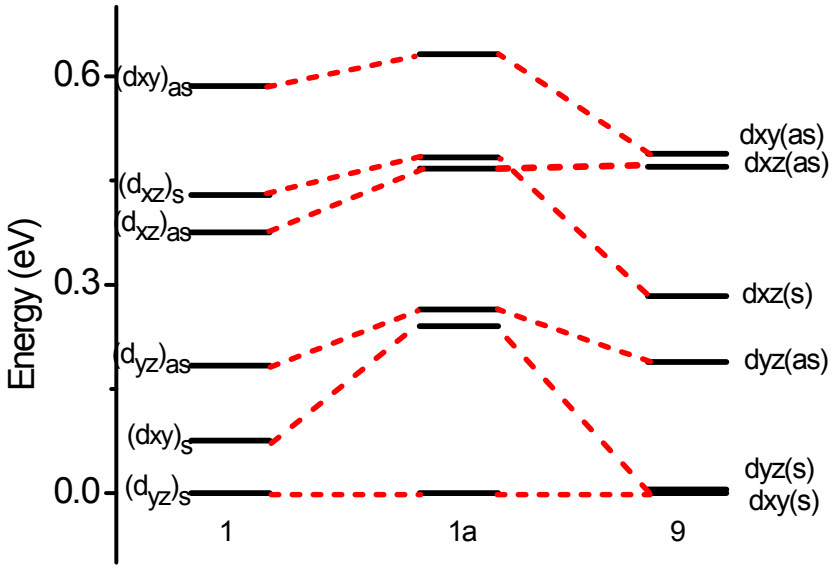

Figure S29. MO energy level splitting for **1**, **1a** and **9**.

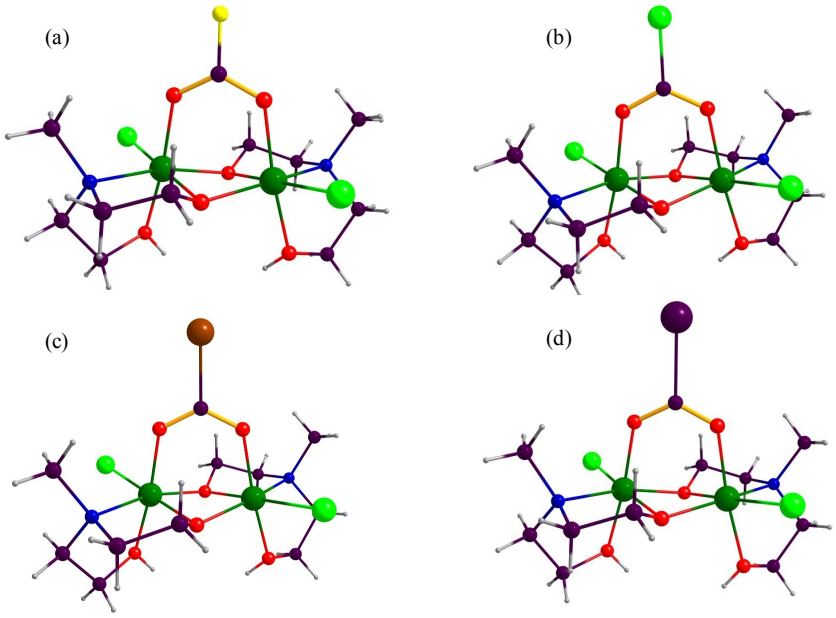

Figure S30. Halogen substitution in **1**. Substitution with fluorine (a), chlorine (b), bromine (c) and iodine (d).

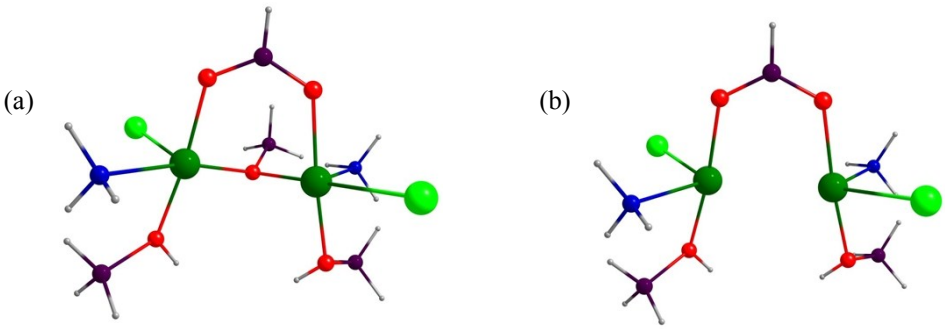

Figure S31. (a) Structure of complex **1b**. (b) Structure of complex **1c**.

