

Chiral Metal Down to 4.2K - a BDH-TTP Radical-Cation Salt with Spiroboronate Anion B(2-chloromandelate)₂⁻

Toby J. Blundell,^a Michael Brannan,^a Hiroshi Nishimoto,^b Tomofumi Kadoya,^b Jun-ichi Yamada,^b Hiroki Akutsu,^c Yasuhiro Nakazawa,^c Lee Martin^{*a}

Table S1 Short (>sum VdW Radii – 3.7 Å) S-S contacts for I. Symmetry operations a = 1 – x, 0.5 + y, 1 – z; b = 2 – x, 0.5 + y, 1 – z; c = –1 – x, –0.5 + y, 1 – z; d = –x, –1/2 + y, 1 – z.

I	Length
S(4)–S(12)	3.5694 (15)
S(6)–S(10)	3.5984 (15)
S(10)–S(13) ^a	3.5787 (16)
S(2)–S(9) ^a	3.5497 (16)
S(4)–S(7) ^b	3.5785 (16)

Table S2 Hydrogen bonding interactions in I.

D-H	d(H..A)	<DHA	d(D..A)	A
I				
C1-H1B	2.477	159.53	3.423	O2 [-x+1, y+1/2, -z+1]
C2-H2A	2.598	160.05	3.545	O6 [-x+1, y+1/2, -z+1]
C2-H2B	2.402	151	3.303	O5 [-x+1, y-1/2, -z+1]
C9 ^a -H9B ^a	2.284	127.6	2.992	O2 [x+1, y, z]
C9A ^b -H9AA ^b	2.474	110.21	2.966	O2 [x+1, y, z]
C10A ^b -H10C ^b	2.625	111.9	3.132	O2 [x+1, y, z]
C11-H11B	2.632	153.88	3.548	O1
C19-H19A	2.605	175.16	3.593	O2 [-x, y+1/2, -z+1]
C19-H19B	2.825	155.09	3.746	Cl1 [-x+1, y-1/2, -z+1]
C20-H20A	2.265	175.02	3.253	O5 [-x+1, y-1/2, -z+1]
C20-H20B	2.932	131.42	3.663	Cl2 [-x, y+1/2, -z+1]

