

Appendix B: Refined framework atomic coordinates, bond lengths and angles for TNU-7, Ga-MAZ and Ga-MOR

(1) Na-TNU-7 (from synchrotron data)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso} (x 100)
T(1)	-0.2500	0.16294(4)	-0.00396(3)	2.07(3)
T(2)	-0.2500	0.0747(5)	0.1037(5)	2.07(3)
T(3)	-0.2500	0.1607(4)	0.2119(3)	2.07(3)
T(4)	0.035(1)	0.1617(3)	-0.0893(2)	2.07(3)
T(5)	0.0472(1)	-0.0203(3)	0.1447(3)	2.07(3)
T(6)	0.043(1)	0.0577(3)	0.2489(5)	2.07(3)
T(7)	0.2500	0.1637(4)	0.3958(3)	2.07(3)
T(8)	0.2500	0.1675(4)	0.5187(3)	2.07(3)
T(9)	-0.047(1)	0.0524(3)	0.3633(2)	2.07(3)
T(10)	0.050(1)	-0.0513(3)	0.4516(2)	2.07(3)
O(1)	-0.2500	0.2500	0.012(1)	3.9(1)
O(2)	-0.2500	0.113(1)	0.0479(5)	3.9(1)
O(3)	-0.2500	0.130(1)	0.1523(4)	3.9(1)
O(4)	-0.2500	0.2500	0.203(1)	3.9(1)
O(5)	-0.078(1)	0.134(1)	-0.0376(4)	3.9(1)
O(6)	-0.064(1)	0.028(1)	0.1017(4)	3.9(1)
O(7)	-0.079(1)	0.1348(5)	0.2473(2)	3.9(1)
O(8)	-0.019(3)	0.2500	-0.105(1)	3.9(1)
O(9)	-0.015(2)	-0.006(1)	0.2064(4)	3.9(1)
O(10)	0.2500	0.156(1)	-0.074(1)	3.9(1)
O(11)	0.2500	-0.004(1)	0.137(1)	3.9(1)
O(12)	0.2500	0.084(1)	0.251(1)	3.9(1)
O(13)	-0.004(2)	0.1108(4)	-0.1413(4)	3.9(1)
O(14)	-0.001(2)	0.018(1)	0.3051(3)	3.9(1)
O(15)	0.2500	0.2500	0.377(1)	3.9(1)
O(16)	0.2500	0.2500	0.545(1)	3.9(1)
O(17)	0.2500	0.159(1)	0.4571(3)	3.9(1)

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O(18)	0.071(1)	0.127(1)	0.372(1)	3.9(1)
O(19)	0.075(1)	0.1253(5)	0.5387(5)	3.9(1)
O(20)	0.014(1)	-0.021(1)	0.3928(3)	3.9(1)
O(21)	0.0000	0.0000	0.5000	3.9(1)
O(22)	-0.2500	0.069(1)	0.374(1)	3.9(1)
O(23)	-0.2500	0.089(1)	0.538(1)	3.9(1)

Bond length (Å)

