Supplementary Material (ESI) for Chemical Communications

Crystallography of hydrogen-containing compounds: realizing the potential of neutron powder diffraction

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Refined fractional coordinates for $Bi(NO_3)_3.5H_2O$ from NPD data (*P*-1,*a* = 6.41605(22) Å, *b* = 8.58647(28) Å, *c* = 10.6268(4) Å, α = 100.1569(18)°, β = 80.9292(18)°, γ = 104.6216(16)°, *V* = 553.656(33) Å^3)

Atom	x	y	z	Ui/Ue*100 (Å^2)
Bi1	0.1860(10)	0.3503(6)	0.2334(5)	0.76(18)
N1	0.0958(9)	0.6623(7)	0.2050(6)	1.34(8)
O1	0.1487(16)	0.5762(12)	0.1007(9)	1.14(9)
O2	0.0937(14)	0.6091(11)	0.3082(8)	1.14(9)
O3	0.0606(16)	0.8029(12)	0.2022(9)	1.14(9)
N2	-0.1645(9)	0.1771(7)	0.4154(5)	1.34(8)
O4	-0.1628(14)	0.3214(12)	0.4005(10)	1.14(9)
O5	-0.0247(16)	0.1071(11)	0.3503(8)	1.14(9)
O6	-0.3107(15)	0.1095(11)	0.4981(8)	1.14(9)
N3	0.3330(9)	0.1626(7)	-0.0428(5)	1.34(8)
O7	0.3604(15)	0.3140(12)	-0.0020(9)	1.14(9)
O8	0.2274(14)	0.0636(11)	0.0292(8)	1.14(9)
O9	0.4116(13)	0.1116(11)	-0.1592(9)	1.14(9)
O10	0.5268(15)	0.5272(12)	0.2069(9)	0.35(9)
O11	0.2860(14)	0.4409(12)	0.4344(8)	0.35(9)
O12	0.4373(17)	0.1838(13)	0.2569(9)	0.35(9)
O13	0.8355(15)	0.2525(12)	0.1042(9)	0.35(9)
O14	0.6796(14)	0.7662(12)	0.4058(9)	0.35(9)
H1	0.5632(28)	0.6066(20)	0.2838(17)	2.63(15)
H2	0.8389(24)	0.3166(20)	0.0406(17)	2.63(15)
H3	0.5598(28)	0.5689(18)	0.1327(17)	2.63(15)
H4	0.2339(28)	0.5232(20)	0.4930(16)	2.63(15)
H5	0.8031(26)	0.8269(19)	0.3702(15)	2.63(15)
H6	0.8370(24)	0.1424(21)	0.0470(17)	2.63(15)
H7	0.4068(27)	0.0816(23)	0.2380(17)	2.63(15)
H8	0.5828(28)	0.2139(19)	0.2151(16)	2.63(15)
H9	0.3056(24)	0.3623(20)	0.4896(17)	2.63(15)
H10	0.5691(26)	0.8247(21)	0.4493(16)	2.63(15)

Selected bond lengths and angles for $Bi(NO_3)_3.5H_2O$ from NPD data

Bond	Length	Bond	Length
Bi1_O1	2.666(11)	O10_H1	0.985(22)
Bi1_O2	2.411(10)	O10_H3	0.896(24)
Bi1_O4	2.617(12)	O11_H4	0.947(23)
Bi1_O5	2.587(10)	O11_H9	1.010(22)
Bi1_O7	2.573(11)	O12_H7	0.844(26)
Bi1_O10	2.334(11)	O12_H8	0.961(23)
Bi1_O11	2.275(10)	O13_H2	0.938(22)
Bi1_O12	2.475(11)	O13_H6	1.031(24)
Bi1_O13	2.695(11)	O14_H5	0.900(21)
		O14_H10	0.982(20)
N1_O2	1.257(11)		
N1_O3	1.288(11)		
N2_O4	1.273(11)		
N2_O5	1.255(10)	Bond	Angle (deg)
N2_O6	1.279(10)	H1_O10_H3	114.5(15)
N3_O7	1.272(10)	H2_O13_H6	99.6(15)
N3_O8	1.242(10)	H5_O14_H10	116.3(16)
N3_O9	1.304(11)	H7_O12_H8	102.5(16)

Refined fractional coordinates for La acetate sesquihydrate from NPD data (a = 8.54367(28)Å, b = 10.02365(34)Å, c = 13.3359(5)Å, α = 87.5147(20)°, β = 76.3247(22)°, γ = 75.4844(20)°)[1]

