Electronic Supplementary Information for

Magneto-Structural Correlations in Oxalate-Bridged Sr(II)Cr(III) Coordination Polymers: Structure, Magnetization, X-band and High-Field ESR studies

L. Androš Dubraja,[a] M. Jurić,[a] J. Popović,[a] D. Pajić,[b] Y. Krupskaya,[c] V. Kataev,[c] B. Bűchner,[c] and D. Žilić*[a,c]

[a] *Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb, Croatia.*
[b] *University of Zagreb, Faculty of Science, Department of Physics, Bijenička 32, 10000 Zagreb, Croatia.*
[c] *IFW Dresden, Institute for Solid State Research, Helmholtzstrasse 20, D-01069 Dresden, Germany.*
**E-mail: dzilic@irb.hr* (D. Žilić)

Structural analysis

Table S1 Molecular geometry and differences between corresponding lengths and angles in two chromium octahedra of SrCrPhen complex.

Cr1 octahedron		Cr2 octahedron		Difference
		Angle Θ (°)		
N1-Cr1-O6	171.56	N3-Cr2-O13	170.38	|ΔΘ|=1.18
O2-Cr1-O9	168.97	O10-Cr2-O17	170.58	|ΔΘ|=1.61
N2-Cr1-O5	174.94	N4-Cr2-O14	173.00	|ΔΘ|=1.94
				Sum |ΔΘ|=4.73
		Bond distance x (Å)		
Cr1-N1	2.069	Cr2-N3	2.070	|Δx|=0.001
Cr1-N2	2.071	Cr2-N4	2.061	|Δx|=0.01
Cr1-O2	1.973	Cr2-O17	1.965	|Δx|=0.008
Cr1-O9	1.980	Cr2-O10	1.964	|Δx|=0.016
Cr1-O5	1.954	Cr2-O14	1.960	|Δx|=0.006
Cr1-O6	1.952	Cr1-O13	1.961	|Δx|=0.009
				Sum |Δx|=0.050

Table S2 Molecular geometry and differences between corresponding lengths and angles in two chromium octahedra of SrCrBpy complex.

Cr1 octahedron		Cr2 octahedron		Difference
		Angle Θ (°)		
N1-Cr1-O6	173.09	N3-Cr2-O13	173.78	|ΔΘ|=0.69
O2-Cr1-O9	172.05	O10-Cr2-O17	169.54	|ΔΘ|=2.51
N2-Cr1-O5	172.95	N4-Cr2-O14	172.94	|ΔΘ|=0.01
				Sum |ΔΘ|=3.21
		Bond distance x (Å)		
Cr1-N1	2.062	Cr2-N3	2.052	|Δx|=0.01
Cr1-N2	2.049	Cr2-N4	2.053	|Δx|=0.004
Cr1-O2	1.970	Cr2-O17	1.977	|Δx|=0.007
Cr1-O5	1.968	Cr2-O14	1.954	|Δx|=0.014
Cr1-O6	1.966	Cr2-O13	1.961	|Δx|=0.005
Cr1-O9	1.966	Cr1-O10	1.979	|Δx|=0.013
				Sum |Δx|=0.053

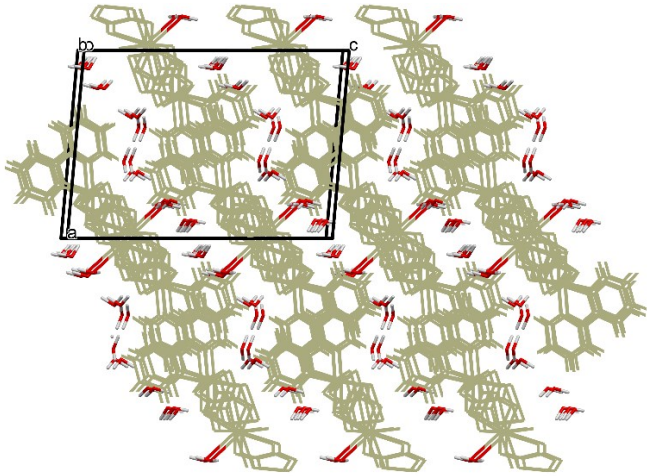

Fig. S1 Zig-zag channels in the crystal packing of SrCrBpy filled with water molecules.