T(1)-O(1)	1.63(1)	T(5)-O(6)	1.63(1)	T(9)-O(14)	1.66(1)	Na(C)-O(19)	3.09(2)
T(1)-O(2)	1.61(1)	T(5)-O(9)	1.67(1)	T(9)-O(18)	1.61(1)	Na(C)-O(23)	3.06(2)
T(1)-O(5)	1.65(1)	T(5)-O(11)	1.63(1)	T(9)-O(20)	1.58(1)	Na(D)-O(9)	2.11(2)
		T(5)-O(13)	1.66(1)	T(9)-O(22)	1.61(1)	Na(D)-O(13)	3.17(2)
T(2)-O(2)	1.61(1)					Na(D)-O(14)	3.05(2)
T(2)-O(3)	1.61(1)	T(6)-O(7)	1.67(1)	T(10)-O(19)	1.65(1)	Na(E)-O(8)	2.34(2)
T(2)-O(6)	1.65(1)	T(6)-O(9)	1.65(1)	T(10)-O(20)	1.63(1)	Na(E)-O(13)	2.30(3)
		T(6)-O(12)	1.64(1)	T(10)-O(21)	1.60(1)	Na(F)-O(1)	2.22(3)
T(3)-O(3)	1.65(1)	T(6)-O(14)	1.66(1)	T(10)-O(23)	1.67(1)	Na(F)-O(2)	2.89(3)
T(3)-O(4)	1.63(1)					Na(F)-O(3)	2.52(3)
T(3)-O(7)	1.66(1)	T(7)-O(15)	1.63(1)	Na(A)-O(2)	2.98(1)	Na(F)-O(4)	2.71(2)
		T(7)-O(17)	1.59(1)	Na(A)-O(5)	2.69(1)		
T(4)-O(5)	1.67(1)	T(7)-O(18)	1.63(1)	Na(A)-O(6)	2.72(1)	Na(A)-Na(A)	3.786(1)
T(4)-O(8)	1.70(1)			Na(B)-O(7)	2.73(2)	Na(E)-Na(E)	2.2(1)
T(4)-O(10)	1.68(1)	T(8)-O(16)	1.63(1)	Na(B)-O(15)	2.40(3)	Na(B)-Na(B)	2.71(1)
T(4)-O(13)	1.66(1)	T(8)-O(17)	1.61(1)	Na(B)-O(18)	2.88(2)	Na(C)-Na(C)	1.01(1)
		T(8)-O(19)	1.61(5)				

O-T-O bond angles (°)

O(1)-T(1)-O(2)	111(1)	O(6)-T(5)-O(9)	116(1)	O(16)-T(8)-O(17)	117(1)
O(1)-T(1)-O(5)	117(1)	O(6)-T(5)-O(11)	104(1)	O(16)-T(8)-O(19)	110(1)
O(2)-T(1)-O(5)	103(1)	O(6)-T(5)-O(13)	116(1)	O(17)-T(8)-O(19)	106(1)
O(5)-T(1)-O(5)	103(2)	O(9)-T(5)-O(11)	113(2)	O(19)-T(8)-O(19)	108(1)

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O(2)-T(2)-O(3)	118(1)	O(9)-T(5)-O(13)	100(1)	O(14)-T(9)-O(18)	108(1)
O(2)-T(2)-O(6)	100(1)	O(11)-T(5)-O(13)	109(1)	O(14)-T(9)-O(20)	98(1)
O(3)-T(2)-O(6)	111(1)	O(7)-T(6)-O(9)	114(1)	O(14)-T(9)-O(22)	113(1)
O(6)-T(2)-O(6)	119(1)	O(7)-T(6)-O(12)	106(1)	O(18)-T(9)-O(20)	119(1)
O(3)-T(3)-O(4)	100(1)	O(7)-T(6)-O(14)	107(1)	O(18)-T(9)-O(22)	112(1)
O(3)-T(3)-O(7)	115(1)	O(9)-T(6)-O(12)	104(1)	O(20)-T(9)-O(22)	108(1)
O(4)-T(3)-O(7)	110(1)	O(9)-T(6)-O(14)	104(1)	O(19)-T(10)-O(20)	108(1)
O(7)-T(3)-O(7)	105(1)	O(12)-T(6)-O(14)	106(1)	O(19)-T(10)-O(21)	101(1)
O(5)-T(4)-O(8)	111(1)	O(15)-T(7)-O(17)	109(1)	O(19)-T(10)-O(23)	101(1)
O(5)-T(4)-O(10)	107(1)	O(15)-T(7)-O(18)	106(1)	O(20)-T(10)-O(21)	119(1)
O(5)-T(4)-O(13)	113(1)	O(17)-T(7)-O(18)	112(1)	O(20)-T(10)-O(23)	117(1)
O(8)-T(4)-O(10)	110(1)	O(18)-T(7)-O(18)	112(1)	O(21)-T(10)-O(23)	109(1)
O(8)-T(4)-O(13)	105(1)				
O(10)-T(4)-O(13)	111(1)				

(2) Na-Ga-MAZ (from synchrotron data)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} (x100)
T(1)	0.4865(2)	0.1537(2)	0.25	3.4(1)
T(2)	0.0937(2)	0.3553(2)	0.0451(3)	3.4(1)
O(1)	0.7468(2)	1.4936(4)	0.25	6.7(3)
O(2)	0.5799(3)	1.130(1)	0.25	6.7(3)
O(3)	0.093(1)	0.377(1)	0.25	6.7(3)
O(4)	0.1005(3)	0.4332(3)	0.923(1)	6.7(3)
O(5)	0.159(1)	0.318(1)	1.006(1)	6.7(3)
O(6)	0.2771(2)	0	0	6.7(3)