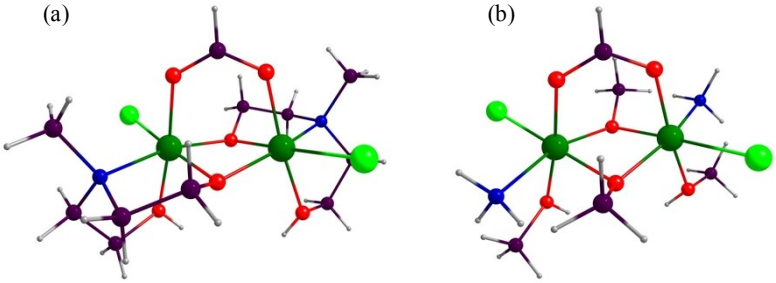

Figure S32. (a) Structure of complex **1** (J = 6.3 cm^{-1}). (b) Structure of the model complex derived from complex **1** (J = 7.4 cm^{-1}) for the magneto-structural correlation.

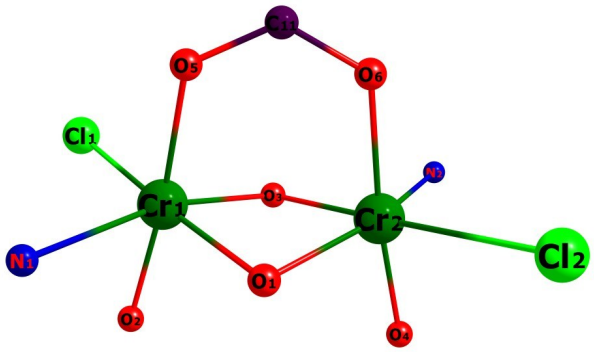

Figure S33. Model complex showing the atomic numbering scheme for spin density calculations.

Table S5. DFT computed spin densities of the chromium ions and atoms bonded to chromium ions for **1**-**9**.

	1		**2**		**3**		**4**		**5**	
	HS	**BS**	**HS**	**BS**	**HS**	**HS**	**HS**	**BS**	**HS**	**BS**
Cr1	3.015	3.012	3.014	3.010	3.006	3.006	3.009	3.004	3.009	3.005
Cr2	3.009	-3.006	3.011	-3.007	3.002	3.002	3.009	-3.004	3.012	-3.007
O1	0.008	-0.003	0.000	-0.000	-0.000	-0.000	-0.001	-0.001	-0.002	-0.000
O2	-0.012	-0.011	-0.012	-0.012	-0.013	-0.013	-0.012	-0.012	-0.013	-0.013
O3	-0.000	0.001	-0.002	0.002	0.010	0.010	0.000	0.002	-0.001	0.002
O4	-0.012	0.011	-0.013	-0.012	-0.014	-0.014	-0.012	0.011	-0.012	0.011
O5	-0.014	-0.037	-0.013	-0.033	-0.014	-0.014	-0.012	-0.029	-0.012	-0.030
O6	-0.014	0.036	-0.013	0.032	-0.013	-0.013	-0.014	0.030	-0.012	0.028
N1	-0.043	-0.045	-0.042	-0.043	-0.042	-0.042	-0.042	-0.043	-0.041	-0.041
N2	-0.043	0.045	-0.042	0.043	-0.043	-0.043	-0.042	0.043	-0.040	-0.040
Cl1	0.026	0.024	0.026	0.024	0.030	0.030	0.029	0.027	0.029	0.027
Cl2	0.029	-0.026	0.030	-0.028	0.032	0.032	0.032	-0.029	0.026	-0.024

	6		**7**		**8**		**9**	
	HS	**BS**	**HS**	**BS**	**HS**	**BS**	**HS**	**BS**
Cr1	3.014	3.011	3.009	3.005	3.006	3.004	3.015	3.010
Cr2	3.005	-2.998	3.012	-3.007	3.001	-2.997	3.015	-3.010
O1	-0.001	-0.001	-0.002	-0.000	-0.001	0.000	-0.000	0.001
O2	-0.012	-0.012	-0.013	-0.013	-0.011	-0.011	-0.010	-0.009
O3	0.014	0.003	-0.001	0.002	0.002	0.001	-0.000	-0.001
O4	-0.012	0.012	-0.012	0.011	-0.013	0.013	-0.010	0.009
O5	-0.013	-0.034	-0.012	-0.030	-0.014	-0.037	0.011(Cl3)	0.011(Cl3)
O6	-0.015	0.033	-0.012	0.028	-0.012	0.037	0.020(Cl4)	0.020(Cl4)
N1	-0.044	-0.045	-0.041	-0.041	-0.043	-0.045	-0.037	0.038
N2	-0.041	0.042	-0.040	-0.040	-0.038	0.038	-0.038	-0.038
Cl1	0.024	0.021	0.029	0.027	0.032	0.030	-0.011	0.011
Cl2	0.032	-0.032	0.026	-0.024	0.036	-0.034	0.020	-0.020

Table S6. Spin density for models **4a** and **4b**.