Table S3 Geometric parameters of the aromatic stacking interactions for compounds SrCrPhen and SrCrBpy.

Compound	Cg(*i*)···Cg(*j*)	Cg(*i*)···Cg(*j*)/Å[a]	*α*/°[b]	*β*/°[c]	Cg(*i*)···plane [Cg(*j*)]/Å[d]	Symmetry operator
SrCrPhen	(N3→C24)···(C16→C24)	3.842(4)	3.4(3)	16.5	3.679(2)	−1 − *x*, −1 − *y*, −*z*
	(N3→C24)···(N3→C24)	4.050(3)	0.0(3)	23.3	3.719(2)	−1 − *x*, −1 − *y*, −*z*
	(N2→C11)···(C4→C12)	3.758(4)	1.4(3)	17.2	3.605(2)	1 − *x*, 1 − *y*, 1 − *z*
	(N1→C12)···(C4→C12)	3.772(4)	2.9(3)	19.9	3.595(2)	−*x*, 1 − *y*, 1 − *z*
	(N1→C12)···(N1→C12)	3.832(3)	0.0(3)	20.7	3.585(2)	−*x*, 1− *y*, 1 − *z*
SrCrBpy	(N1→C5)···(N4→C20)	3.901(2)	6.93(14)	18.2	3.5772(13)	1 − *x*, 1 − *y*, 2 − *z*
	(N2→C10)···(N3→C15)	3.623(2)	3.41(12)	16.1	3.5304(10)	1 − *x*, 1 − *y*, 2 − *z*
	(N1→C5)···(N1→C5)	4.215(3)	11.2	11.2	4.1351(13)	1 − *x*, 1 − *y*, 2 − *z*
	(N3→C15)···(N3→C15)	4.094(2)	0.02(12)	17.7	3.9013(10)	1 − *x*, 2 − *y*, 2− *z*

[a] Cg = centre of gravity of the aromatic ring. [b] *α* = angle between the planes of two aromatic rings. [c] *β* = angle between the Cg···Cg line and the normal to the plane of the first aromatic ring.

Table S4 Hydrogen-bonding geometry in compounds SrCrPhen and SrCrBpy.

Compound	*D*−H···*A*	*D*−H/Å	H···*A*/Å	*D*···*A*/Å	*D*−H···*A*/°	Symm. op. on *A*
SrCrPhen	O1−H1A···O8	0.89(7)	2.09(6)	2.958(6)	164(6)	1 − *x*, 1 − *y*, 1 − *z*
	O1−H1B···O10	0.86(4)	2.06(4)	2.895(6)	161(5)	−*x*, −*y*, 1 − *z*
SrCrBpy	O1−H1A···O2	0.88(2)	1.99(2)	2.840(3)	163(4)	−*x*, 1 − *y*, 2 − *z*
	O1−H1B···O15	0.88(4)	1.92(6)	2.740(3)	154(6)	−*x*, 1 − *y*, 2 − *z*
	O18−H18A···O17	0.889(19)	2.022(19)	2.887(3)	164(3)	1 + *x*,1/2 − *y*,1/2 + *z*
	O18−H18B···O4	0.89(3)	2.04(3)	2.806(3)	144(3)	1 − *x*, −1/2 + *y*, 3/2 − *z*
	O20−H20A···O13	0.90(4)	2.08(4)	2.968(3)	172(3)	−*x*, 1 − *y*, 1 − *z*
	O20−H20B···O16	0.88(3)	2.05(4)	2.888(4)	159(5)	−*x*, -1/2 + *y*, 1/2 − *z*
	O21−H21A···O11	0.88(4)	2.00(4)	2.852(3)	164(3)	1 − *x*, 1 − *y*, 1 − *z*
	O21−H21B···O18	0.89(3)	1.93(3)	2.797(3)	164(3)	*x*, 1/2 − *y*, -1/2 + *z*
	O22−H22A···O8	0.91(4)	2.02(4)	2.875(3)	156(4)	*x*, *y*, *z*
	O22−H22B···O21	0.89(3)	1.95(2)	2.801(3)	159(5)	−*x*, 1 − *y*, 1 − *z*
	O19−H19A···O6	0.84	2.29	3.117(4)	168	*x*, *y*, *z*
	O19−H19B···O3	0.84	2.14	2.818(4)	138	−*x*, 1 − *y*, 2 − *z*