	Bond length (Å)	O-T-O bond angles (°)
T(1)-O(1)	1.651(3)	O(1)-T(1)-O(2) 103.2(4)
T(1)-O(2)	1.638(3)	O(1)-T(1)-O(4) 111.6(3)
T(1)-O(4)	1.649(3)	O(2)-T(1)-O(4) 111.6(3)

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		O(4)-T(1)-O(4)	107(1)
T(2)-O(3)	1.618(3)		
T(2)-O(4)	1.642(4)	O(3)-T(2)-O(4)	111.5(4)
T(2)-O(5)	1.660(4)	O(3)-T(2)-O(5)	111(1)
T(2)-O(6)	1.572(3)	O(3)-T(2)-O(6)	105.5(4)
		O(4)-T(2)-O(5)	120(1)
Na(A)-O(4)	2.73(1)	O(4)-T(2)-O(6)	99(1)
Na(D)-O(5)	2.34(1)	O(5)-T(2)-O(6)	108.6(4)
Na(A)-Na(A)	3.8427(1)		

(3) Na-Ga-MOR (from synchrotron data)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso} ($\times 100$)
T(1)	0.20113(1)	0.4281(2)	0.54193(4)	2.32(4)
T(2)	0.1934(2)	0.1904(2)	0.5427(5)	2.32(4)
T(3)	0.0861(1)	0.3846(2)	0.25	2.32(4)
T(4)	0.0849(2)	0.2261(1)	0.25	2.32(4)
O(1)	0.1289(4)	0.4134(4)	0.426(1)	4.4(1)
O(2)	0.1170(3)	0.195(1)	0.429(1)	4.4(1)
O(3)	0.2661(3)	0.3827(3)	0.478(1)	4.4(1)
O(4)	0.0939(5)	0.3051(3)	0.25	4.4(1)
O(5)	0.1721(5)	0.199(1)	0.75	4.4(1)
O(6)	0.181(1)	0.415(1)	0.75	4.4(1)
O(7)	0.232(1)	0.5	0.5	4.4(1)
O(8)	0.25	0.25	0.5	4.4(1)
O(9)	0	0.407(1)	0.25	4.4(1)
O(10)	0	0.200(1)	0.25	4.4(1)

Bond length (Å)				O-T-O bond angles (°)	
T(1)-O(1)	1.59(1)	Na(B _{mor})-O(1)	2.97(1)	O(1)-T(1)-O(3)	109.5(4)
T(1)-O(3)	1.56(1)	Na(B _{mor})-O(9)	2.65(1)	O(1)-T(1)-O(6)	108(1)
T(1)-O(6)	1.622(4)	Na(C)-O(2)	2.52(1)	O(1)-T(1)-O(7)	111(1)
T(1)-O(7)	1.595(4)	Na(C)-O(10)	2.72(2)	O(3)-T(1)-O(6)	112(1)
		Na(D)-O(3)	2.72(2)	O(3)-T(1)-O(7)	103(1)
T(2)-O(2)	1.62(1)	Na(D)-O(7)	2.65(2)		
T(2)-O(3)	1.66(1)	Na(B _{mor})-Na(B _{mor})	3.746(1)	O(2)-T(2)-O(3)	112(1)
T(2)-O(5)	1.609(4)	Na(C)-Na(C)	2.1(1)	O(2)-T(2)-O(5)	107.3(4)
T(2)-O(8)	1.613(4)	Na(D)-Na(D)	3.94(2)	O(2)-T(2)-O(8)	112.8(4)
				O(3)-T(2)-O(5)	107(1)
T(3)-O(1)	1.636(4)			O(3)-T(2)-O(8)	112.0(3)
T(3)-O(4)	1.62(1)			O(5)-T(2)-O(8)	105(1)
T(3)-O(9)	1.62(1)			O(1)-T(3)-O(1)	108(1)
				O(1)-T(3)-O(4)	108.3(4)
T(4)-O(2)	1.291(4)			O(1)-T(3)-O(9)	110.5(4)
T(4)-O(4)	1.61(1)			O(4)-T(3)-O(9)	112(1)
T(4)-O(10)	1.62(1)			O(2)-T(4)-O(2)	115(1)
				O(2)-T(4)-O(4)	110.9(4)
				O(2)-T(4)-O(10)	102.6(4)
				O(4)-T(4)-O(10)	115(1)

