Supplementary Information

Synchrotron Charge Density Studies in Materials Chemistry:

16 K X-ray Charge Density of a New Magnetic Metal Organic Framework Material,

$Mn_2(C_8H_4O_4)_2(C_3H_7NO)_2$

R. D. Poulsen, A. Bentien, B. B. Iversen*

Department of Chemistry, University of Aarhus, DK-8000 Århus C, Denmark

*Corresponding author: bo@chem.au.dk

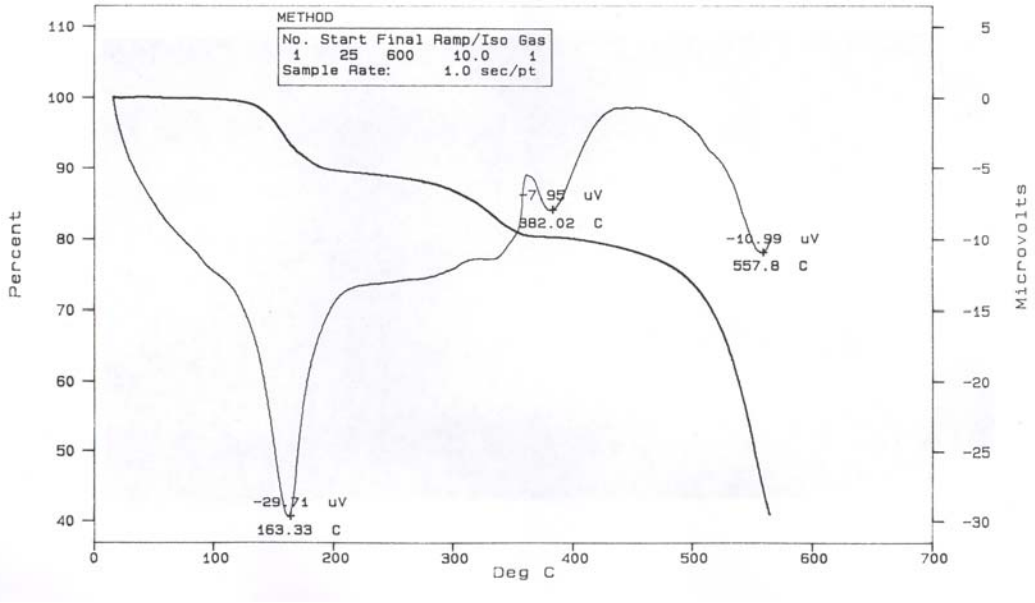
Topological properties in the ligand bonds. R is the refined internulcear distance (Å), whereas $d_{ij} = d_1 + d_2$ is the sum of the distances from the bond critical point to the attractors (Å). ρ is the electron density (e/Å^3)and $\nabla^2\rho$ the Laplacian (e/Å^5).