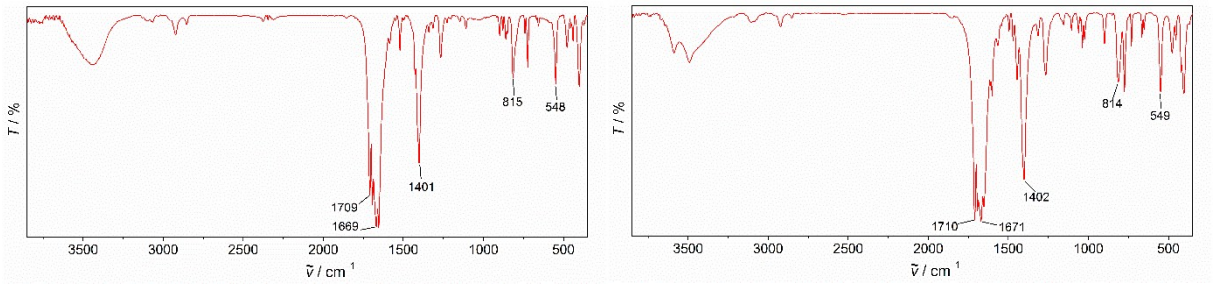

Fig. S2 IR spectra of compounds SrCrPhen (left) and SrCrBpy (right).

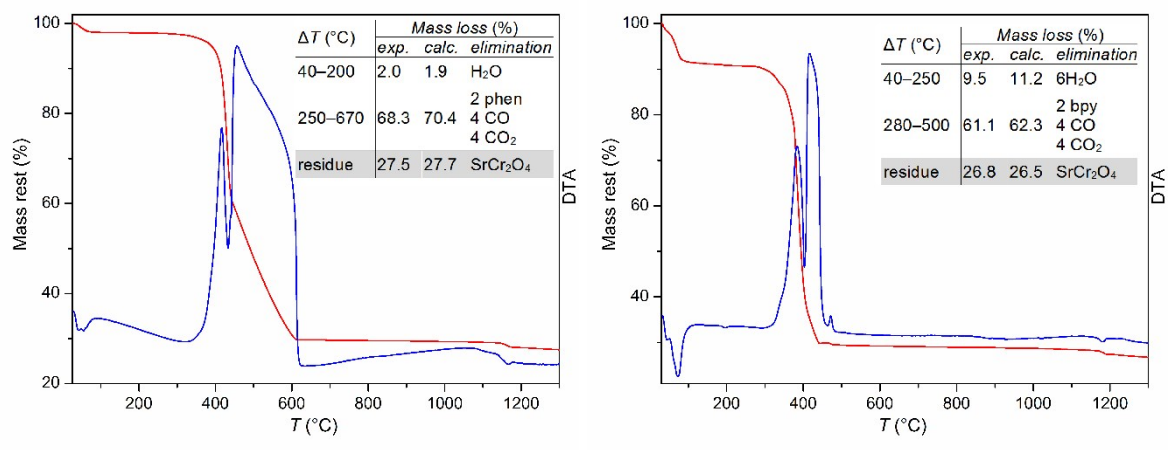

Fig. S3 The TG/DTA curves and thermoanalytical data for compounds SrCrPhen (left) and SrCrBpy (right) measured in the nitrogen atmosphere.