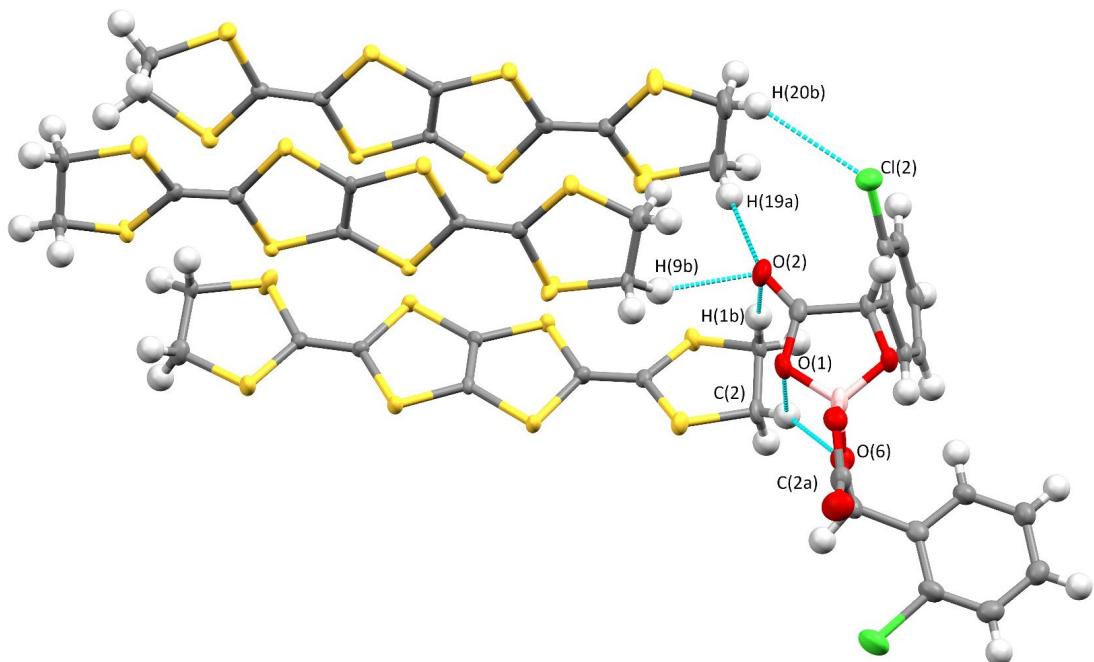


Fig. S1 Hydrogen bonding interactions viewed along the b axis. Thermal ellipsoids set at 50% probability, minor disordered components omitted for clarity.