	4a		4b	
	HS	**BS**	**HS**	**BS**
Cr1	2.869	2.866	3.002	2.996
Cr2	2.862	-2.868	2.999	-2.993
O1	-0.010	-0.000	0.004	-0.001
O2	-0.011	-0.010	-0.015	-0.014
O3	-0.010	0.001	0.006	0.001
O4	-0.011	0.010	-0.014	0.014
O5	0.162	0.143	-0.008	-0.009
O6	0.158	-0.140	-0.007	0.008
N1	-0.032	-0.033	-0.048	-0.049
N2	-0.033	0.034	-0.049	0.050
Cl1	0.013	0.011	0.035	0.033
Cl2	0.015	-0.012	0.039	-0.037

	1-F		1-Cl		1-Br		1-I	
	HS	**BS**	**HS**	**BS**	**HS**	**BS**	**HS**	**BS**
Cr1	3.009	3.005	3.011	3.007	3.012	3.009	3.014	3.010
Cr2	3.004	-2.999	3.005	-3.002	3.006	-3.003	3.008	-3.004
O1	0.002	-0.003	0.002	-0.003	0.001	-0.002	0.001	-0.003
O2	-0.013	-0.012	-0.013	-0.012	-0.012	-0.012	-0.012	-0.012
O3	0.001	0.001	0.000	0.001	0.000	0.001	0.000	0.001
O4	-0.012	0.011	-0.012	0.011	-0.012	0.012	-0.012	0.011
O5	-0.009	-0.026	-0.009	-0.029	-0.010	-0.030	-0.011	-0.031
O6	-0.009	0.025	-0.010	0.028	-0.010	0.029	-0.011	0.030
N1	-0.044	-0.045	-0.044	-0.046	-0.044	-0.045	-0.044	-0.045
N2	-0.045	0.046	-0.044	0.046	-0.044	0.046	-0.044	0.046
Cl1	0.028	0.026	0.027	0.025	0.027	0.025	0.027	0.025
Cl2	0.030	-0.028	0.030	-0.028	0.030	-0.028	0.030	-0.027
F/Cl/Br/I	-0.001	0.000	-0.006	0.000	3.012	3.009	-0.010	0.000

Table S7. Overlap integral with magneto-structural correlations.

<u>Cr-O-Cr angle:</u>

Φ = 83°

Alpha Beta	**d_{xy}**	**d_{xz}**	**d_{yz}**
d_{xy}	-0.079	0.126	-0.084
d_{xz}	-0.150	-0.292	-0.309
d_{yz}	0.112	-0.426	-0.073

Φ = 88°

Alpha Beta	**d_{xy}**	**d_{xz}**	**d_{yz}**
d_{xy}	-0.092	0.044	-0.124

d_{xz}	-0.093	-0.342	-0.263
d_{yz}	0.167	-0.399	0.020

Φ = 93°

Alpha Beta	**d_{xy}**	**d_{xz}**	**d_{yz}**
d_{xy}	-0.069	-0.033	-0.131
d_{xz}	-0.036	-0.365	-0.197
d_{yz}	0.176	-0.329	0.056

Φ = 98°

Alpha Beta	**d_{xy}**	**d_{xz}**	**d_{yz}**
d_{xy}	-0.017	-0.093	-0.135
d_{xz}	0.011	-0.345	-0.136
d_{yz}	0.157	-0.215	0.052

Φ = 103°

Alpha Beta	**d_{xy}**	**d_{xz}**	**d_{yz}**
d_{xy}	0.038	0.125	-0.158
d_{xz}	-0.043	-0.255	-0.108
d_{yz}	0.155	-0.124	-0.041

Φ = 108°

Alpha Beta	**d_{xy}**	**d_{xz}**	**d_{yz}**
d_{xy}	0.051	-0.118	0.176
d_{xz}	0.047	-0.113	-0.114
d_{yz}	-0.175	0.087	0.041

Cr-O-Cr-O dihedral angle:

Ψ = 0.1°

Alpha Beta	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	0.197	0.183	0.285
d_{xz}	-0.104	0.737	-0.950
d_{yz}	-0.428	-0.082	-0.084