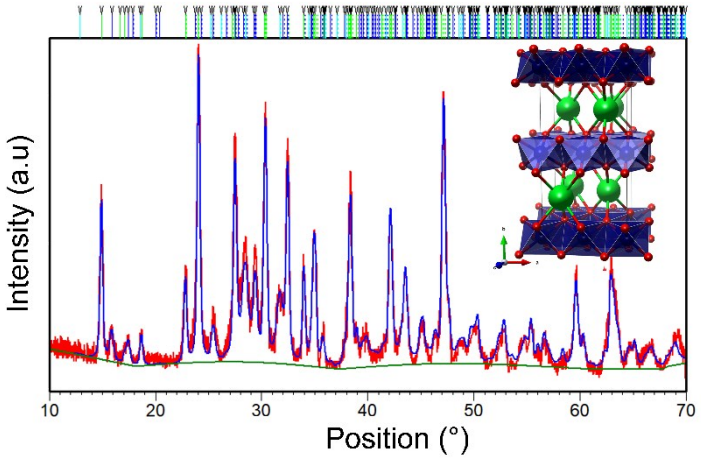

Fig. S4 Graphical result of the Rietveld refinement of the product (α-$SrCr_2O_4$, $SrCrO_4$ and Cr_2O_3) obtained by heat treatment of SrCrBpy at 1300°C. Experimental data are given in red, calculated pattern in blue. Positions of diffraction lines corresponding to α-$SrCr_2O_4$ is shown with green vertical marks. Positions of minor phases are maked in teal and turquoise. Inset: structure of α-$SrCr_2O_4$; CrO_6 octahedra are given in dark blue, Sr cations are represented as green balls while oxygen by red once.

ESR spectroscopy

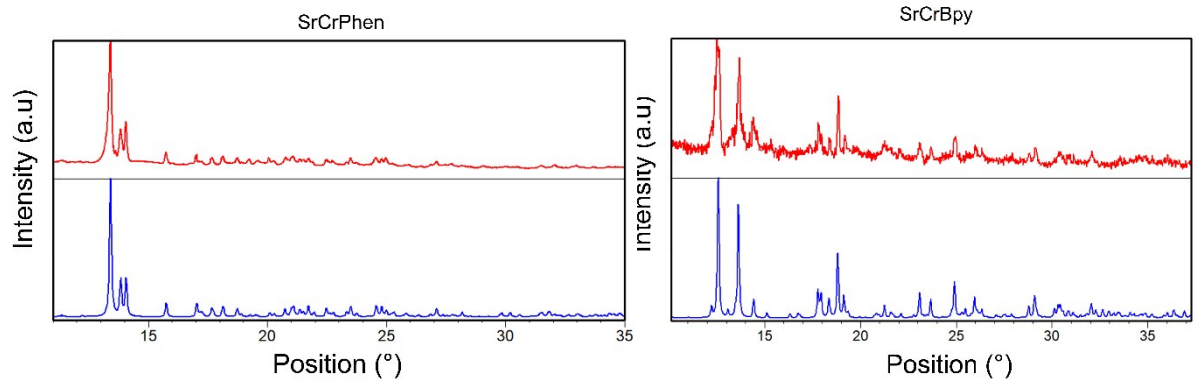

Fig. S5 Comparison of the powder X-ray diffraction patterns of polycrystalline samples (SrCrPhen and SrCrBpy) ground into powder and used for HF-ESR measurements (red lines) with those calculated from their single-crystal X-ray diffraction data (blue lines).