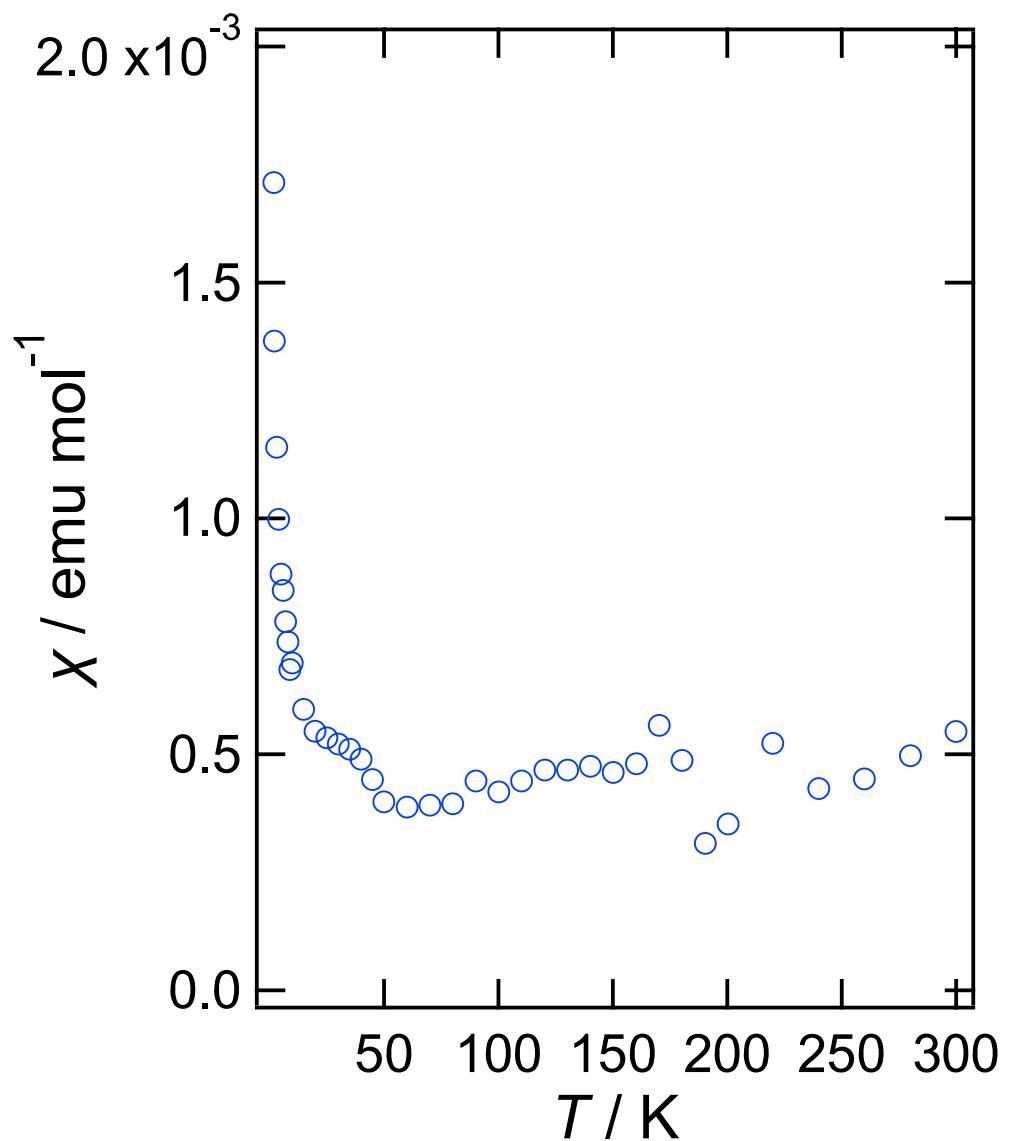


Fig. S2 Temperature-dependent magnetic susceptibility of **1**.

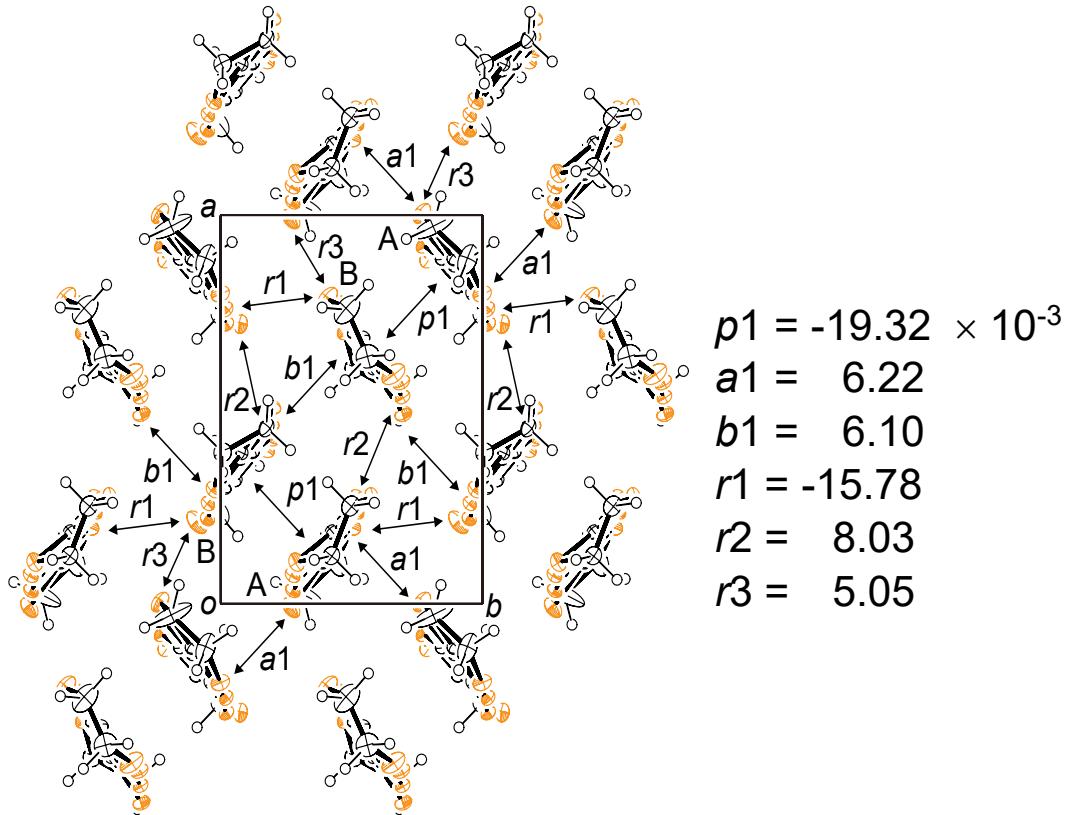


Fig. S3 Transfer integrals for I. Band calculation for I at 150K is shown in Fig. 7.