(4) Na-TNU-7 (from neutron data)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} (x 100)
T(1)	-0.2500	0.1638(3)	-0.0053(4)	2.2(1)
T(2)	-0.2500	0.069(1)	0.1043(5)	2.2(1)
T(3)	-0.2500	0.159(1)	0.2080(5)	2.2(1)
T(4)	0.037(1)	0.1661(5)	-0.0828(4)	2.2(1)
T(5)	0.036(1)	-0.0201(5)	0.1481(4)	2.2(1)
T(6)	0.040(1)	0.062(1)	0.2519(4)	2.2(1)

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T(7)	0.2500	0.163(1)	0.3969(5)	2.2(1)
T(8)	0.2500	0.164(1)	0.5178(4)	2.2(1)
T(9)	-0.041(1)	0.0514(5)	0.3619(4)	2.2(1)
T(10)	0.046(1)	-0.0513(5)	0.4539(3)	2.2(1)
O(1)	-0.2500	0.2500	0.011(1)	1.9(1)
O(2)	-0.2500	0.109(1)	0.0433(4)	1.9(1)
O(3)	-0.2500	0.129(1)	0.1495(4)	1.9(1)
O(4)	-0.2500	0.2500	0.209(1)	1.9(1)
O(5)	-0.079(1)	0.1375(4)	-0.0381(4)	1.9(1)
O(6)	-0.069(1)	0.0176(4)	0.100(4)	1.9(1)
O(7)	-0.082(1)	0.1339(5)	0.2405(3)	1.9(1)
O(8)	0.007(2)	0.2500	-0.0961(5)	1.9(1)
O(9)	-0.017(1)	-0.0011(4)	0.2056(3)	1.9(1)
O(10)	0.2500	0.157(1)	-0.0761(5)	1.9(1)
O(11)	0.2500	-0.011(1)	0.1295(5)	1.9(1)
O(12)	0.2500	0.075(1)	0.247(4)	1.9(1)
O(13)	-0.0137(1)	0.1110(5)	-0.1338(4)	1.9(1)
O(14)	-0.024(1)	0.0253(5)	0.3041(3)	1.9(1)
O(15)	0.2500	0.2500	0.377(1)	1.9(1)
O(16)	0.2500	0.2500	0.538(1)	1.9(1)
O(17)	0.2500	0.158(1)	0.4542(4)	1.9(1)
O(18)	0.078(1)	0.1234(4)	0.3661(3)	1.9(1)
O(19)	0.075(1)	0.1234(5)	0.5343(4)	1.9(1)
O(20)	0.019(1)	-0.0172(5)	0.3985(4)	1.9(1)
O(21)	0.0000	0.0000	0.5000	1.9(1)
O(22)	-0.2500	0.080(1)	0.3749(4)	1.9(1)
O(23)	-0.2500	0.088(1)	0.532(1)	1.9(1)

Bond length (Å)

T(1)-O(1)	1.56(1)	T(5)-O(6)	1.63(1)	T(9)-O(14)	1.57(1)	Na(C)-O(23)	2.95(1)
T(1)-O(2)	1.64(1)	T(5)-O(9)	1.58(1)	T(9)-O(18)	1.59(1)	Na(D)-O(9)	2.68(4)
T(1)-O(5)	1.64(1)	T(5)-O(11)	1.70(1)	T(9)-O(20)	1.63(1)		

