Crystal structure and magnetic properties of $Cr_3Te_5O_{13}Cl_3$

Supplementary data

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Table S1   Atomic coordinates and equivalent isotropic displacement parameters for $Cr_3Te_5O_{13}Cl_3$.

Atom label	Wyckoff	x	y	z	Uiso
Te1	4a	0.02223(8)	0.18754(2)	0.636719(19)	0.00663(8)
Te2	4a	0.51184(8)	0.09010(2)	0.958538(19)	0.00730(8)
Te3	4a	0.08679(8)	0.42206(2)	0.59614(2)	0.00781(8)
Te4	4a	0.44666(8)	0.48277(2)	0.77890(2)	0.00654(8)
Te5	4a	0.03461(8)	0.29518(2)	0.85212(2)	0.00625(7)
Cr1	4a	0.0294(2)	0.09199(5)	0.81774(5)	0.00632(18)
Cr2	4a	0.5305(2)	0.31746(5)	0.70439(5)	0.00654(18)
Cr3	4a	0.52906(19)	0.17087(5)	0.77836(5)	0.00567(17)
Cl1	4a	0.0360(4)	0.35427(12)	0.46707(10)	0.0267(4)
Cl2	4a	0.8731(4)	0.47766(12)	0.88752(10)	0.0244(4)
Cl3	4a	0.4751(4)	0.31916(12)	0.96190(11)	0.0300(4)
O1	4a	0.2255(8)	0.3472(3)	0.7756(3)	0.0083(9)
O2	4a	0.2005(8)	0.1951(3)	0.8374(2)	0.0077(9)
O3	4a	0.2148(8)	0.0498(3)	0.9049(3)	0.0112(9)
O4	4a	0.6480(9)	0.5724(3)	0.7445(2)	0.0075(9)
O5	4a	0.8531(8)	0.1338(2)	0.7221(2)	0.0076(8)
O6	4a	0.7025(8)	0.1307(3)	0.8712(2)	0.0061(8)
O7	4a	0.2961(9)	0.4954(3)	0.5360(3)	0.0139(10)
O8	4a	0.6812(8)	0.4176(3)	0.7267(3)	0.0091(9)
O9	4a	0.8530(9)	0.2823(3)	0.6439(3)	0.0116(9)
O10	4a	0.3488(8)	0.2153(2)	0.6888(2)	0.0072(9)
O11	4a	0.3736(9)	0.3584(3)	0.6129(2)	0.0105(9)
O12	4a	0.7147(8)	0.2691(2)	0.7926(2)	0.0072(9)
O13	4a	0.1768(8)	0.4934(3)	0.6934(2)	0.0086(9)

Table S2 Selected bond lengths (Å).

Te1 – O9^i	1.845(5)	Cr1 – O3	1.924(4)
Te1 – O10	1.905(4)	Cr1 – O4^{iii}	1.952(4)
Te1 – O5^i	1.949(4)	Cr1 – O6^i	1.974(4)
Te1 – Cl1^{ii}	3.0856(19)	Cr1 – O13^{vii}	1.995(5)
Te2 – O3	1.869(4)	Cr1 – O2	2.004(5)
Te2 – O7^{iii}	1.896(5)	Cr1 – O5^i	2.021(4)
Te2 – O6	1.928(4)	Cr1 – Cr3	2.8891(13)
Te2 – Cl2^{iv}	3.0223(18)	Cr1 – Cr3^i	2.8918(13)
Te2 – Cl3^v	3.095(2)	Cr2 – O11	1.915(4)
Te3 – O3^{vi}	2.663(5)	Cr2 – O8	1.927(5)
Te3 – O7	1.945(5)	Cr2 – O12	1.978(4)
Te3 – O11	1.812(4)	Cr2 – O9	1.999(4)
Te3 – O13	2.154(4)	Cr2 – O10	2.001(4)
Te3 – Cl1	2.5630(16)	Cr2 – O1	2.016(4)
Te4 – O1	5.589(5)	Cr2 – Cr3	2.8539(12)
Te4 – O4	1.937(4)	Cr3 – O12	1.947(4)
Te4 – O8	1.854(4)	Cr3 – O4^{iii}	1.958(4)
Te4 – O13	2.008(4)	Cr3 – O10	1.960(4)
Te4 – Cl2	2.8298(18)	Cr3 – O2	1.960(4)
Te5 – O1	1.868(4)	Cr3 – O6	1.965(4)
Te5 – O2	1.934(4)	Cr3 – O5	1.977(4)
Te5 – O12^i	1.937(4)		
Te5 – Cl3	2.9229(19)		

symmetrie codes: i) x–1, y , z; ii) x–0.5, –y+0.5, –z+1; iii) –x+1, y–0.5, –z+1.5; iv) x–0.5, –y+0.5, –z+2; v) x+0.5, –y+0.5, –z+2; vi) –x, y+0.5, –z+1.5; vii) –x, y–0.5, –z+1.5.

Table S3 Selected bond angles (^{o}).