Bond	**R**	$\mathbf{r_{ij}}$	$\mathbf{d_1}$	$\mathbf{d_2}$	ρ	$\nabla^2\rho$
O(1) -C(1)	1.263(1)	1.263	0.854	0.409	2.48(4)	-8.7(2)
O(2) -C(1)	1.261(1)	1.263	0.847	0.415	2.50(4)	-13.0(2)
O(8) -C(8)	1.265(1)	1.265	0.848	0.416	2.36(4)	-8.6(2)
O(9) -C(8)	1.273(1)	1.275	0.858	0.417	2.37(3)	-9.6(2)
O(11) -C(11)	1.271(1)	1.272	0.851	0.420	2.37(4)	-7.0(2)
O(12) -C(11)	1.261(1)	1.262	0.851	0.411	2.46(4)	-5.7(2)
O(18) -C(18)	1.262(1)	1.262	0.837	0.425	2.58(4)	-22.6(2)
O(19) -C(18)	1.261(1)	1.262	0.848	0.414	2.50(4)	-13.0(2)
O(21) -C(21)	1.247(1)	1.247	0.832	0.416	2.58(4)	-14.6(2)
O(31) -C(31)	1.247(1)	1.247	0.838	0.409	2.71(4)	-12.7(2)
N(21) -C(21)	1.332(1)	1.333	0.913	0.421	2.16(4)	-4.6(2)
N(31) -C(31)	1.336(1)	1.336	0.910	0.427	2.21(4)	-9.7(2)
N(21) -C(22)	1.462(1)	1.462	0.923	0.540	1.63(4)	-9.8(1)
N(21) -C(23)	1.459(1)	1.460	0.960	0.500	1.66(4)	-14.3(1)
N(31) -C(32)	1.460(1)	1.462	0.916	0.545	1.68(3)	-14.0(1)
N(31) -C(33)	1.458(1)	1.462	0.990	0.472	1.51(4)	-6.1(2)
C(2) -C(3)	1.402(1)	1.402	0.727	0.675	2.11(3)	-22.0(1)
C(2) -C(7)	1.401(1)	1.401	0.715	0.686	2.17(3)	-21.5(1)
C(3) -C(4)	1.393(1)	1.393	0.688	0.705	2.08(4)	-21.4(1)
C(4) -C(5)	1.406(1)	1.406	0.672	0.734	2.04(3)	-19.8(1)
C(5) -C(6)	1.404(1)	1.405	0.753	0.652	2.09(3)	-20.7(1)
C(6) -C(7)	1.396(1)	1.396	0.730	0.666	2.14(4)	-20.2(1)
C(12) -C(13)	1.402(1)	1.402	0.747	0.655	2.10(3)	-21.1(1)
C(12) -C(17)	1.403(1)	1.403	0.739	0.665	2.13(3)	-20.5(1)
C(13) -C(14)	1.401(1)	1.401	0.736	0.666	2.15(3)	-21.7(1)
C(14) -C(15)	1.402(1)	1.402	0.745	0.657	2.09(3)	-20.1(1)
C(15) -C(16)	1.402(1)	1.403	0.726	0.677	2.14(3)	-22.1(1)
C(16) -C(17)	1.397(1)	1.397	0.668	0.728	2.13(4)	-21.2(1)
C(1) -C(2)	1.505(1)	1.505	0.778	0.727	1.85(2)	-16.2(1)
C(5) -C(8)	1.491(1)	1.491	0.663	0.828	1.78(3)	-17.3(1)
C(11) -C(12)	1.507(1)	1.507	0.738	0.769	1.69(2)	-11.9(1)
C(15) -C(18)	1.515(1)	1.515	0.770	0.745	1.71(2)	-14.1(1)

Bond angles around the Mn sites

O(1)	Mn(1)	O(8)	84.24(4)
O(1)	Mn(1)	O(8)'	86.15(3)
O(1)	Mn(1)	O(9)	100.86(3)
O(1)	Mn(1)	O(11)	87.52(4)
O(1)	Mn(1)	O(21)	172.22(3)
O(8)	Mn(1)	O(8)'	77.72(3)
O(8)	Mn(1)	O(9)	55.81(2)
O(8)	Mn(1)	O(11)	170.08(3)
O(8)	Mn(1)	O(21)	97.97(4)
O(8)'	Mn(1)	O(9)	131.50(4)
O(8)'	Mn(1)	O(11)	107.27(3)
O(8)'	Mn(1)	O(21)	87.03(3)
O(9)	Mn(1)	O(11)	120.84(3)
O(9)	Mn(1)	O(21)	86.48(3)
O(11)	Mn(1)	O(21)	90.93(4)
O(2)	Mn(2)	O(9)	82.77(3)
O(2)	Mn(2)	O(12)	90.30(3)
O(2)	Mn(2)	O(18)	83.83(3)
O(2)	Mn(2)	O(19)	163.06(4)
O(2)	Mn(2)	O(31)	84.24(3)
O(9)	Mn(2)	O(12)	86.43(3)
O(9)	Mn(2)	O(18)	166.60(3)
O(9)	Mn(2)	O(19)	82.32(3)
O(9)	Mn(2)	O(31)	90.74(3)
O(12)	Mn(2)	O(18)	93.99(4)
O(12)	Mn(2)	O(19)	96.76(4)
O(12)	Mn(2)	O(31)	174.13(3)
O(18)	Mn(2)	O(19)	110.88(3)
O(18)	Mn(2)	O(31)	87.58(4)
O(19)	Mn(2)	O(31)	87.95(4)

DTA and TGA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Sample Rate: 1.0 sec/pt
-7.95 uV
382.02 C
-10.99 uV
557.8 C
-29.71 uV
163.33 C
Percent
Microvolts
Deg C
110
100
90
80
70
60
50
40
5
0
-5
-10
-15
-20
-25
-30
0
100
200
300
400
500
600
700