Ψ = 4.8°

Alpha Beta	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	-0.163	-0.102	0.234
d_{xz}	0.000	0.758	0.288
d_{yz}	-0.412	0.034	-0.059

Ψ = 8.7°

Alpha Beta	**d_{xy}**	**d_{yz}**	**d_{xz}**

d_{xy}	0.072	-0.139	0.159
d_{xz}	0.070	-0.777	-0.064
d_{yz}	-0.193	-0.123	-0.094

Ψ = 13.4°

Alpha Beta	d_{xy}	d_{yz}	d_{xz}
d_{xy}	0.005	-0.105	0.122
d_{xz}	0.024	-0.618	-0.006
d_{yz}	-0.153	0.006	-0.016

Ψ = 18.3°

Alpha Beta	d_{xy}	d_{yz}	d_{xz}
d_{xy}	-0.017	-0.093	-0.135
d_{xz}	0.011	-0.345	-0.136
d_{yz}	-0.157	-0.215	0.052

Ψ = 23.1°

Alpha Beta	d_{xy}	d_{yz}	d_{xz}
d_{xy}	-0.014	-0.472	-0.161
d_{xz}	0.140	-0.737	-0.236
d_{yz}	-0.249	-0.164	0.007

Cr-O_{carb} distance:

τ = 1.6 Å

Alpha Beta	d_{xy}	d_{yz}	d_{xz}
d_{xy}	-0.039	-0552	-0.105
d_{xz}	0.157	0.735	0.050
d_{yz}	0.230	0.145	-0.066

τ = 1.7 Å

Alpha Beta	d_{xy}	d_{yz}	d_{xz}
d_{xy}	-0.013	-0.363	-0.102
d_{xz}	0.127	0.772	0.056
d_{yz}	0.206	0.036	0.034

τ = 1.8 Å

Alpha Beta	d_{xy}	d_{yz}	d_{xz}
d_{xy}	-0.003	-0.147	-0.108
d_{xz}	0.073	0.487	0.082
d_{yz}	0.177	-0.248	0.068

τ = 1.9 Å

Alpha Beta	d_{xy}	d_{yz}	d_{xz}

d_{xy}	-0.017	-0.093	-0.135
d_{xz}	0.011	-0.345	-0.136
d_{yz}	-0.157	-0.215	0.052

τ = 2.0 Å

Alpha Beta	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	-0.138	0.148	-0.244
d_{xz}	0.175	0.202	-0.199
d_{yz}	0.214	-0.052	0.007

τ = 2.1 Å

Alpha Beta	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	-0.054	-0.311	0.452
d_{xz}	0.413	0.054	0.137
d_{yz}	0.411	0.389	-0.022

τ = 2.2 Å

Alpha Beta	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	-0.445	0.168	0.180
d_{xz}	-0.369	-0.511	0.032
d_{yz}	0.093	0.205	-0.445

<u>Out of plane shift:</u>

θ = 55.70°

Alpha Beta	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	-0.056	-0.035	-0.178
d_{xz}	0.028	-0.131	-0.222
d_{yz}	0.087	-0.194	0.020

θ = 50.74°

Alpha Beta	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	-0.042	-0.062	-0.154
d_{xz}	0.019	-0.194	-0.186
d_{yz}	0.108	-0.213	0.033

θ = 45.76°

Alpha Beta	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	-0.030	-0.080	-0.141
d_{xz}	0.013	-0.261	-0.159
d_{yz}	0.132	-0.217	0.044

θ = 40.79°

Alpha	**d_{xy}**	**d_{yz}**	**d_{xz}**

Beta			
d_{xy}	-0.017	-0.093	-0.135
d_{xz}	0.011	-0.345	-0.136
d_{yz}	-0.157	-0.215	0.052

θ = 35.89°

Alpha **Beta**	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	-0.047	0.103	-0.135
d_{xz}	0.011	-0.452	-0.110
d_{yz}	-0.185	-0.214	0.060

θ = 30.96°

Alpha **Beta**	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	0.062	0.113	-0.138
d_{xz}	-0.010	-0.553	0.083
d_{yz}	0.212	-0.212	0.069

θ = 26.03°

Alpha **Beta**	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	0.015	0.123	-0.142
d_{xz}	-0.021	-0.624	0.063
d_{yz}	0.236	0.208	0.077

θ = 21.20°

Alpha **Beta**	**d_{xy}**	**d_{yz}**	**d_{xz}**
d_{xy}	0.021	0.131	-0.144
d_{xz}	0.016	-0.662	0.053
d_{yz}	0.258	-0.202	-0.081