O9^i – Te1 – O10	96.9(2)	O8 – Cr2 – O12	92.73(18)
O9^i – Te1 – O5^i	100.46(18)	O11 – Cr2 – O9	89.21(18)
O10 – Te1 – O5^i	96.28(17)	O8 – Cr2 – O9	94.57(19)
O3 – Te2 – O7^{ii}	95.1(2)	O12 – Cr2 – O9	85.66(18)
O3 – Te2 – O6	96.58(19)	O11 – Cr2 – O10	92.00(18)
O7^{ii} – Te2 – O6	96.64(19)	O8 – Cr2 – O10	174.70(18)
O11 – Te3 – O7	94.43(19)	O12 – Cr2 – O10	86.25(17)
O11 – Te3 – O13	93.58(18)	O9 – Cr2 – O10	90.55(19)
O7 – Te3 – O13	86.91(18)	O11 – Cr2 – O1	97.28(18)
O11 – Te3 – Cl1	86.52(14)	O8 – Cr2 – O1	85.85(18)
O7 – Te3 – Cl1	82.64(14)	O12 – Cr2 – O1	87.84(18)
O13 – Te3 – Cl1	169.52(13)	O9 – Cr2 – O1	173.50(18)
O8 – Te4 – O4	91.13(18)	O10 – Cr2 – O1	88.91(18)
O8 – Te4 – O13	95.52(19)	O12 – Cr3 – O4^{ii}	175.36(17)
O4 – Te4 – O13	91.69(18)	O12 – Cr3 – O10	88.23(18)
O1 – Te5 – O2	97.31(18)	O4^{ii} – Cr3 – O10	88.79(18)
O1 – Te5 – O12^i	97.53(18)	O12 – Cr3 – O2	97.42(18)
O2 – Te5 – O12^i	93.39(18)	O4^{ii} – Cr3 – O2	86.05(18)
		O10 – Cr3 – O2	88.23(18)
O3 – Cr1 – O4^{ii}	89.77(18)	O12 – Cr3 – O6	90.11(18)
O3 – Cr1 – O6^i	97.76(18)	O4^{ii} – Cr3 – O6	93.01(18)
O4^{ii} – Cr1 – O6^i	169.33(19)	O10 – Cr3 – O6	177.09(19)
O3 – Cr1 – O13^{iii}	89.52(18)	O2 – Cr3 – O6	89.62(17)
O4^{ii} – Cr1 – O13^{iii}	101.90(18)	O12 – Cr3 – O5	88.43(18)
O6^i – Cr1 – O13^{iii}	85.79(19)	O4^{ii} – Cr3 – O5	88.30(17)
O3 – Cr1 – O2	90.25(18)	O10 – Cr3 – O5	95.18(18)
O4^{ii} – Cr1 – O2	85.00(18)	O2 – Cr3 – O5	173.34(18)
O6^i – Cr1 – O2	87.40(18)	O6 – Cr3 – O5	87.16(18)
O13^{iii} – Cr1 – O2	173.10(18)		
O3 – Cr1 – O5^i	176.52(19)	Cr3 – O2 – Cr1	93.55(18)
O4^{ii} – Cr1 – O5^i	86.82(17)	Cr1^{iv} – O4 – Cr3^{iv}	95.29(19)
O6^i – Cr1 – O5^i	85.71(18)	Cr3 – O5 – Cr1^v	92.64(18)
O13^{iii} – Cr1 – O5^i	90.53(18)	Cr3 – O6 – Cr1^v	94.48(17)
O2 – Cr1 – O5^i	90.12(17)	Cr3 – O10 – Cr2	92.20(17)
O11 – Cr2 – O8	89.47(19)	Cr3 – O12 – Cr2	93.28(17)
O11 – Cr2 – O12	174.56(19)		

<u>Symmetrie codes:</u>   i) x–1, y, z; ii) –x+1, y–0.5, –z+1.5; iii) –x, y–0.5, –z+1.5;
iv) –x+1, y+0.5, –z+1.5; v) x+1, y, z.

Table S4 Bond valance sum calculations

Te1

Te1 – O5	1.016
Te1 – O9	1.346
Te1 – O10	1.145
Te1 – Cl1	0.144
$\sum$	**3.7**

Te2

Te2 – O3	1.261
Te2 – O6	1.076
Te2 – O7	1.176
Te2 – Cl2	0.172
Te2 – Cl3	0.141
$\sum$	**3.8**

Te3

Te3 – O3	0.148
Te3 – O7	1.027
Te3 – O11	1.476
Te3 – O13	0.586
Te3 – Cl1	0.594
$\sum$	**3.8**

Te4

Te4 – O1	0.180
Te4 – O4	1.050
Te4 – O8	1.346
Te4 – O13	0.867
Te4 – Cl2	0.288
$\sum$	**3.7**

Te5

Te5 – O1	1.265
Te5 – O2	1.058
Te5 – O12	1.050
Te5 – Cl3	0.224
$\sum$	**3.7**

Cr1

Cr1 – O2	0.468
Cr1 – O3	0.584
Cr1 – O4	0.541
Cr1 – O5	0.447
Cr1 – O6	0.509
Cr1 – O13	0.480
$\sum$	**3.0**

Cr2

Cr2 – O1	0.455
Cr2 – O8	0.578
Cr2 – O9	0.476
Cr2 – O10	0.473
Cr2 – O11	0.595
Cr2 – O12	0.503
∑	**3.1**

Cr3

Cr3 – O1	0.528
Cr3 – O8	0.533
Cr3 – O9	0.505
Cr3 – O10	0.521
Cr3 – O11	0.528
Cr3 – O12	0.547
∑	**3.2**

The bond valence sum calculations are performed according to Brown and Altermatt [S1]

References

[S1]   I.D. Brown, D. Altermatt, *Acta Cryst.*, 1985, **B41**, 244–247.