Electronic Supplementary Information for Dalton Transactions

Supporting information

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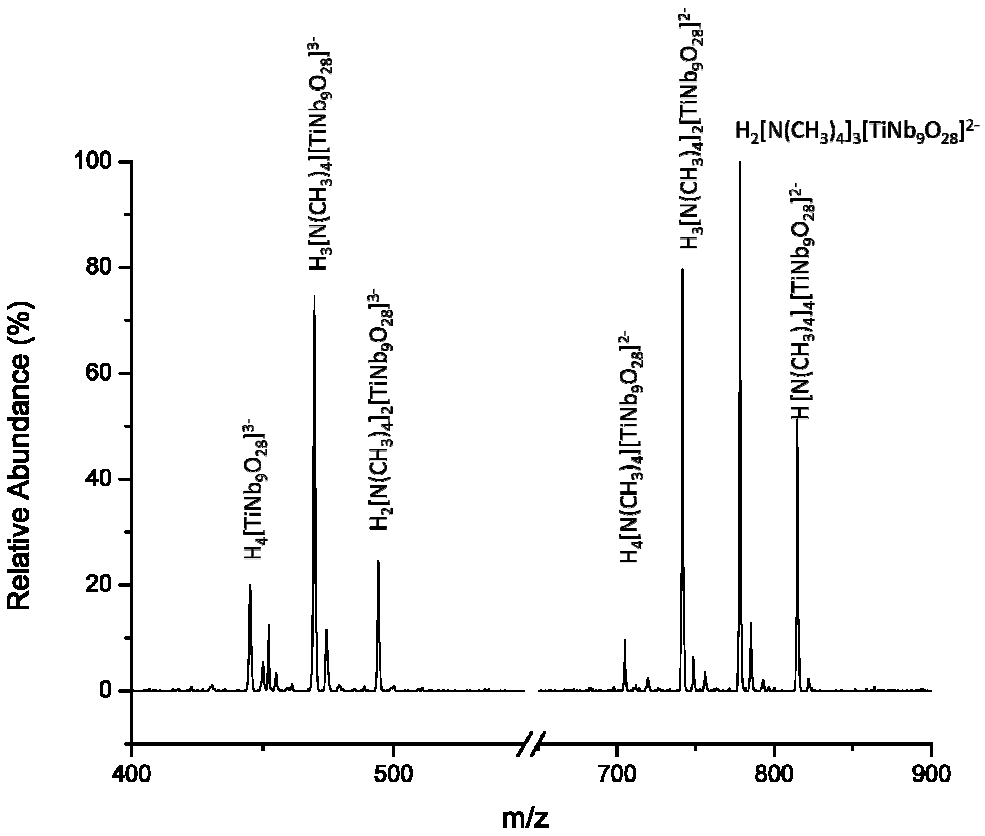


Fig. S.1. ESI-MS spectrum (Cone voltage -20 V, negative mode) of $[N(CH_3)_4]_7[TiNb_9O_{28}]$ in water. The main impurity is $[Ti_2Nb_8O_{28}]^{8-}$.

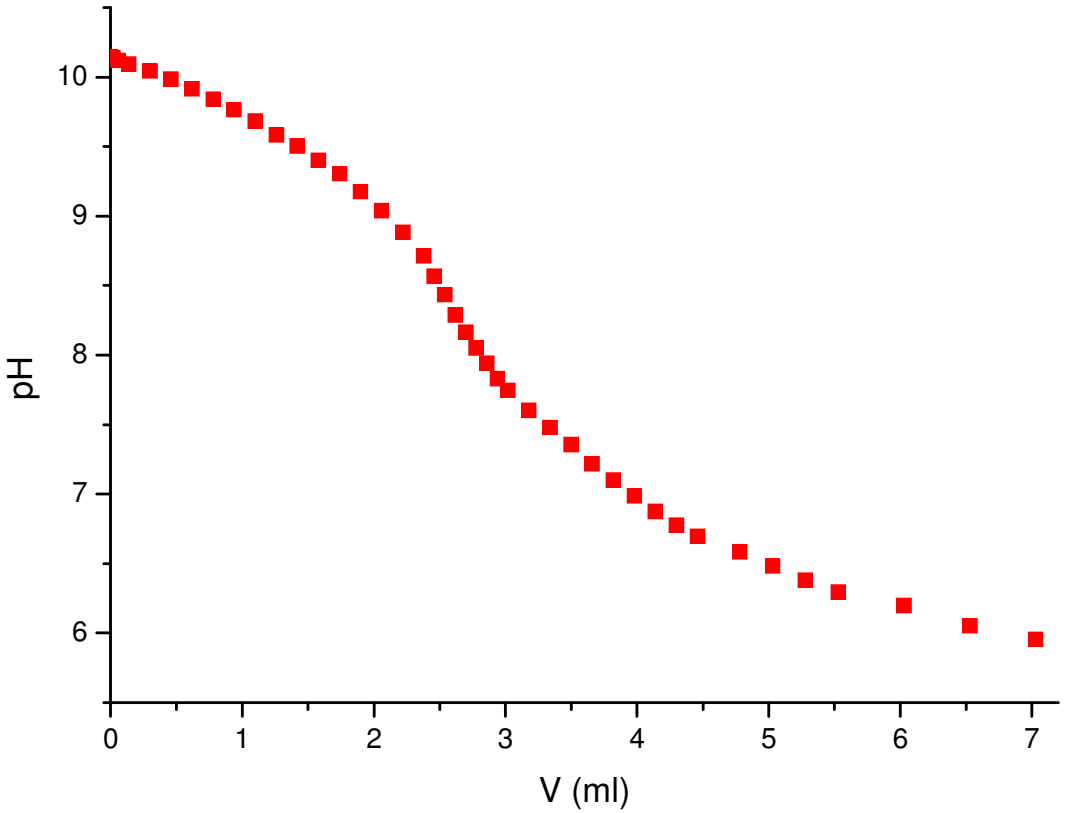


Fig. S.2. Titration of a solution of $[N(CH_3)_4]_7[TiNb_9O_{28}]$ (5 mM) at 23 ˚C using HCl (5 mM). $[N(CH_3)_4]Cl$ (0.1 M) was used as background salt, and $[N(CH_3)_4]OH$ (3 ml, 11 mM) was added prior to titration.

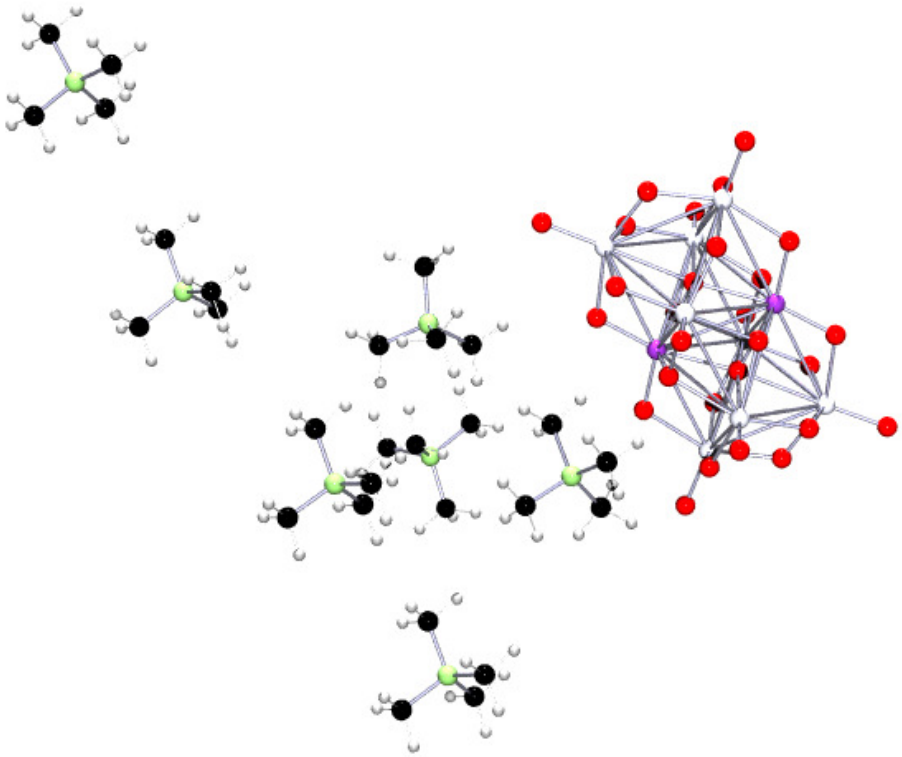
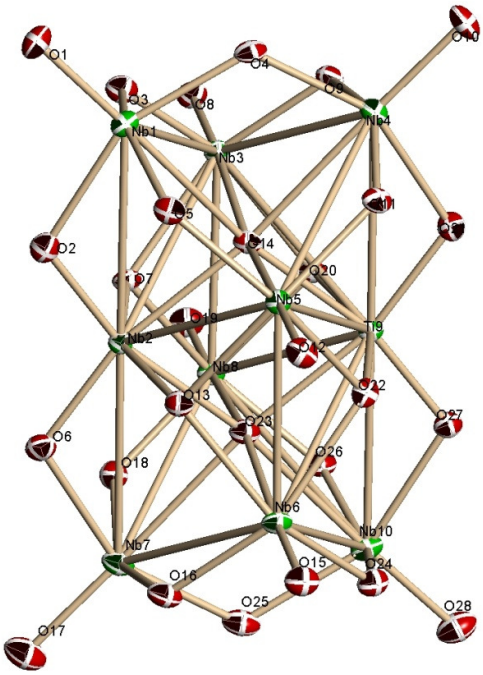


Fig. S.3. Content of unit cell for $[N(CH_3)_4]_7[TiNb_9O_{28}]$. Waters removed. Hydrogen, carbon, nitrogen, oxygen, niobium atoms in grey, black, green, red and silver, respectively. Sites in purple have 50% occupancy of titanium and 50% occupancy of niobium.

$[N(CH_3)_4]_7[TiNb_9O_{28}]\cdot 22\ H_2O$

A colorless block with approximate orthogonal dimensions 0.50 x 0.35 x 0.22mm^3 was placed and optically centered on the Bruker APEX II[1] CCD system at 90(2)K. The initial unit cell was indexed using a least-squares analysis of a random set of reflections collected from three series of 0.3° wide ω-scans, 10 seconds per frame, and 30 frames per series that were well distributed in reciprocal space. Four ω-scan data frame series were collected [MoKα] with 0.3° wide scans, 15 seconds per frame and 606 frames were collected, at varying phi angles (phi=0°, 90°, 180°, 270°), for each series. The crystal to detector distance was 5.28cm, thus providing a complete sphere of data with processing to $2\theta_{max}$=55.24°.