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	T(5)-O(13)	1.70(1)	T(9)-O(22)	1.70(1)	Na(D)-O(14)	2.33(4)	
T(2)-O(2)	1.74(1)				Na(E)-O(8)	2.25(2)	
T(2)-O(3)	1.60(1)	T(6)-O(7)	1.63(1)	T(10)-O(19)	1.63(1)	Na(E)-O(13)	2.78(3)
T(2)-O(6)	1.66(1)	T(6)-O(9)	1.71(1)	T(10)-O(20)	1.58(1)	Na(F)-O(1)	2.3(4)
		T(6)-O(12)	1.61(1)	T(10)-O(21)	1.55(1)	Na(F)-O(1)	2.16(2)
T(3)-O(3)	1.61(1)	T(6)-O(14)	1.58(1)	T(10)-O(23)	1.72(1)	Na(F)-O(2)	2.88(1)
T(3)-O(4)	1.64(1)				Na(F)-O(3)	2.60(1)	
T(3)-O(7)	1.60(1)	T(7)-O(15)	1.65(1)	Na(A)-O(2)	2.96(1)	Na(F)-O(4)	2.60(2)
		T(7)-O(17)	1.48(1)	Na(A)-O(5)	2.74(1)		
T(4)-O(5)	1.54(1)	T(7)-O(18)	1.69(1)	Na(A)-O(6)	2.66(1)	Na(A)-Na(A)	3.791(1)
T(4)-O(8)	1.57(1)			Na(B)-O(4)	2.86(3)	Na(B)-Na(B)	4.1(1)
T(4)-O(10)	1.63(1)	T(8)-O(16)	1.63(1)	Na(B)-O(7)	2.53(2)	Na(C)-Na(C)	0.5(2)
T(4)-O(13)	1.70(1)	T(8)-O(17)	1.65(1)	Na(B)-O(15)	2.93(3)	Na(E)-Na(E)	0.8(1)
		T(8)-O(19)	1.58(1)	Na(B)-O(18)	3.12(2)		

O-T-O bond angles (°)

O(1)-T(1)-O(2)	114(1)	O(6)-T(5)-O(9)	119(1)	O(16)-T(8)-O(17)	113(1)
O(1)-T(1)-O(5)	117(1)	O(6)-T(5)-O(11)	102(1)	O(16)-T(8)-O(19)	111(1)
O(2)-T(1)-O(5)	101(1)	O(6)-T(5)-O(13)	101(1)	O(17)-T(8)-O(19)	104(1)
O(5)-T(1)-O(5)	105(1)	O(9)-T(5)-O(11)	119(2)	O(19)-T(8)-O(19)	114(1)
O(2)-T(2)-O(3)	112(1)	O(9)-T(5)-O(13)	113(1)	O(14)-T(9)-O(18)	105(1)
O(2)-T(2)-O(6)	100(1)	O(11)-T(5)-O(13)	99(1)	O(14)-T(9)-O(20)	108(1)
O(3)-T(2)-O(6)	116(1)	O(7)-T(6)-O(9)	105(1)	O(14)-T(9)-O(22)	111(1)
O(6)-T(2)-O(6)	111(1)	O(7)-T(6)-O(12)	116(1)	O(18)-T(9)-O(20)	115(1)
O(3)-T(3)-O(4)	111(1)	O(7)-T(6)-O(14)	108(1)	O(18)-T(9)-O(22)	105(1)
O(3)-T(3)-O(7)	113(1)	O(9)-T(6)-O(12)	107(1)	O(20)-T(9)-O(22)	112(1)
O(4)-T(3)-O(7)	106(1)	O(9)-T(6)-O(14)	104(1)	O(19)-T(10)-O(20)	114(1)
O(7)-T(3)-O(7)	106(1)	O(12)-T(6)-O(14)	116(1)	O(19)-T(10)-O(21)	102(1)
O(5)-T(4)-O(8)	114(1)	O(15)-T(7)-O(17)	112(1)	O(19)-T(10)-O(23)	99(1)
O(5)-T(4)-O(10)	117(1)	O(15)-T(7)-O(18)	105(1)	O(20)-T(10)-O(21)	116(1)
O(5)-T(4)-O(13)	105(1)	O(17)-T(7)-O(18)	116(1)	O(20)-T(10)-O(23)	117(1)
O(8)-T(4)-O(10)	105(1)	O(18)-T(7)-O(18)	101(1)	O(21)-T(10)-O(23)	106(1)

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O(8)-T(4)-O(13) 112(1)

O(10)-T(4)-O(13) 105(1)