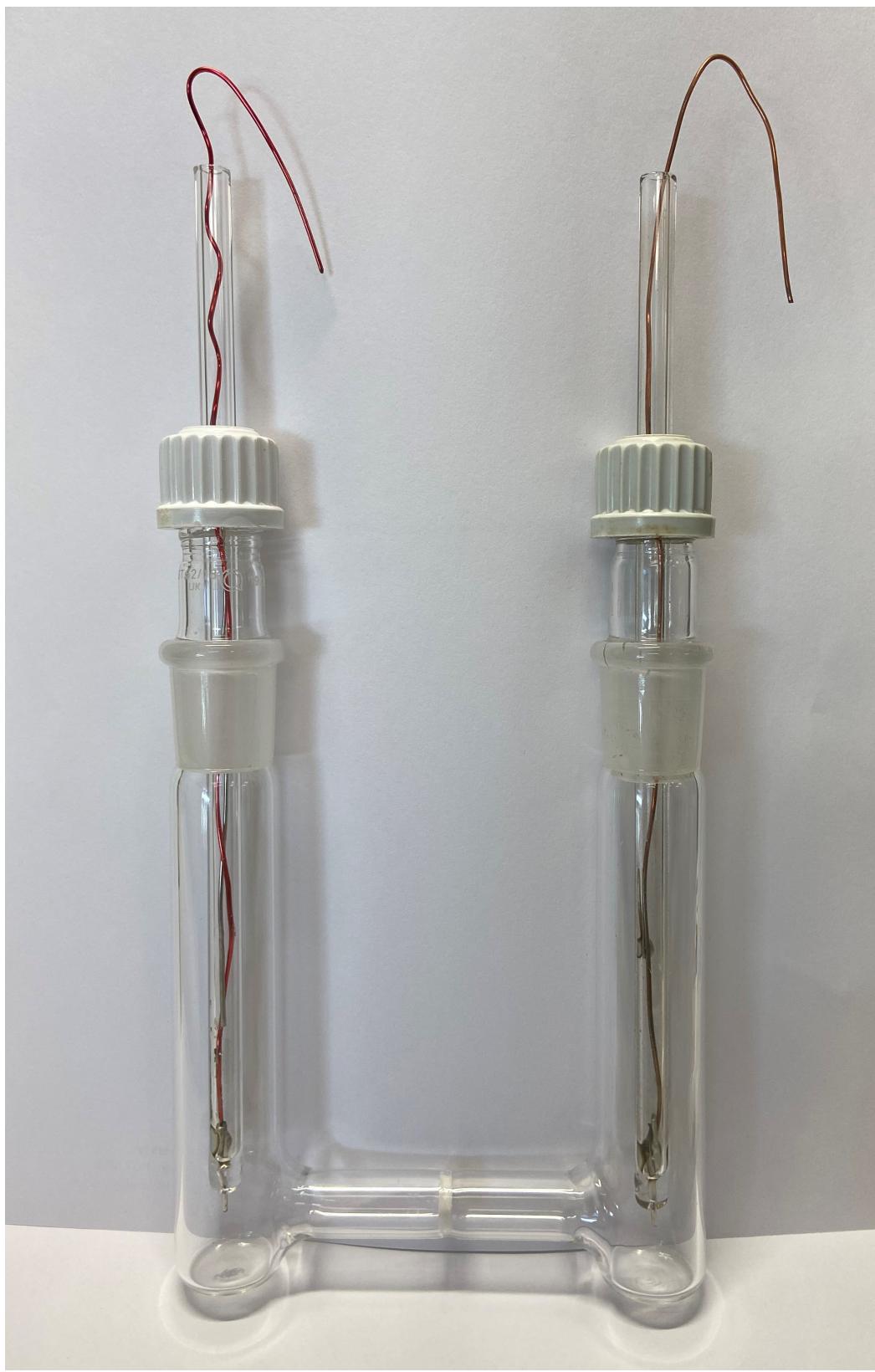


Fig. S4 H-shaped electrochemical cell