Structural determination and Refinement:

All crystallographic calculations were performed on a Personal computer (PC) with a Pentium 3.20GHz processor and 4GB of extended memory. A total of 49929 reflections were collected and corrected for Lorentz and polarization effects and numerical, face based, absorption using Blessing's method as incorporated into the program SADABS[2, 3] with 18438 unique. The SHELXTL[4] program package was implemented to determine the probable space group and set up the initial files. The unit cell appears monoclinic with both alpha and gamma near 90.0 degrees. However, system symmetry and lack of systematic absences generated three possibilities, P2, Pm, or P2/m and after all three had had exhaustive attempts with strange fruitless results in each, the triclinic system was attempted. System symmetry, lack of systematic absences and intensity statistics indicated the potential centrosymmetric triclinic space group P-1 (no. 2). The structure was determined by direct methods with the successful location of a majority of the molecule of interest using the program XS[5]. The structure was refined with XL[5]. An initial result in P-1 proved appealing and when the twin law -1 0 0 0 1 0 0 0 -1 was included the structure converged quickly. When viewed down the 010 axis it becomes apparent that the molecule does not possess two-fold symmetry about this axis but is skewed from it. The tetramethylammonium anions are also problematic with a two fold rotation but are well ordered in P-1. It was therefore concluded that this system possesses a nearly monoclinic cell but is actually triclinic in nature. A multitude of refinement difference-Fourier cycles were required to locate the remaining non-hydrogen atoms. Water molecules were optimized when believed to be partial occupancy and hydrogen atoms were located whenever possible with difference-Fourier maps. All hydrogen atoms were optimized to have minimal interactions with neighboring water molecules. The data collected were merged based upon identical indices yielding 12276

data [R(int)=0.0212] that were truncated to $2\theta_{max}$=55.00° resulting in 12262 data that were further merged in least-squares refinement to 6255 unique data [R(int)=0.0240]. All non-hydrogen atoms were refined anisotropically. The final structure was refined to convergence with R(F)=4.62%, wR(F^2)=10.91%, GOF=1.053 for all 18438 unique reflections [R(F)=4.03%, wR(F^2)=10.56% for those 16888 data with Fo > 4σ(Fo)]. The final difference-Fourier map was possessed a multitude of peaks near the heavy atoms within the structure while the remainder of the map was featureless indicating that the structure is both correct and complete.

References:

1. Bruker (2007) APEX (Version 2.2.0) and SAINT (Version 7.23a). Bruker AXS Inc., Madison, Wisconsin, USA.

2. An Empirical Correction for Absorption Anisotropy, Blessing, R. H. (1995). Acta Cryst., A51, 33-38.

3. Sheldrick, G.M., SADABS (2007) Version 2007/3, 'Siemens Area Detector Absorption Correction' Universität Göttingen: Göttingen, Germany.

4. Sheldrick, G.M., (2002). SHELXTL. Version 6.1. Bruker AXS Inc., Madison, Wisconsin, USA.

5. Sheldrick, G. M., (1997). SHELXS97 and SHELXL97. Universität Göttingen: Göttingen, Germany.

Table S.1. Crystal data and structure refinement for $[Nb9TiO_{28}][C_4H_{12}N]_7[H_2O]_{22}$.

Identification code	jf1660ffmi (Rotational TWIN)	
Empirical formula	C28 H128 N7 Nb9 O50 Ti	
Formula weight	2247.46	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 13.583(2) Å	α= 90.020(2)°.
	b = 19.893(4) Å	β= 105.549(2)°.
	c = 15.513(3) Å	γ = 89.966(2)°.
Volume	4038.4(12) $Å^3$	
Z	2	
Density (calculated)	1.848 Mg/m^3	
Absorption coefficient	1.416 mm^{-1}	
F(000)	2272	
Crystal size	0.50 x 0.35 x 0.22 mm^3	
Crystal color and habit	Colorless Block	
Diffractometer	Bruker APEX-II CCD	
Theta range for data collection	2.91 to 27.48°.	
Index ranges	-17<=h<=17, -25<=k<=25, -20<=l<=20	
Reflections collected	35282	
Independent reflections	18438 [R(int) = 0.0350]	

Observed reflections (I > 2sigma(I))	16888
Completeness to theta = 27.48°	99.5 %
Absorption correction	Numerical
Max. and min. transmission	0.7477 and 0.5402
Solution method	SHELXS-97 (Sheldrick, 2008)
Refinement method	SHELXL-97 (Sheldrick, 2008) Full-matrix least-squares on F^2
Data / restraints / parameters	18438 / 54 / 955
Goodness-of-fit on F^2	1.053
Final R indices [I>2sigma(I)]	R1 = 0.0403, wR2 = 0.1056
R indices (all data)	R1 = 0.0462, wR2 = 0.1091
Largest diff. peak and hole	2.721 and -1.778 e.Å^{-3}

Table S.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jf1660ffmi. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Nb(1)	1304(1)	5881(1)	2213(1)	13(1)
Nb(2)	1414(1)	7503(1)	2296(1)	10(1)
Ti(2)	1414(1)	7503(1)	2296(1)	10(1)
Nb(3)	-645(1)	6768(1)	945(1)	11(1)
Nb(4)	-966(1)	5935(1)	2715(1)	13(1)
Nb(5)	1085(1)	6664(1)	4075(1)	11(1)
Nb(6)	1156(1)	8304(1)	4150(1)	13(1)
Nb(7)	1514(1)	9128(1)	2397(1)	16(1)
Nb(8)	-527(1)	8409(1)	1018(1)	12(1)
Nb(9)	-876(1)	7562(1)	2794(1)	10(1)
Ti(9)	-876(1)	7562(1)	2794(1)	10(1)
Nb(10)	-785(1)	9180(1)	2858(1)	15(1)
O(1)	2076(4)	5226(2)	1990(3)	19(1)
O(2)	2080(3)	6747(2)	2112(3)	16(1)
O(3)	428(3)	6126(2)	1016(3)	16(1)
O(4)	142(3)	5417(2)	2444(3)	14(1)
O(5)	1834(3)	6040(2)	3538(3)	15(1)
O(6)	2182(3)	8225(2)	2191(3)	16(1)

O(7)	423(3)	7553(2)	1083(2)	13(1)
O(8)	-1255(3)	6794(2)	-213(3)	15(1)
O(9)	-1482(3)	6171(2)	1413(3)	14(1)
O(10)	-1793(3)	5313(2)	2900(3)	18(1)
O(11)	-68(3)	6095(2)	3938(3)	15(1)
O(12)	1710(3)	6591(2)	5228(3)	16(1)
O(13)	1818(3)	7470(2)	3652(2)	14(1)
O(14)	222(3)	6833(2)	2508(3)	11(1)
O(15)	1770(3)	8291(2)	5311(3)	17(1)
O(16)	1992(4)	8891(2)	3680(3)	17(1)
O(17)	2408(4)	9734(2)	2271(3)	26(1)
O(18)	628(3)	8979(2)	1167(3)	15(1)
O(19)	-1143(3)	8479(2)	-134(3)	17(1)
O(20)	-1287(3)	7600(2)	1444(2)	11(1)
O(21)	-1646(3)	6839(2)	2904(3)	13(1)
O(22)	109(3)	7507(2)	4011(2)	13(1)
O(23)	307(3)	8235(2)	2584(3)	14(1)
O(24)	70(3)	8935(2)	4068(3)	15(1)
O(25)	401(4)	9650(2)	2658(3)	18(1)
O(26)	-1278(3)	9027(2)	1555(3)	16(1)
O(27)	-1565(3)	8315(2)	2969(3)	14(1)
O(28)	-1581(4)	9822(2)	3072(3)	22(1)
C(31)	9912(6)	8965(4)	6181(5)	29(2)

N(31)	8768(5)	8977(3)	5809(4)	25(1)
C(32)	8467(6)	9617(4)	5312(4)	28(2)
C(33)	8461(8)	8387(4)	5200(5)	38(2)
C(34)	8280(6)	8929(4)	6567(5)	30(2)
C(35)	9819(6)	5897(4)	6030(5)	31(2)
N(35)	8692(4)	5907(3)	5685(3)	18(1)
C(36)	8356(6)	6519(4)	5142(5)	26(2)
C(37)	8380(7)	5303(4)	5098(5)	34(2)
C(38)	8234(5)	5886(4)	6457(4)	25(1)
C(39)	5750(5)	7590(5)	5205(5)	36(2)
N(39)	4636(5)	7663(4)	4816(4)	38(2)
C(40)	4381(9)	8363(8)	4513(14)	128(8)
C(41)	4299(7)	7152(7)	4044(7)	75(4)
C(42)	4078(5)	7491(5)	5483(5)	32(2)
C(43)	9254(7)	822(5)	1083(6)	50(3)
N(43)	8180(5)	797(3)	612(4)	29(1)
C(44)	7864(7)	1425(4)	64(5)	37(2)
C(45)	8020(8)	200(4)	-32(6)	47(2)
C(46)	7507(8)	700(5)	1224(7)	53(3)
C(47)	4399(6)	6310(4)	1869(6)	36(2)
N(47)	4983(5)	5666(3)	2160(5)	33(1)
C(48)	5975(6)	5670(4)	1924(6)	34(2)
C(49)	4385(8)	5080(5)	1651(10)	68(4)

C(50)	5199(13)	5605(6)	3141(7)	83(5)
C(51)	8202(6)	3938(4)	1703(5)	32(2)
N(51)	8547(4)	3975(3)	868(4)	19(1)
C(52)	8068(8)	4571(4)	336(5)	43(2)
C(53)	9682(5)	4039(4)	1137(5)	26(2)
C(54)	8241(6)	3345(4)	334(5)	28(2)
C(55)	4813(5)	7927(4)	-44(5)	35(2)
N(55)	5933(4)	7942(3)	364(4)	26(1)
C(56)	6268(7)	8614(5)	734(8)	53(2)
C(57)	6480(6)	7743(4)	-332(5)	34(2)
C(58)	6203(5)	7442(4)	1107(4)	30(2)
O(61)	4195(4)	9396(4)	1741(4)	115(4)
O(62)	4159(6)	7998(4)	1920(6)	68(2)
O(63)	5972(8)	9768(6)	4057(11)	138(6)
O(64)	6467(6)	8546(5)	3216(7)	74(2)
O(65)	6519(4)	7104(3)	3363(4)	35(1)
O(66)	6360(3)	4646(1)	5559(4)	40(1)
O(67)	6683(3)	5930(3)	75(3)	28(1)
O(68)	5992(3)	9882(4)	6121(4)	94(3)
O(69)	4567(1)	6113(3)	9659(1)	35(1)
O(70)	7390(3)	8981(2)	8393(4)	47(2)
O(71)	7454(3)	6027(2)	8543(3)	24(1)
O(72)	9429(6)	7635(3)	8674(4)	54(2)

O(73)	9593(4)	7363(3)	7014(4)	39(1)
O(74)	5940(4)	6674(3)	7300(4)	37(1)
O(75)	5977(5)	8123(3)	7324(4)	41(1)
O(76)	5411(4)	5883(3)	5676(4)	43(1)
O(77)	4180(4)	6445(3)	7816(3)	30(1)
O(78)	2817(3)	5730(2)	6554(3)	23(1)
O(79)	4217(4)	8602(1)	7745(3)	43(2)
O(80)	3057(4)	7566(3)	8092(3)	35(1)
O(81)	2828(4)	9283(2)	6417(3)	26(1)
O(82)	1470(4)	7442(3)	6564(3)	22(1)

Table S.3. Bond lengths [Å] and angles [°] for jf1660ffmi.