Bond	Length (A)	Bond	Length (A)
La1 -O4	2.5095(16)	La2 - O2	2.5524(18)
O4 - C3	1.2725(27)	O2 - C1	1.2795(29)
C3 - O3	1.2668(28)	C1 - O1	1.2671(29)
C3 - C4	1.4864(32)	C1 - C2	1.485(4)
C4 - H4A	1.0500(26)	C2 - H2A	1.0485(26)
C4 - H4B	1.0524(26)	C2 - H2B	1.0495(26)
C4 - H4C	1.0485(26)	C2 - H2C	1.0492(26)
La1 - O11	2.6369(16)	La2 - O6	2.5573(17)
La1 - O11'	2.4702(17)	O6 - C5	1.2512(28)
O11 - C9	1.2812(29)	C5 - O5	1.2705(27)
C9 - O10	1.2520(29)	C5 - C6	1.4957(32)
C9 - C10	1.4945(31)	C6 - H6A	1.0494(26)
C10 - H8A	1.0493(26)	C6 - H6B	1.0515(26)
C10 - H8B	1.0488(26)	C6 - H6C	1.0508(26)
C10 - H8C	1.0490(26)		
La1 - O12	2.6201(16)	La2 - O9	2.7367(18)
La1 - O12'	2.4842(17)	La2 - O9'	2.5573(16)
O12 - C11	1.2825(28)	O9 - C7	1.2684(27)
C11 - O8	1.2538(29)	C7 - O7	1.2741(29)
C11 - C12	1.4993(31)	C7 - C8	1.489(4)
C12 - H12A	1.0502(26)	C8 - H8A	1.0510(26)
C12 - H12B	1.0490(26)	C8 - H8B	1.0496(26)
C12 - H12C	1.0496(26)	C8 - H8C	1.0481(26)
La1 ... OW2	2.5137(18)	**Bond**	**Angle (deg)**
OW2 - H1	1.029(16)	H2-OW2-	107.3(12)
OW2 - H2	0.992(16)	H4-OW1-	105.6(13)
		H6-OW3-	107.5(13)
La2 ... OW1	2.5132(18)		
OW1 - H3	0.971(16)		
OW1 - H4	0.980(16)		
La2 ... OW3	4.3484(18)		
OW3 - H5	1.020(16)		
OW3 - H6	0.913(15)		

[1] *NB: Atoms O11 and O11', O12 and O12' are related by the P-1 inversion centre.*

Comparison of refined bond lengths for the atoms in Zeise's salt from (a) NPD data ($P2_1/c$, a = 11.1378(4) Å, b = 8.2444(3) Å, c = 9.4749(3) Å, β = 106.5041(23)°, V = 834.19(5) Å^3) and (b) SND ($P2_1/c$, a = 11.212(3) Å, b = 8.424(6) Å, c = 9.696(6) Å, β = 107.52(4)°)

Atoms	Distance /Å	
	NPD	SXD
Pt–Cl(1) Trans	2.343(4)	2.340(2)
Pt–Cl(2) Cis	2.317(6)	2.302 (2)
Pt–Cl(3) Cis	2.287(6)	2.303(2)
Pt–C(1)	2.125(5)	2.128 (3)
Pt–C(2)	2.155(5)	2.135(3)
C(1) –H(1)	1.131(12)	1.096(7)
C(1) –H(2)	1.112(12)	1.087(7)
C(2) –H(3)	1.064(12)	1.079(8)
C(2) –H(4)	1.047(13)	1.086(8)
O–H(5)	1.005(13)	0.975(9)
O–H(6)	1.025(14)	0.940(8)
H(5).....Cl(2)	2.214(11)	2.288(8)
H(6)...Cl(3)	2.266(12)	2.380(8)
K---Cl(1)	3.538(8)	3.768(5)
K---Cl(1)'	3.207(8)	3.237(5)
K---Cl(1)''	3.179(8)	3.236(5)
K---Cl(1)'''	3.408(8)	3.397(5)
K---Cl(2)	3.234(8)	3.299(5)
K---Cl(3)	3.102(8)	3.199(5)
K----O	2.767(9)	2.761(6)
K---O'	2.714(10)	2.798(6)
Cl(1)-Pt-Cl(2)	89.71(19)	90.05(8)
Cl(1)-Pt-Cl(3)	90.28(20)	90.43(8)
Cl(2)-Pt-Cl(3)	177.07(20)	177.65(9)
C(1)-Pt-C(2)	37.94(16)	37.6(1)
Pt-C(1)-C(2)	72.2(3)	71.4(2)
Pt-C(2)-C(1)	69.9(3)	70.9(2)
H(1)-C(1)-H(2)	117.3(7)	115.2(5)
H(1)-C(1)-C(2)	120.8(7)	121.7(4)
H(2)-C(1)-C(2)	120.7(7)	120.6(4)
H(3)-C(2)-H(4)	119.0(7)	114.6(6)
H(3)-C(2)-C(1)	118.3(8)	121.2(5)
H(4)-C(2)-C(1)	120.9(8)	120.8(5)
H(5)-O-H(6)	100.9(9)	103.6(6)
O-H(5)---Cl(2)	162.8(10)	161.6(7)
O-H(6)--Cl(3)	177.0(9)	179.4(7)
Pt-Cl(2)--H(5)	100.4(4)	103.6(2)
Pt-Cl(3)---H(6)	102.1(3)	102.5(2)