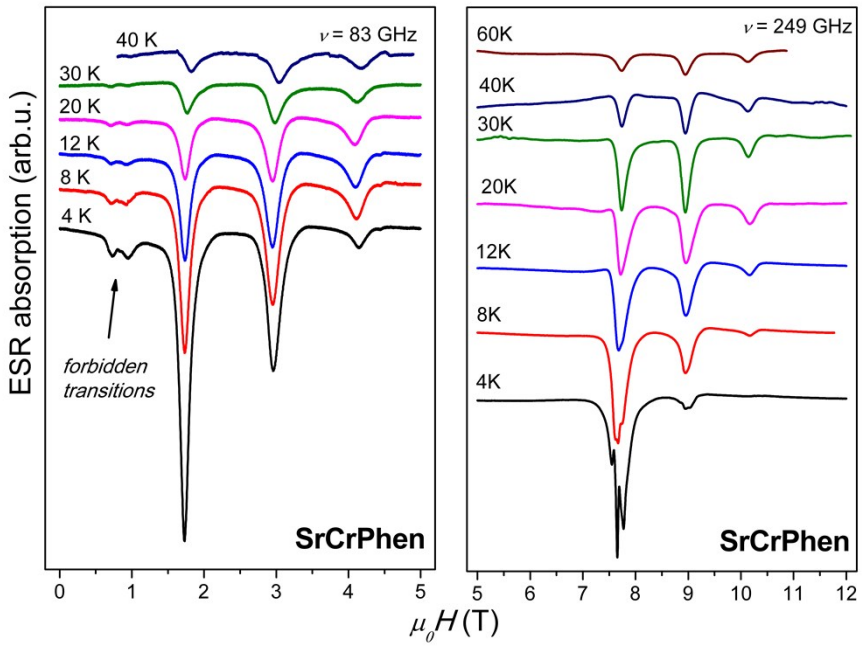

Fig. S6 Temperature dependence of ESR spectra of SrCrPhen complexes at indicated frequencies.

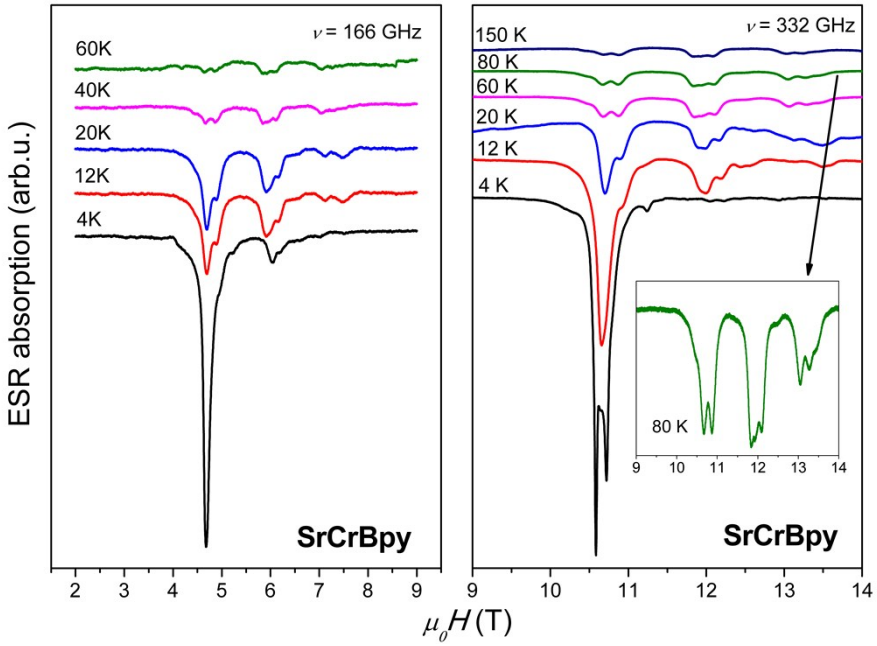

Fig. S7 Temperature dependence of ESR spectra of SrCrBpy complexes at indicated frequencies.