Nb(1)-O(1)	1.763(4)	Nb(3)-O(20)	2.112(4)
Nb(1)-O(4)	1.943(4)	Nb(3)-O(14)	2.398(4)
Nb(1)-O(3)	1.979(4)	Nb(3)-Nb(8)	3.2686(9)
Nb(1)-O(5)	2.012(4)	Nb(3)-Nb(4)	3.3362(8)
Nb(1)-O(2)	2.048(5)	Nb(4)-O(10)	1.746(4)
Nb(1)-O(14)	2.512(4)	Nb(4)-O(4)	1.960(4)
Nb(1)-Nb(2)	3.2314(10)	Nb(4)-O(11)	1.986(4)
Nb(1)-Nb(3)	3.3466(8)	Nb(4)-O(9)	2.009(4)
Nb(2)-O(6)	1.809(4)	Nb(4)-O(21)	2.078(4)
Nb(2)-O(2)	1.815(4)	Nb(4)-O(14)	2.486(4)
Nb(2)-O(7)	2.001(4)	Nb(4)-Nb(9)	3.2405(10)
Nb(2)-O(13)	2.028(4)	Nb(4)-Nb(5)	3.3415(8)
Nb(2)-O(14)	2.190(4)	Nb(5)-O(12)	1.768(4)
Nb(2)-O(23)	2.222(4)	Nb(5)-O(11)	1.898(4)
Nb(2)-Nb(7)	3.2381(10)	Nb(5)-O(5)	1.929(4)
Nb(2)-Nb(3)	3.3486(9)	Nb(5)-O(13)	2.086(4)
Nb(2)-Nb(5)	3.3574(9)	Nb(5)-O(22)	2.124(4)
Nb(3)-O(8)	1.766(4)	Nb(5)-O(14)	2.423(4)
Nb(3)-O(9)	1.918(4)	Nb(5)-Nb(6)	3.2655(9)
Nb(3)-O(3)	1.919(5)	Nb(6)-O(15)	1.770(4)
Nb(3)-O(7)	2.104(4)	Nb(6)-O(16)	1.906(4)

Nb(6)-O(24)	1.914(4)	Nb(9)-O(22)	2.003(4)
Nb(6)-O(22)	2.102(4)	Nb(9)-O(20)	2.020(4)
Nb(6)-O(13)	2.127(4)	Nb(9)-O(23)	2.183(4)
Nb(6)-O(23)	2.398(4)	Nb(9)-O(14)	2.209(4)
Nb(6)-Nb(7)	3.3220(9)	Nb(9)-Nb(10)	3.2210(10)
Nb(6)-Nb(9)	3.3336(9)	Nb(10)-O(28)	1.761(5)
Nb(6)-Nb(10)	3.3429(8)	Nb(10)-O(25)	1.958(5)
Nb(7)-O(17)	1.759(5)	Nb(10)-O(26)	1.975(4)
Nb(7)-O(25)	1.963(5)	Nb(10)-O(24)	1.986(4)
Nb(7)-O(16)	1.977(4)	Nb(10)-O(27)	2.052(4)
Nb(7)-O(18)	1.986(4)	Nb(10)-O(23)	2.500(4)
Nb(7)-O(6)	2.076(5)	C(31)-N(31)	1.505(10)
Nb(7)-O(23)	2.487(4)	C(31)-H(31A)	0.9800
Nb(7)-Nb(8)	3.3367(8)	C(31)-H(31B)	0.9800
Nb(8)-O(19)	1.764(4)	C(31)-H(31C)	0.9800
Nb(8)-O(18)	1.900(4)	N(31)-C(32)	1.486(9)
Nb(8)-O(26)	1.925(4)	N(31)-C(33)	1.495(8)
Nb(8)-O(20)	2.111(4)	N(31)-C(34)	1.500(9)
Nb(8)-O(7)	2.121(4)	C(32)-H(32A)	0.9800
Nb(8)-O(23)	2.414(4)	C(32)-H(32B)	0.9800
Nb(8)-Nb(10)	3.3403(9)	C(32)-H(32C)	0.9800
Nb(9)-O(21)	1.814(4)	C(33)-H(33A)	0.9800
Nb(9)-O(27)	1.824(4)	C(33)-H(33B)	0.9800

C(33)-H(33C)	0.9800	C(39)-H(39C)	0.9800
C(34)-H(34A)	0.9800	N(39)-C(42)	1.478(9)
C(34)-H(34B)	0.9800	N(39)-C(40)	1.482(14)
C(34)-H(34C)	0.9800	N(39)-C(41)	1.543(13)
C(35)-N(35)	1.480(9)	C(40)-H(40A)	0.9800
C(35)-H(35A)	0.9800	C(40)-H(40B)	0.9800
C(35)-H(35B)	0.9800	C(40)-H(40C)	0.9800
C(35)-H(35C)	0.9800	C(41)-H(41A)	0.9800
N(35)-C(36)	1.483(8)	C(41)-H(41B)	0.9800
N(35)-C(38)	1.490(8)	C(41)-H(41C)	0.9800
N(35)-C(37)	1.499(9)	C(42)-H(42A)	0.9800
C(36)-H(36A)	0.9800	C(42)-H(42B)	0.9800
C(36)-H(36B)	0.9800	C(42)-H(42C)	0.9800
C(36)-H(36C)	0.9800	C(43)-N(43)	1.446(10)
C(37)-H(37A)	0.9800	C(43)-H(43A)	0.9800
C(37)-H(37B)	0.9800	C(43)-H(43B)	0.9800
C(37)-H(37C)	0.9800	C(43)-H(43C)	0.9800
C(38)-H(38A)	0.9800	N(43)-C(46)	1.496(9)
C(38)-H(38B)	0.9800	N(43)-C(44)	1.508(9)
C(38)-H(38C)	0.9800	N(43)-C(45)	1.528(11)
C(39)-N(39)	1.478(9)	C(44)-H(44A)	0.9800
C(39)-H(39A)	0.9800	C(44)-H(44B)	0.9800
C(39)-H(39B)	0.9800	C(44)-H(44C)	0.9800

C(45)-H(45A)	0.9800	C(51)-H(51A)	0.9800
C(45)-H(45B)	0.9800	C(51)-H(51B)	0.9800
C(45)-H(45C)	0.9800	C(51)-H(51C)	0.9800
C(46)-H(46A)	0.9800	N(51)-C(52)	1.490(9)
C(46)-H(46B)	0.9800	N(51)-C(53)	1.491(8)
C(46)-H(46C)	0.9800	N(51)-C(54)	1.498(8)
C(47)-N(47)	1.510(10)	C(52)-H(52A)	0.9800
C(47)-H(47A)	0.9800	C(52)-H(52B)	0.9800
C(47)-H(47B)	0.9800	C(52)-H(52C)	0.9800
C(47)-H(47C)	0.9800	C(53)-H(53A)	0.9800
N(47)-C(50)	1.475(12)	C(53)-H(53B)	0.9800
N(47)-C(48)	1.488(9)	C(53)-H(53C)	0.9800
N(47)-C(49)	1.518(11)	C(54)-H(54A)	0.9800
C(48)-H(48A)	0.9800	C(54)-H(54B)	0.9800
C(48)-H(48B)	0.9800	C(54)-H(54C)	0.9800
C(48)-H(48C)	0.9800	C(55)-N(55)	1.483(8)
C(49)-H(49A)	0.9800	C(55)-H(55A)	0.9800
C(49)-H(49B)	0.9800	C(55)-H(55B)	0.9800
C(49)-H(49C)	0.9800	C(55)-H(55C)	0.9800
C(50)-H(50A)	0.9800	N(55)-C(56)	1.477(11)
C(50)-H(50B)	0.9800	N(55)-C(58)	1.491(9)
C(50)-H(50C)	0.9800	N(55)-C(57)	1.518(9)
C(51)-N(51)	1.493(8)	C(56)-H(56A)	0.9800

C(56)-H(56B)	0.9800	O(70)-H(70B)	0.8444
C(56)-H(56C)	0.9800	O(71)-H(71A)	0.84(6)
C(57)-H(57A)	0.9800	O(71)-H(71B)	0.84(5)
C(57)-H(57B)	0.9800	O(72)-H(72A)	0.84(6)
C(57)-H(57C)	0.9800	O(72)-H(72B)	0.84(10)
C(58)-H(58A)	0.9800	O(73)-H(73A)	0.84(3)
C(58)-H(58B)	0.9800	O(73)-H(73B)	0.84(6)
C(58)-H(58C)	0.9800	O(74)-H(74A)	0.84(3)
O(61)-H(61A)	0.8434	O(74)-H(74B)	0.84(8)
O(61)-H(61B)	0.8411	O(75)-H(75A)	0.84(5)
O(64)-H(64A)	0.84(5)	O(75)-H(75B)	0.85(8)
O(64)-H(64B)	0.85(7)	O(77)-H(77A)	0.84(6)
O(65)-H(65A)	0.84(2)	O(77)-H(77B)	0.84(4)
O(65)-H(65B)	0.84(6)	O(78)-H(78A)	0.84(6)
O(66)-H(66A)	0.8469	O(78)-H(78B)	0.84(6)
O(66)-H(66B)	0.8422	O(79)-H(79A)	0.8404
O(67)-H(67A)	0.8604	O(79)-H(79B)	0.8393
O(67)-H(67B)	0.8558	O(81)-H(81A)	0.85(7)
O(68)-H(68A)	0.8404	O(81)-H(81B)	0.84(7)
O(68)-H(68B)	0.8402	O(82)-H(82A)	0.84(4)
O(69)-H(69A)	0.8406	O(82)-H(82B)	0.84(6)
O(69)-H(69B)	0.8402		
O(70)-H(70A)	0.8414	O(1)-Nb(1)-O(4)	103.92(19)

O(1)-Nb(1)-O(3)	103.71(19)	O(5)-Nb(1)-Nb(3)	121.85(12)
O(4)-Nb(1)-O(3)	88.65(18)	O(2)-Nb(1)-Nb(3)	81.57(12)
O(1)-Nb(1)-O(5)	104.34(19)	O(14)-Nb(1)-Nb(3)	45.63(9)
O(4)-Nb(1)-O(5)	88.45(18)	Nb(2)-Nb(1)-Nb(3)	61.172(18)
O(3)-Nb(1)-O(5)	151.66(18)	O(6)-Nb(2)-O(2)	108.64(17)
O(1)-Nb(1)-O(2)	105.1(2)	O(6)-Nb(2)-O(7)	97.71(18)
O(4)-Nb(1)-O(2)	150.95(17)	O(2)-Nb(2)-O(7)	97.57(18)
O(3)-Nb(1)-O(2)	85.04(17)	O(6)-Nb(2)-O(13)	96.72(18)
O(5)-Nb(1)-O(2)	83.94(17)	O(2)-Nb(2)-O(13)	97.37(18)
O(1)-Nb(1)-O(14)	178.57(18)	O(7)-Nb(2)-O(13)	154.68(15)
O(4)-Nb(1)-O(14)	77.37(15)	O(6)-Nb(2)-O(14)	164.87(18)
O(3)-Nb(1)-O(14)	75.62(16)	O(2)-Nb(2)-O(14)	86.47(18)
O(5)-Nb(1)-O(14)	76.25(15)	O(7)-Nb(2)-O(14)	80.41(16)
O(2)-Nb(1)-O(14)	73.60(16)	O(13)-Nb(2)-O(14)	80.24(16)
O(1)-Nb(1)-Nb(2)	136.15(15)	O(6)-Nb(2)-O(23)	86.32(18)
O(4)-Nb(1)-Nb(2)	119.92(12)	O(2)-Nb(2)-O(23)	165.03(18)
O(3)-Nb(1)-Nb(2)	78.55(13)	O(7)-Nb(2)-O(23)	80.51(16)
O(5)-Nb(1)-Nb(2)	78.57(12)	O(13)-Nb(2)-O(23)	79.77(16)
O(2)-Nb(1)-Nb(2)	31.04(12)	O(14)-Nb(2)-O(23)	78.56(13)
O(14)-Nb(1)-Nb(2)	42.56(10)	O(6)-Nb(2)-Nb(1)	144.22(15)
O(1)-Nb(1)-Nb(3)	133.80(15)	O(2)-Nb(2)-Nb(1)	35.58(14)
O(4)-Nb(1)-Nb(3)	78.80(12)	O(7)-Nb(2)-Nb(1)	90.02(13)
O(3)-Nb(1)-Nb(3)	30.32(13)	O(13)-Nb(2)-Nb(1)	90.34(13)

O(14)-Nb(2)-Nb(1)	50.89(11)	Nb(1)-Nb(2)-Nb(5)	61.361(19)
O(23)-Nb(2)-Nb(1)	129.46(11)	Nb(7)-Nb(2)-Nb(5)	118.06(2)
O(6)-Nb(2)-Nb(7)	36.24(14)	Nb(3)-Nb(2)-Nb(5)	91.40(2)
O(2)-Nb(2)-Nb(7)	144.88(14)	O(8)-Nb(3)-O(9)	103.87(19)
O(7)-Nb(2)-Nb(7)	90.26(13)	O(8)-Nb(3)-O(3)	102.72(19)
O(13)-Nb(2)-Nb(7)	89.18(13)	O(9)-Nb(3)-O(3)	94.83(18)
O(14)-Nb(2)-Nb(7)	128.64(11)	O(8)-Nb(3)-O(7)	101.81(17)
O(23)-Nb(2)-Nb(7)	50.08(11)	O(9)-Nb(3)-O(7)	152.17(16)
Nb(1)-Nb(2)-Nb(7)	179.40(2)	O(3)-Nb(3)-O(7)	89.80(17)
O(6)-Nb(2)-Nb(3)	134.07(14)	O(8)-Nb(3)-O(20)	102.86(17)
O(2)-Nb(2)-Nb(3)	84.70(14)	O(9)-Nb(3)-O(20)	90.08(16)
O(7)-Nb(2)-Nb(3)	36.36(12)	O(3)-Nb(3)-O(20)	151.93(16)
O(13)-Nb(2)-Nb(3)	125.74(12)	O(7)-Nb(3)-O(20)	73.82(15)
O(14)-Nb(2)-Nb(3)	45.63(10)	O(8)-Nb(3)-O(14)	175.03(17)
O(23)-Nb(2)-Nb(3)	85.15(11)	O(9)-Nb(3)-O(14)	80.24(16)
Nb(1)-Nb(2)-Nb(3)	61.110(18)	O(3)-Nb(3)-O(14)	79.51(16)
Nb(7)-Nb(2)-Nb(3)	118.93(2)	O(7)-Nb(3)-O(14)	73.65(14)
O(6)-Nb(2)-Nb(5)	132.61(13)	O(20)-Nb(3)-O(14)	74.13(14)
O(2)-Nb(2)-Nb(5)	84.18(14)	O(8)-Nb(3)-Nb(8)	90.64(14)
O(7)-Nb(2)-Nb(5)	126.41(12)	O(9)-Nb(3)-Nb(8)	129.36(13)
O(13)-Nb(2)-Nb(5)	35.89(12)	O(3)-Nb(3)-Nb(8)	129.30(13)
O(14)-Nb(2)-Nb(5)	46.11(10)	O(7)-Nb(3)-Nb(8)	39.50(11)
O(23)-Nb(2)-Nb(5)	85.10(11)	O(20)-Nb(3)-Nb(8)	39.29(10)

O(14)-Nb(3)-Nb(8)	84.55(9)	Nb(4)-Nb(3)-Nb(2)	88.47(2)
O(8)-Nb(3)-Nb(4)	136.31(14)	Nb(1)-Nb(3)-Nb(2)	57.72(2)
O(9)-Nb(3)-Nb(4)	32.66(12)	O(10)-Nb(4)-O(4)	103.1(2)
O(3)-Nb(3)-Nb(4)	83.48(13)	O(10)-Nb(4)-O(11)	102.39(19)
O(7)-Nb(3)-Nb(4)	121.60(10)	O(4)-Nb(4)-O(11)	88.78(18)
O(20)-Nb(3)-Nb(4)	85.97(10)	O(10)-Nb(4)-O(9)	105.32(18)
O(14)-Nb(3)-Nb(4)	48.04(10)	O(4)-Nb(4)-O(9)	89.34(17)
Nb(8)-Nb(3)-Nb(4)	118.94(2)	O(11)-Nb(4)-O(9)	151.92(17)
O(8)-Nb(3)-Nb(1)	134.04(14)	O(10)-Nb(4)-O(21)	105.1(2)
O(9)-Nb(3)-Nb(1)	84.64(13)	O(4)-Nb(4)-O(21)	151.74(17)
O(3)-Nb(3)-Nb(1)	31.38(12)	O(11)-Nb(4)-O(21)	84.79(17)
O(7)-Nb(3)-Nb(1)	85.21(11)	O(9)-Nb(4)-O(21)	83.72(17)
O(20)-Nb(3)-Nb(1)	122.46(10)	O(10)-Nb(4)-O(14)	178.03(17)
O(14)-Nb(3)-Nb(1)	48.48(10)	O(4)-Nb(4)-O(14)	77.72(15)
Nb(8)-Nb(3)-Nb(1)	118.83(2)	O(11)-Nb(4)-O(14)	75.81(15)
Nb(4)-Nb(3)-Nb(1)	60.734(18)	O(9)-Nb(4)-O(14)	76.42(15)
O(8)-Nb(3)-Nb(2)	135.18(14)	O(21)-Nb(4)-O(14)	74.02(15)
O(9)-Nb(3)-Nb(2)	120.94(12)	O(10)-Nb(4)-Nb(9)	136.21(16)
O(3)-Nb(3)-Nb(2)	76.16(13)	O(4)-Nb(4)-Nb(9)	120.62(12)
O(7)-Nb(3)-Nb(2)	34.33(10)	O(11)-Nb(4)-Nb(9)	78.27(12)
O(20)-Nb(3)-Nb(2)	77.63(10)	O(9)-Nb(4)-Nb(9)	78.67(12)
O(14)-Nb(3)-Nb(2)	40.73(10)	O(21)-Nb(4)-Nb(9)	31.12(12)
Nb(8)-Nb(3)-Nb(2)	61.116(18)	O(14)-Nb(4)-Nb(9)	42.90(10)

O(10)-Nb(4)-Nb(3)	135.99(14)	O(5)-Nb(5)-O(22)	151.87(15)
O(4)-Nb(4)-Nb(3)	78.88(12)	O(13)-Nb(5)-O(22)	73.85(15)
O(11)-Nb(4)-Nb(3)	121.61(12)	O(12)-Nb(5)-O(14)	176.65(17)
O(9)-Nb(4)-Nb(3)	31.01(12)	O(11)-Nb(5)-O(14)	78.90(16)
O(21)-Nb(4)-Nb(3)	81.20(11)	O(5)-Nb(5)-O(14)	79.90(16)
O(14)-Nb(4)-Nb(3)	45.83(9)	O(13)-Nb(5)-O(14)	73.78(14)
Nb(9)-Nb(4)-Nb(3)	61.469(17)	O(22)-Nb(5)-O(14)	73.45(14)
O(10)-Nb(4)-Nb(5)	131.96(14)	O(12)-Nb(5)-Nb(6)	92.50(14)
O(4)-Nb(4)-Nb(5)	78.77(12)	O(11)-Nb(5)-Nb(6)	128.02(13)
O(11)-Nb(4)-Nb(5)	29.89(12)	O(5)-Nb(5)-Nb(6)	130.00(13)
O(9)-Nb(4)-Nb(5)	122.73(12)	O(13)-Nb(5)-Nb(6)	39.64(11)
O(21)-Nb(4)-Nb(5)	82.08(11)	O(22)-Nb(5)-Nb(6)	39.16(11)
O(14)-Nb(4)-Nb(5)	46.32(9)	O(14)-Nb(5)-Nb(6)	84.18(9)
Nb(9)-Nb(4)-Nb(5)	61.699(18)	O(12)-Nb(5)-Nb(4)	134.14(14)
Nb(3)-Nb(4)-Nb(5)	91.90(2)	O(11)-Nb(5)-Nb(4)	31.42(13)
O(12)-Nb(5)-O(11)	102.91(19)	O(5)-Nb(5)-Nb(4)	84.01(12)
O(12)-Nb(5)-O(5)	102.67(19)	O(13)-Nb(5)-Nb(4)	121.55(11)
O(11)-Nb(5)-O(5)	94.79(19)	O(22)-Nb(5)-Nb(4)	84.77(11)
O(12)-Nb(5)-O(13)	103.91(18)	O(14)-Nb(5)-Nb(4)	47.91(10)
O(11)-Nb(5)-O(13)	150.83(17)	Nb(6)-Nb(5)-Nb(4)	117.90(2)
O(5)-Nb(5)-O(13)	90.37(17)	O(12)-Nb(5)-Nb(2)	137.60(14)
O(12)-Nb(5)-O(22)	103.66(17)	O(11)-Nb(5)-Nb(2)	119.48(13)
O(11)-Nb(5)-O(22)	88.86(17)	O(5)-Nb(5)-Nb(2)	76.24(12)

O(13)-Nb(5)-Nb(2)	34.74(11)	O(22)-Nb(6)-Nb(5)	39.64(11)
O(22)-Nb(5)-Nb(2)	77.71(10)	O(13)-Nb(6)-Nb(5)	38.74(11)
O(14)-Nb(5)-Nb(2)	40.62(10)	O(23)-Nb(6)-Nb(5)	84.57(10)
Nb(6)-Nb(5)-Nb(2)	61.490(19)	O(15)-Nb(6)-Nb(7)	135.06(15)
Nb(4)-Nb(5)-Nb(2)	88.23(2)	O(16)-Nb(6)-Nb(7)	31.82(13)
O(15)-Nb(6)-O(16)	103.5(2)	O(24)-Nb(6)-Nb(7)	84.33(13)
O(15)-Nb(6)-O(24)	102.8(2)	O(22)-Nb(6)-Nb(7)	122.14(10)
O(16)-Nb(6)-O(24)	95.74(19)	O(13)-Nb(6)-Nb(7)	85.34(11)
O(15)-Nb(6)-O(22)	102.39(17)	O(23)-Nb(6)-Nb(7)	48.30(10)
O(16)-Nb(6)-O(22)	151.55(16)	Nb(5)-Nb(6)-Nb(7)	118.30(2)
O(24)-Nb(6)-O(22)	89.95(17)	O(15)-Nb(6)-Nb(9)	136.05(15)
O(15)-Nb(6)-O(13)	103.22(18)	O(16)-Nb(6)-Nb(9)	120.47(13)
O(16)-Nb(6)-O(13)	89.16(18)	O(24)-Nb(6)-Nb(9)	75.83(13)
O(24)-Nb(6)-O(13)	151.60(17)	O(22)-Nb(6)-Nb(9)	34.72(10)
O(22)-Nb(6)-O(13)	73.47(15)	O(13)-Nb(6)-Nb(9)	77.58(11)
O(15)-Nb(6)-O(23)	175.84(17)	O(23)-Nb(6)-Nb(9)	40.82(10)
O(16)-Nb(6)-O(23)	79.66(16)	Nb(5)-Nb(6)-Nb(9)	61.534(18)
O(24)-Nb(6)-O(23)	79.48(16)	Nb(7)-Nb(6)-Nb(9)	88.87(2)
O(22)-Nb(6)-O(23)	74.01(14)	O(15)-Nb(6)-Nb(10)	134.28(15)
O(13)-Nb(6)-O(23)	73.91(15)	O(16)-Nb(6)-Nb(10)	84.58(14)
O(15)-Nb(6)-Nb(5)	91.32(15)	O(24)-Nb(6)-Nb(10)	31.65(12)
O(16)-Nb(6)-Nb(5)	127.90(14)	O(22)-Nb(6)-Nb(10)	85.87(11)
O(24)-Nb(6)-Nb(5)	129.59(13)	O(13)-Nb(6)-Nb(10)	122.04(11)

O(23)-Nb(6)-Nb(10)	48.25(10)	O(6)-Nb(7)-Nb(2)	31.01(12)
Nb(5)-Nb(6)-Nb(10)	119.22(2)	O(23)-Nb(7)-Nb(2)	43.23(10)
Nb(7)-Nb(6)-Nb(10)	61.089(19)	O(17)-Nb(7)-Nb(6)	133.36(16)
Nb(9)-Nb(6)-Nb(10)	57.69(2)	O(25)-Nb(7)-Nb(6)	78.60(12)
O(17)-Nb(7)-O(25)	104.7(2)	O(16)-Nb(7)-Nb(6)	30.54(13)
O(17)-Nb(7)-O(16)	103.0(2)	O(18)-Nb(7)-Nb(6)	121.92(12)
O(25)-Nb(7)-O(16)	88.98(19)	O(6)-Nb(7)-Nb(6)	82.23(12)
O(17)-Nb(7)-O(18)	104.7(2)	O(23)-Nb(7)-Nb(6)	46.05(9)
O(25)-Nb(7)-O(18)	88.55(18)	Nb(2)-Nb(7)-Nb(6)	62.147(18)
O(16)-Nb(7)-O(18)	151.84(18)	O(17)-Nb(7)-Nb(8)	134.62(16)
O(17)-Nb(7)-O(6)	103.5(2)	O(25)-Nb(7)-Nb(8)	78.75(13)
O(25)-Nb(7)-O(6)	151.83(18)	O(16)-Nb(7)-Nb(8)	122.32(13)
O(16)-Nb(7)-O(6)	84.80(18)	O(18)-Nb(7)-Nb(8)	30.09(12)
O(18)-Nb(7)-O(6)	84.25(17)	O(6)-Nb(7)-Nb(8)	81.49(12)
O(17)-Nb(7)-O(23)	177.6(2)	O(23)-Nb(7)-Nb(8)	46.19(9)
O(25)-Nb(7)-O(23)	77.59(16)	Nb(2)-Nb(7)-Nb(8)	61.545(18)
O(16)-Nb(7)-O(23)	76.15(16)	Nb(6)-Nb(7)-Nb(8)	91.96(2)
O(18)-Nb(7)-O(23)	75.92(16)	O(19)-Nb(8)-O(18)	103.18(19)
O(6)-Nb(7)-O(23)	74.24(16)	O(19)-Nb(8)-O(26)	103.02(19)
O(17)-Nb(7)-Nb(2)	134.47(18)	O(18)-Nb(8)-O(26)	94.70(19)
O(25)-Nb(7)-Nb(2)	120.82(12)	O(19)-Nb(8)-O(20)	103.80(18)
O(16)-Nb(7)-Nb(2)	78.94(12)	O(18)-Nb(8)-O(20)	150.99(16)
O(18)-Nb(7)-Nb(2)	78.33(12)	O(26)-Nb(8)-O(20)	89.47(16)

O(19)-Nb(8)-O(7)	103.26(17)	O(18)-Nb(8)-Nb(10)	83.93(13)
O(18)-Nb(8)-O(7)	90.10(17)	O(26)-Nb(8)-Nb(10)	31.51(12)
O(26)-Nb(8)-O(7)	151.41(16)	O(20)-Nb(8)-Nb(10)	84.83(10)
O(20)-Nb(8)-O(7)	73.50(15)	O(7)-Nb(8)-Nb(10)	121.94(10)
O(19)-Nb(8)-O(23)	176.30(17)	O(23)-Nb(8)-Nb(10)	48.27(10)
O(18)-Nb(8)-O(23)	79.26(16)	Nb(3)-Nb(8)-Nb(10)	118.19(2)
O(26)-Nb(8)-O(23)	79.41(16)	Nb(7)-Nb(8)-Nb(10)	60.968(18)
O(20)-Nb(8)-O(23)	73.31(14)	O(21)-Nb(9)-O(27)	107.77(17)
O(7)-Nb(8)-O(23)	73.83(14)	O(21)-Nb(9)-O(22)	97.14(18)
O(19)-Nb(8)-Nb(3)	92.21(14)	O(27)-Nb(9)-O(22)	98.28(17)
O(18)-Nb(8)-Nb(3)	129.22(13)	O(21)-Nb(9)-O(20)	96.99(17)
O(26)-Nb(8)-Nb(3)	128.77(13)	O(27)-Nb(9)-O(20)	96.49(17)
O(20)-Nb(8)-Nb(3)	39.31(10)	O(22)-Nb(9)-O(20)	155.35(15)
O(7)-Nb(8)-Nb(3)	39.12(11)	O(21)-Nb(9)-O(23)	165.29(18)
O(23)-Nb(8)-Nb(3)	84.10(9)	O(27)-Nb(9)-O(23)	86.93(18)
O(19)-Nb(8)-Nb(7)	134.63(15)	O(22)-Nb(9)-O(23)	80.90(16)
O(18)-Nb(8)-Nb(7)	31.61(12)	O(20)-Nb(9)-O(23)	80.31(15)
O(26)-Nb(8)-Nb(7)	83.92(13)	O(21)-Nb(9)-O(14)	86.31(17)
O(20)-Nb(8)-Nb(7)	121.22(10)	O(27)-Nb(9)-O(14)	165.87(17)
O(7)-Nb(8)-Nb(7)	85.61(11)	O(22)-Nb(9)-O(14)	80.64(16)
O(23)-Nb(8)-Nb(7)	48.03(10)	O(20)-Nb(9)-O(14)	80.23(15)
Nb(3)-Nb(8)-Nb(7)	118.39(2)	O(23)-Nb(9)-O(14)	78.98(14)
O(19)-Nb(8)-Nb(10)	134.38(14)	O(21)-Nb(9)-Nb(10)	143.90(13)

O(27)-Nb(9)-Nb(10)	36.14(13)	O(28)-Nb(10)-O(24)	103.49(19)
O(22)-Nb(9)-Nb(10)	90.86(13)	O(25)-Nb(10)-O(24)	88.26(18)
O(20)-Nb(9)-Nb(10)	89.52(11)	O(26)-Nb(10)-O(24)	151.88(18)
O(23)-Nb(9)-Nb(10)	50.79(11)	O(28)-Nb(10)-O(27)	103.7(2)
O(14)-Nb(9)-Nb(10)	129.77(11)	O(25)-Nb(10)-O(27)	151.51(18)
O(21)-Nb(9)-Nb(4)	36.30(13)	O(26)-Nb(10)-O(27)	85.20(17)
O(27)-Nb(9)-Nb(4)	144.07(14)	O(24)-Nb(10)-O(27)	84.20(17)
O(22)-Nb(9)-Nb(4)	89.43(13)	O(28)-Nb(10)-O(23)	177.71(19)
O(20)-Nb(9)-Nb(4)	90.10(11)	O(25)-Nb(10)-O(23)	77.35(16)
O(23)-Nb(9)-Nb(4)	129.00(11)	O(26)-Nb(10)-O(23)	76.38(15)
O(14)-Nb(9)-Nb(4)	50.02(11)	O(24)-Nb(10)-O(23)	75.69(16)
Nb(10)-Nb(9)-Nb(4)	179.60(2)	O(27)-Nb(10)-O(23)	74.17(15)
O(21)-Nb(9)-Nb(6)	133.85(13)	O(28)-Nb(10)-Nb(9)	135.25(17)
O(27)-Nb(9)-Nb(6)	85.05(13)	O(25)-Nb(10)-Nb(9)	119.91(13)
O(22)-Nb(9)-Nb(6)	36.71(12)	O(26)-Nb(10)-Nb(9)	79.38(12)
O(20)-Nb(9)-Nb(6)	126.14(11)	O(24)-Nb(10)-Nb(9)	77.97(12)
O(23)-Nb(9)-Nb(6)	45.92(11)	O(27)-Nb(10)-Nb(9)	31.60(12)
O(14)-Nb(9)-Nb(6)	85.87(10)	O(23)-Nb(10)-Nb(9)	42.57(10)
Nb(10)-Nb(9)-Nb(6)	61.301(19)	O(28)-Nb(10)-Nb(8)	134.75(15)
Nb(4)-Nb(9)-Nb(6)	118.86(2)	O(25)-Nb(10)-Nb(8)	78.70(13)
O(28)-Nb(10)-O(25)	104.8(2)	O(26)-Nb(10)-Nb(8)	30.63(13)
O(28)-Nb(10)-O(26)	104.3(2)	O(24)-Nb(10)-Nb(8)	121.76(13)
O(25)-Nb(10)-O(26)	88.77(18)	O(27)-Nb(10)-Nb(8)	82.06(11)

O(23)-Nb(10)-Nb(8)	46.11(9)	Nb(2)-O(14)-Nb(9)	101.32(16)
Nb(9)-Nb(10)-Nb(8)	61.788(17)	Nb(2)-O(14)-Nb(3)	93.64(15)
O(28)-Nb(10)-Nb(6)	133.66(15)	Nb(9)-O(14)-Nb(3)	93.64(14)
O(25)-Nb(10)-Nb(6)	78.10(13)	Nb(2)-O(14)-Nb(5)	93.27(14)
O(26)-Nb(10)-Nb(6)	122.04(13)	Nb(9)-O(14)-Nb(5)	93.47(15)
O(24)-Nb(10)-Nb(6)	30.39(13)	Nb(3)-O(14)-Nb(5)	168.93(18)
O(27)-Nb(10)-Nb(6)	81.63(11)	Nb(2)-O(14)-Nb(4)	171.6(2)
O(23)-Nb(10)-Nb(6)	45.71(9)	Nb(9)-O(14)-Nb(4)	87.08(15)
Nb(9)-Nb(10)-Nb(6)	61.010(19)	Nb(3)-O(14)-Nb(4)	86.13(13)
Nb(8)-Nb(10)-Nb(6)	91.53(2)	Nb(5)-O(14)-Nb(4)	85.77(13)
Nb(2)-O(2)-Nb(1)	113.4(2)	Nb(2)-O(14)-Nb(1)	86.55(15)
Nb(3)-O(3)-Nb(1)	118.3(2)	Nb(9)-O(14)-Nb(1)	172.1(2)
Nb(1)-O(4)-Nb(4)	119.86(19)	Nb(3)-O(14)-Nb(1)	85.89(13)
Nb(5)-O(5)-Nb(1)	117.2(2)	Nb(5)-O(14)-Nb(1)	85.91(12)
Nb(2)-O(6)-Nb(7)	112.7(2)	Nb(4)-O(14)-Nb(1)	85.05(12)
Nb(2)-O(7)-Nb(3)	109.30(18)	Nb(6)-O(16)-Nb(7)	117.6(2)
Nb(2)-O(7)-Nb(8)	109.42(18)	Nb(8)-O(18)-Nb(7)	118.3(2)
Nb(3)-O(7)-Nb(8)	101.38(16)	Nb(9)-O(20)-Nb(8)	109.33(17)
Nb(3)-O(9)-Nb(4)	116.3(2)	Nb(9)-O(20)-Nb(3)	108.90(18)
Nb(5)-O(11)-Nb(4)	118.7(2)	Nb(8)-O(20)-Nb(3)	101.41(15)
Nb(2)-O(13)-Nb(5)	109.36(19)	Nb(9)-O(21)-Nb(4)	112.6(2)
Nb(2)-O(13)-Nb(6)	109.17(19)	Nb(9)-O(22)-Nb(6)	108.57(18)
Nb(5)-O(13)-Nb(6)	101.62(15)	Nb(9)-O(22)-Nb(5)	109.76(19)

Nb(6)-O(22)-Nb(5)	101.19(16)	N(31)-C(31)-H(31C)	109.5
Nb(9)-O(23)-Nb(2)	101.13(16)	H(31A)-C(31)-H(31C)	109.5
Nb(9)-O(23)-Nb(6)	93.26(15)	H(31B)-C(31)-H(31C)	109.5
Nb(2)-O(23)-Nb(6)	94.21(15)	C(32)-N(31)-C(33)	110.7(6)
Nb(9)-O(23)-Nb(8)	94.17(15)	C(32)-N(31)-C(34)	110.1(6)
Nb(2)-O(23)-Nb(8)	92.98(15)	C(33)-N(31)-C(34)	109.8(6)
Nb(6)-O(23)-Nb(8)	168.48(19)	C(32)-N(31)-C(31)	109.0(6)
Nb(9)-O(23)-Nb(7)	172.2(2)	C(33)-N(31)-C(31)	108.3(6)
Nb(2)-O(23)-Nb(7)	86.69(15)	C(34)-N(31)-C(31)	109.0(6)
Nb(6)-O(23)-Nb(7)	85.66(13)	N(31)-C(32)-H(32A)	109.5
Nb(8)-O(23)-Nb(7)	85.79(13)	N(31)-C(32)-H(32B)	109.5
Nb(9)-O(23)-Nb(10)	86.64(15)	H(32A)-C(32)-H(32B)	109.5
Nb(2)-O(23)-Nb(10)	172.2(2)	N(31)-C(32)-H(32C)	109.5
Nb(6)-O(23)-Nb(10)	86.04(13)	H(32A)-C(32)-H(32C)	109.5
Nb(8)-O(23)-Nb(10)	85.62(13)	H(32B)-C(32)-H(32C)	109.5
Nb(7)-O(23)-Nb(10)	85.55(12)	N(31)-C(33)-H(33A)	109.5
Nb(6)-O(24)-Nb(10)	118.0(2)	N(31)-C(33)-H(33B)	109.5
Nb(10)-O(25)-Nb(7)	119.5(2)	H(33A)-C(33)-H(33B)	109.5
Nb(8)-O(26)-Nb(10)	117.9(2)	N(31)-C(33)-H(33C)	109.5
Nb(9)-O(27)-Nb(10)	112.3(2)	H(33A)-C(33)-H(33C)	109.5
N(31)-C(31)-H(31A)	109.5	H(33B)-C(33)-H(33C)	109.5
N(31)-C(31)-H(31B)	109.5	N(31)-C(34)-H(34A)	109.5
H(31A)-C(31)-H(31B)	109.5	N(31)-C(34)-H(34B)	109.5

H(34A)-C(34)-H(34B)	109.5	N(35)-C(37)-H(37B)	109.5
N(31)-C(34)-H(34C)	109.5	H(37A)-C(37)-H(37B)	109.5
H(34A)-C(34)-H(34C)	109.5	N(35)-C(37)-H(37C)	109.5
H(34B)-C(34)-H(34C)	109.5	H(37A)-C(37)-H(37C)	109.5
N(35)-C(35)-H(35A)	109.5	H(37B)-C(37)-H(37C)	109.5
N(35)-C(35)-H(35B)	109.5	N(35)-C(38)-H(38A)	109.5
H(35A)-C(35)-H(35B)	109.5	N(35)-C(38)-H(38B)	109.5
N(35)-C(35)-H(35C)	109.5	H(38A)-C(38)-H(38B)	109.5
H(35A)-C(35)-H(35C)	109.5	N(35)-C(38)-H(38C)	109.5
H(35B)-C(35)-H(35C)	109.5	H(38A)-C(38)-H(38C)	109.5
C(35)-N(35)-C(36)	110.3(6)	H(38B)-C(38)-H(38C)	109.5
C(35)-N(35)-C(38)	108.9(5)	N(39)-C(39)-H(39A)	109.5
C(36)-N(35)-C(38)	110.4(6)	N(39)-C(39)-H(39B)	109.5
C(35)-N(35)-C(37)	107.9(6)	H(39A)-C(39)-H(39B)	109.5
C(36)-N(35)-C(37)	108.6(5)	N(39)-C(39)-H(39C)	109.5
C(38)-N(35)-C(37)	110.8(5)	H(39A)-C(39)-H(39C)	109.5
N(35)-C(36)-H(36A)	109.5	H(39B)-C(39)-H(39C)	109.5
N(35)-C(36)-H(36B)	109.5	C(42)-N(39)-C(39)	110.7(6)
H(36A)-C(36)-H(36B)	109.5	C(42)-N(39)-C(40)	108.6(8)
N(35)-C(36)-H(36C)	109.5	C(39)-N(39)-C(40)	110.4(8)
H(36A)-C(36)-H(36C)	109.5	C(42)-N(39)-C(41)	106.8(7)
H(36B)-C(36)-H(36C)	109.5	C(39)-N(39)-C(41)	108.1(7)
N(35)-C(37)-H(37A)	109.5	C(40)-N(39)-C(41)	112.2(11)

N(39)-C(40)-H(40A)	109.5	H(43B)-C(43)-H(43C)	109.5
N(39)-C(40)-H(40B)	109.5	C(43)-N(43)-C(46)	112.9(7)
H(40A)-C(40)-H(40B)	109.5	C(43)-N(43)-C(44)	110.6(7)
N(39)-C(40)-H(40C)	109.5	C(46)-N(43)-C(44)	109.5(6)
H(40A)-C(40)-H(40C)	109.5	C(43)-N(43)-C(45)	107.8(7)
H(40B)-C(40)-H(40C)	109.5	C(46)-N(43)-C(45)	108.0(7)
N(39)-C(41)-H(41A)	109.5	C(44)-N(43)-C(45)	107.8(6)
N(39)-C(41)-H(41B)	109.5	N(43)-C(44)-H(44A)	109.5
H(41A)-C(41)-H(41B)	109.5	N(43)-C(44)-H(44B)	109.5
N(39)-C(41)-H(41C)	109.5	H(44A)-C(44)-H(44B)	109.5
H(41A)-C(41)-H(41C)	109.5	N(43)-C(44)-H(44C)	109.5
H(41B)-C(41)-H(41C)	109.5	H(44A)-C(44)-H(44C)	109.5
N(39)-C(42)-H(42A)	109.5	H(44B)-C(44)-H(44C)	109.5
N(39)-C(42)-H(42B)	109.5	N(43)-C(45)-H(45A)	109.5
H(42A)-C(42)-H(42B)	109.5	N(43)-C(45)-H(45B)	109.5
N(39)-C(42)-H(42C)	109.5	H(45A)-C(45)-H(45B)	109.5
H(42A)-C(42)-H(42C)	109.5	N(43)-C(45)-H(45C)	109.5
H(42B)-C(42)-H(42C)	109.5	H(45A)-C(45)-H(45C)	109.5
N(43)-C(43)-H(43A)	109.5	H(45B)-C(45)-H(45C)	109.5
N(43)-C(43)-H(43B)	109.5	N(43)-C(46)-H(46A)	109.5
H(43A)-C(43)-H(43B)	109.5	N(43)-C(46)-H(46B)	109.5
N(43)-C(43)-H(43C)	109.5	H(46A)-C(46)-H(46B)	109.5
H(43A)-C(43)-H(43C)	109.5	N(43)-C(46)-H(46C)	109.5

H(46A)-C(46)-H(46C)	109.5	N(47)-C(49)-H(49C)	109.5
H(46B)-C(46)-H(46C)	109.5	H(49A)-C(49)-H(49C)	109.5
N(47)-C(47)-H(47A)	109.5	H(49B)-C(49)-H(49C)	109.5
N(47)-C(47)-H(47B)	109.5	N(47)-C(50)-H(50A)	109.5
H(47A)-C(47)-H(47B)	109.5	N(47)-C(50)-H(50B)	109.5
N(47)-C(47)-H(47C)	109.5	H(50A)-C(50)-H(50B)	109.5
H(47A)-C(47)-H(47C)	109.5	N(47)-C(50)-H(50C)	109.5
H(47B)-C(47)-H(47C)	109.5	H(50A)-C(50)-H(50C)	109.5
C(50)-N(47)-C(48)	108.2(8)	H(50B)-C(50)-H(50C)	109.5
C(50)-N(47)-C(47)	108.8(7)	N(51)-C(51)-H(51A)	109.5
C(48)-N(47)-C(47)	111.1(6)	N(51)-C(51)-H(51B)	109.5
C(50)-N(47)-C(49)	113.9(9)	H(51A)-C(51)-H(51B)	109.5
C(48)-N(47)-C(49)	105.6(7)	N(51)-C(51)-H(51C)	109.5
C(47)-N(47)-C(49)	109.3(7)	H(51A)-C(51)-H(51C)	109.5
N(47)-C(48)-H(48A)	109.5	H(51B)-C(51)-H(51C)	109.5
N(47)-C(48)-H(48B)	109.5	C(52)-N(51)-C(53)	110.6(6)
H(48A)-C(48)-H(48B)	109.5	C(52)-N(51)-C(51)	109.2(6)
N(47)-C(48)-H(48C)	109.5	C(53)-N(51)-C(51)	107.6(5)
H(48A)-C(48)-H(48C)	109.5	C(52)-N(51)-C(54)	110.1(6)
H(48B)-C(48)-H(48C)	109.5	C(53)-N(51)-C(54)	109.8(5)
N(47)-C(49)-H(49A)	109.5	C(51)-N(51)-C(54)	109.4(5)
N(47)-C(49)-H(49B)	109.5	N(51)-C(52)-H(52A)	109.5
H(49A)-C(49)-H(49B)	109.5	N(51)-C(52)-H(52B)	109.5

H(52A)-C(52)-H(52B)	109.5	C(56)-N(55)-C(58)	108.5(7)
N(51)-C(52)-H(52C)	109.5	C(55)-N(55)-C(58)	109.1(6)
H(52A)-C(52)-H(52C)	109.5	C(56)-N(55)-C(57)	110.7(6)
H(52B)-C(52)-H(52C)	109.5	C(55)-N(55)-C(57)	109.4(6)
N(51)-C(53)-H(53A)	109.5	C(58)-N(55)-C(57)	108.0(5)
N(51)-C(53)-H(53B)	109.5	N(55)-C(56)-H(56A)	109.5
H(53A)-C(53)-H(53B)	109.5	N(55)-C(56)-H(56B)	109.5
N(51)-C(53)-H(53C)	109.5	H(56A)-C(56)-H(56B)	109.5
H(53A)-C(53)-H(53C)	109.5	N(55)-C(56)-H(56C)	109.5
H(53B)-C(53)-H(53C)	109.5	H(56A)-C(56)-H(56C)	109.5
N(51)-C(54)-H(54A)	109.5	H(56B)-C(56)-H(56C)	109.5
N(51)-C(54)-H(54B)	109.5	N(55)-C(57)-H(57A)	109.5
H(54A)-C(54)-H(54B)	109.5	N(55)-C(57)-H(57B)	109.5
N(51)-C(54)-H(54C)	109.5	H(57A)-C(57)-H(57B)	109.5
H(54A)-C(54)-H(54C)	109.5	N(55)-C(57)-H(57C)	109.5
H(54B)-C(54)-H(54C)	109.5	H(57A)-C(57)-H(57C)	109.5
N(55)-C(55)-H(55A)	109.5	H(57B)-C(57)-H(57C)	109.5
N(55)-C(55)-H(55B)	109.5	N(55)-C(58)-H(58A)	109.5
H(55A)-C(55)-H(55B)	109.5	N(55)-C(58)-H(58B)	109.5
N(55)-C(55)-H(55C)	109.5	H(58A)-C(58)-H(58B)	109.5
H(55A)-C(55)-H(55C)	109.5	N(55)-C(58)-H(58C)	109.5
H(55B)-C(55)-H(55C)	109.5	H(58A)-C(58)-H(58C)	109.5
C(56)-N(55)-C(55)	111.0(6)	H(58B)-C(58)-H(58C)	109.5

H(61A)-O(61)-H(61B)	104.2	H(72A)-O(72)-H(72B)	107(10)
H(64A)-O(64)-H(64B)	106(12)	H(73A)-O(73)-H(73B)	106(7)
H(65A)-O(65)-H(65B)	106(7)	H(74A)-O(74)-H(74B)	107(8)
H(66A)-O(66)-H(66B)	121.3	H(75A)-O(75)-H(75B)	112(9)
H(67A)-O(67)-H(67B)	97.9	H(77A)-O(77)-H(77B)	108(7)
H(68A)-O(68)-H(68B)	106.9	H(78A)-O(78)-H(78B)	111(6)
H(69A)-O(69)-H(69B)	105.6	H(79A)-O(79)-H(79B)	107.0
H(70A)-O(70)-H(70B)	121.1	H(81A)-O(81)-H(81B)	106(7)
H(71A)-O(71)-H(71B)	106(6)	H(82A)-O(82)-H(82B)	108(7)

Symmetry transformations used to generate equivalent atoms:

Table S.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for jf1660ffmi. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Nb(1)	15(1)	12(1)	10(1)	0(1)	3(1)	3(1)
Nb(2)	11(1)	10(1)	9(1)	0(1)	2(1)	-1(1)
Ti(2)	11(1)	10(1)	9(1)	0(1)	2(1)	-1(1)
Nb(3)	13(1)	10(1)	9(1)	-1(1)	2(1)	0(1)
Nb(4)	13(1)	13(1)	11(1)	1(1)	1(1)	-2(1)
Nb(5)	12(1)	11(1)	9(1)	1(1)	1(1)	1(1)
Nb(6)	17(1)	11(1)	9(1)	-1(1)	1(1)	-1(1)
Nb(7)	20(1)	13(1)	13(1)	1(1)	3(1)	-4(1)
Nb(8)	15(1)	10(1)	10(1)	1(1)	2(1)	0(1)
Nb(9)	11(1)	10(1)	8(1)	0(1)	1(1)	1(1)
Ti(9)	11(1)	10(1)	8(1)	0(1)	1(1)	1(1)
Nb(10)	20(1)	11(1)	11(1)	-1(1)	3(1)	2(1)
O(1)	21(2)	20(2)	16(2)	-1(2)	8(2)	5(2)
O(2)	16(2)	18(2)	14(2)	0(2)	3(2)	1(2)
O(3)	19(2)	17(2)	11(2)	0(2)	2(2)	-2(2)
O(4)	22(2)	8(2)	12(2)	1(1)	4(2)	1(2)
O(5)	14(2)	15(2)	12(2)	1(2)	-1(2)	0(2)
O(6)	19(2)	16(2)	14(2)	-3(2)	4(2)	-2(2)

O(7)	17(2)	11(2)	10(2)	-2(2)	2(2)	-1(2)
O(8)	17(2)	17(2)	12(2)	-2(2)	2(2)	-1(2)
O(9)	14(2)	14(2)	14(2)	-2(2)	3(2)	-3(2)
O(10)	13(2)	22(2)	15(2)	5(2)	1(2)	-6(2)
O(11)	20(2)	10(2)	15(2)	3(2)	6(2)	-2(2)
O(12)	18(2)	16(2)	14(2)	4(2)	2(2)	0(2)
O(13)	15(2)	12(2)	14(2)	0(2)	3(2)	0(2)
O(14)	11(2)	11(2)	9(2)	0(1)	-1(1)	0(2)
O(15)	23(2)	16(2)	11(2)	2(2)	3(2)	-1(2)
O(16)	23(2)	14(2)	14(2)	0(2)	3(2)	-6(2)
O(17)	31(3)	20(2)	24(2)	4(2)	5(2)	-8(2)
O(18)	17(2)	15(2)	13(2)	1(2)	5(2)	-1(2)
O(19)	19(2)	16(2)	13(2)	1(2)	0(2)	1(2)
O(20)	12(2)	12(2)	8(2)	-1(1)	0(1)	0(2)
O(21)	12(2)	14(2)	13(2)	3(2)	1(2)	2(2)
O(22)	15(2)	14(2)	9(2)	4(2)	3(1)	3(2)
O(23)	18(2)	12(2)	12(2)	0(2)	3(2)	-1(2)
O(24)	21(2)	15(2)	10(2)	1(2)	5(2)	0(2)
O(25)	25(2)	12(2)	15(2)	2(2)	1(2)	-3(2)
O(26)	19(2)	12(2)	16(2)	0(2)	3(2)	0(2)
O(27)	16(2)	12(2)	13(2)	0(2)	3(2)	1(2)
O(28)	28(3)	17(2)	18(2)	0(2)	3(2)	7(2)
C(31)	33(4)	29(4)	27(3)	-3(3)	9(3)	3(3)

N(31)	41(4)	19(3)	17(3)	-4(2)	11(2)	-5(2)
C(32)	41(4)	23(3)	17(3)	-1(3)	4(3)	-8(3)
C(33)	66(6)	22(4)	30(4)	-13(3)	22(4)	-25(4)
C(34)	44(4)	24(3)	26(3)	-3(3)	16(3)	-7(3)
C(35)	24(4)	38(4)	27(4)	8(3)	3(3)	8(3)
N(35)	18(3)	19(3)	16(2)	4(2)	2(2)	-2(2)
C(36)	30(4)	24(3)	21(3)	6(3)	1(3)	7(3)
C(37)	55(5)	23(3)	28(4)	-6(3)	21(4)	-8(3)
C(38)	22(3)	33(4)	23(3)	1(3)	13(3)	-11(3)
C(39)	18(3)	53(5)	34(4)	0(4)	3(3)	-1(3)
N(39)	21(3)	62(5)	33(3)	8(3)	10(3)	7(3)
C(40)	33(6)	136(14)	230(20)	131(14)	53(9)	33(7)
C(41)	23(4)	158(13)	47(5)	-33(7)	16(4)	-17(6)
C(42)	16(3)	46(4)	34(4)	4(4)	8(3)	4(3)
C(43)	39(5)	59(6)	42(5)	22(4)	-6(4)	-19(4)
N(43)	32(3)	33(3)	28(3)	14(3)	19(3)	13(3)
C(44)	58(5)	24(4)	37(4)	14(3)	28(4)	17(4)
C(45)	64(6)	35(5)	42(5)	11(4)	13(5)	-2(4)
C(46)	58(6)	61(6)	57(6)	32(5)	45(5)	26(5)
C(47)	20(3)	39(4)	50(5)	-3(4)	11(3)	3(3)
N(47)	23(3)	30(3)	51(4)	-3(3)	17(3)	-8(3)
C(48)	19(3)	45(5)	42(4)	9(3)	12(3)	0(3)
C(49)	33(5)	39(5)	132(11)	-27(6)	23(6)	-22(4)

C(50)	166(15)	50(6)	54(6)	23(5)	68(8)	35(8)
C(51)	33(4)	46(4)	21(3)	-8(3)	16(3)	-12(3)
N(51)	15(2)	23(3)	19(2)	-1(2)	3(2)	1(2)
C(52)	64(6)	35(4)	25(4)	7(3)	3(4)	17(4)
C(53)	17(3)	34(4)	29(3)	-12(3)	10(3)	-3(3)
C(54)	33(4)	24(3)	28(3)	-12(3)	10(3)	-13(3)
C(55)	11(3)	47(5)	40(4)	8(3)	-4(3)	3(3)
N(55)	11(3)	26(3)	36(3)	3(2)	0(2)	-2(2)
C(56)	34(5)	45(5)	79(7)	-13(5)	12(5)	-8(4)
C(57)	26(4)	44(4)	32(4)	10(3)	10(3)	-3(3)
C(58)	21(3)	45(4)	23(3)	12(3)	2(3)	2(3)
O(61)	93(8)	60(6)	226(14)	-3(7)	105(9)	2(5)
O(62)	44(4)	85(6)	82(6)	-7(4)	30(4)	6(4)
O(63)	54(6)	102(8)	266(17)	54(10)	59(9)	-10(6)
O(64)	36(4)	88(6)	108(7)	-9(6)	38(4)	-22(4)
O(65)	23(3)	47(3)	37(3)	5(3)	12(2)	3(2)
O(66)	26(3)	36(3)	51(4)	2(3)	-2(3)	-2(2)
O(67)	12(2)	42(3)	25(2)	-2(2)	-2(2)	-6(2)
O(68)	62(6)	127(9)	86(7)	8(6)	11(5)	-22(6)
O(69)	19(2)	58(4)	28(3)	6(2)	5(2)	3(2)
O(70)	35(3)	40(3)	47(3)	24(3)	-23(3)	-17(3)
O(71)	16(2)	23(2)	28(2)	-10(2)	-5(2)	3(2)
O(72)	106(6)	29(3)	42(4)	1(3)	45(4)	2(3)

O(73)	44(3)	42(3)	33(3)	-9(2)	15(2)	-13(3)
O(74)	23(3)	51(4)	33(3)	12(3)	2(2)	-1(3)
O(75)	41(3)	42(3)	38(3)	-3(3)	5(3)	-7(3)
O(76)	33(3)	46(3)	41(3)	3(3)	-5(2)	-3(3)
O(77)	25(3)	38(3)	27(3)	-1(2)	5(2)	-3(2)
O(78)	14(2)	21(2)	28(2)	5(2)	-4(2)	-9(2)
O(79)	31(3)	38(3)	50(4)	13(3)	-4(3)	2(3)
O(80)	37(3)	30(3)	29(2)	2(2)	-6(2)	-4(2)
O(81)	25(3)	22(2)	29(2)	-6(2)	1(2)	0(2)
O(82)	26(2)	22(2)	16(2)	0(2)	3(2)	2(2)

Table S.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for jf1660ffmi.

	x	y	z	U(eq)
H(31A)	10131	9362	6558	44
H(31B)	10236	8966	5688	44
H(31C)	10113	8557	6541	44
H(32A)	7722	9632	5076	42
H(32B)	8785	9642	4816	42
H(32C)	8694	9997	5718	42
H(33A)	8642	7970	5543	56
H(33B)	8818	8404	4729	56
H(33C)	7722	8399	4928	56
H(34A)	7536	8916	6328	45
H(34B)	8473	9321	6958	45
H(34C)	8514	8519	6910	45
H(35A)	10031	5493	6393	46
H(35B)	10046	6297	6399	46
H(35C)	10128	5895	5527	46
H(36A)	8540	6918	5522	39
H(36B)	7613	6506	4887	39

H(36C)	8692	6539	4657	39
H(37A)	8701	5321	4603	50
H(37B)	7635	5298	4858	50
H(37C)	8600	4894	5449	50
H(38A)	8509	5500	6838	37
H(38B)	7491	5843	6235	37
H(38C)	8402	6301	6805	37
H(39A)	6111	7758	4780	54
H(39B)	5918	7114	5331	54
H(39C)	5961	7848	5762	54
H(40A)	4130	8606	4962	192
H(40B)	3850	8360	3942	192
H(40C)	4993	8587	4434	192
H(41A)	3561	7078	3914	112
H(41B)	4659	6726	4219	112
H(41C)	4464	7328	3510	112
H(42A)	4310	7782	6008	48
H(42B)	4209	7020	5664	48
H(42C)	3343	7557	5219	48
H(43A)	9658	879	652	75
H(43B)	9452	403	1416	75
H(43C)	9378	1202	1501	75
H(44A)	7929	1814	464	55

H(44B)	7152	1382	-292	55
H(44C)	8306	1488	-336	55
H(45A)	8420	268	-465	71
H(45B)	7294	164	-349	71
H(45C)	8244	-214	306	71
H(46A)	7631	254	1501	80
H(46B)	6789	736	880	80
H(46C)	7659	1046	1690	80
H(47A)	3702	6262	1929	54
H(47B)	4373	6402	1243	54
H(47C)	4742	6681	2246	54
H(48A)	6373	6064	2191	52
H(48B)	5847	5686	1272	52
H(48C)	6358	5260	2154	52
H(49A)	4855	4710	1628	102
H(49B)	4037	5222	1040	102
H(49C)	3879	4928	1954	102
H(50A)	5276	6054	3411	124
H(50B)	5832	5350	3373	124
H(50C)	4633	5370	3292	124
H(51A)	8516	3546	2055	47
H(51B)	7457	3894	1547	47
H(51C)	8409	4348	2056	47

H(52A)	7326	4508	134	64
H(52B)	8341	4622	-185	64
H(52C)	8223	4976	708	64
H(53A)	9879	4440	1510	39
H(53B)	9929	4080	601	39
H(53C)	9984	3640	1476	39
H(54A)	8561	2957	689	42
H(54B)	8465	3370	-215	42
H(54C)	7496	3297	179	42
H(55A)	4627	8271	-512	52
H(55B)	4459	8017	417	52
H(55C)	4615	7483	-306	52
H(56A)	6151	8942	246	80
H(56B)	6997	8600	1047	80
H(56C)	5877	8745	1155	80
H(57A)	6347	7269	-488	50
H(57B)	7217	7813	-88	50
H(57C)	6230	8021	-868	50
H(58A)	5925	7590	1597	46
H(58B)	6948	7405	1324	46
H(58C)	5913	7004	887	46
H(61A)	3664	9495	1897	172
H(61B)	4546	9168	2170	172

H(64A)	6460(90)	8964(15)	3300(100)	111
H(64B)	5850(30)	8430(60)	3010(100)	111
H(65A)	6480(60)	7517(10)	3250(60)	53
H(65B)	7070(40)	6970(30)	3270(60)	53
H(66A)	6073	5019	5596	60
H(66B)	6060	4279	5582	60
H(67A)	6918	5959	-386	41
H(67B)	7242	6004	476	41
H(68A)	5391	9858	6168	140
H(68B)	6007	9662	5662	140
H(69A)	5203	6055	9783	53
H(69B)	4375	6161	9101	53
H(70A)	7898	8777	8718	71
H(70B)	7450	9367	8188	71
H(71A)	7880(40)	6240(30)	8940(40)	37
H(71B)	7760(50)	5680(20)	8440(50)	37
H(72A)	8830(30)	7510(60)	8440(70)	81
H(72B)	9410(70)	7910(50)	9080(60)	81
H(73A)	9620(50)	7400(60)	7559(14)	58
H(73B)	10160(30)	7490(60)	6960(50)	58
H(74A)	5980(60)	6260(10)	7210(70)	56
H(74B)	5430(50)	6730(40)	7500(60)	56
H(75A)	6160(70)	8526(15)	7410(70)	62

H(75B)	6400(60)	7890(40)	7140(70)	62
H(77A)	3800(50)	6260(30)	7360(40)	45
H(77B)	3970(60)	6842(17)	7840(50)	45
H(78A)	2400(40)	5460(30)	6670(40)	19(19)
H(78B)	2530(40)	5990(30)	6140(40)	40(30)
H(79A)	3851	8815	7308	64
H(79B)	4220	8199	7585	64
H(81A)	2440(60)	8950(30)	6230(50)	40
H(81B)	2940(70)	9460(40)	5960(30)	40
H(82A)	1360(90)	7833(17)	6360(50)	70(40)
H(82B)	1520(60)	7190(30)	6140(30)	20(20)

Table S.6. Hydrogen bonds for jf1660ffmi [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(61)-H(61A)...O(17)	0.84	2.00	2.844(6)	180
O(61)-H(61B)...O(62)	0.84	2.39	2.796(12)	110.0
O(64)-H(64A)...O(63)	0.84(5)	2.19(9)	2.921(17)	146(14)
O(64)-H(64B)...O(62)	0.85(7)	2.61(11)	3.418(12)	161(14)
O(65)-H(65A)...O(64)	0.84(2)	2.05(2)	2.875(11)	169(9)
O(65)-H(65B)...O(21)#1	0.84(6)	1.99(6)	2.819(7)	167(7)
O(66)-H(66B)...O(76)#2	0.84	2.41	2.845(7)	113
O(66)-H(66A)...O(76)	0.85	1.96	2.806(7)	180
O(66)-H(66B)...O(76)#2	0.84	2.41	2.845(7)	113
O(67)-H(67A)...O(71)#3	0.86	1.99	2.851(7)	180
O(67)-H(67B)...O(9)#1	0.86	1.97	2.824(6)	179
O(68)-H(68A)...O(63)#4	0.84	1.94	2.698(11)	150
O(68)-H(68B)...O(63)	0.84	2.49	3.202(17)	144
O(69)-H(69A)...O(67)#5	0.84	1.95	2.795(4)	180
O(69)-H(69B)...O(77)	0.84	2.02	2.842(5)	166
O(70)-H(70A)...O(19)#6	0.84	1.99	2.783(5)	156
O(70)-H(70B)...O(17)#4	0.84	1.95	2.798(5)	179
O(71)-H(71A)...O(8)#6	0.84(6)	1.87(6)	2.705(6)	175(7)
O(71)-H(71B)...O(1)#2	0.84(5)	1.96(3)	2.754(6)	157(7)

O(72)-H(72B)...O(19)#6	0.84(10)	1.96(9)	2.759(7)	160(9)
O(73)-H(73A)...O(72)	0.84(3)	1.87(3)	2.697(8)	166(10)
O(73)-H(73B)...O(82)#1	0.84(6)	2.03(4)	2.822(7)	157(10)
O(74)-H(74A)...O(76)	0.84(3)	2.42(9)	2.891(9)	117(8)
O(74)-H(74B)...O(77)	0.84(8)	1.97(7)	2.755(8)	155(7)
O(75)-H(75A)...O(70)	0.84(5)	2.14(8)	2.765(8)	131(10)
O(77)-H(77A)...O(78)	0.84(6)	1.89(3)	2.710(7)	165(9)
O(77)-H(77B)...O(80)	0.84(6)	2.01(4)	2.797(8)	156(9)
O(78)-H(78A)...O(10)#7	0.84(6)	1.95(6)	2.757(6)	163(6)
O(78)-H(78B)...O(12)	0.84(6)	1.96(6)	2.786(6)	174(7)
O(79)-H(79A)...O(81)	0.84	1.92	2.749(6)	170
O(79)-H(79B)...O(80)	0.84	2.32	2.735(8)	111
O(81)-H(81A)...O(15)	0.85(7)	1.97(4)	2.753(6)	153(7)
O(81)-H(81B)...O(63)#4	0.84(7)	2.13(6)	2.722(11)	127(6)
O(82)-H(82A)...O(15)	0.84(4)	2.06(6)	2.687(6)	131(7)
O(82)-H(82B)...O(12)	0.84(6)	1.92(6)	2.761(6)	176(8)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 -x+1,-y+1,-z+1 #3 x,y,z-1 #4 -x+1,-y+2,-z+1

#5 x,y,z+1 #6 x+1,y,z+1 #7 -x,-y+1,-z+1