Electronic Supplementary Information

Section 1 Experimental

Section 2 CIFs

(1) BAF845

(2) BAF847

(3) BAF1011

(4) BAF1013

(5) BAF1074

(6) BAF1125

(7) BAF1152

(8) BAF2021

Section 3. Output from "TOTOPOL" for BAF1125

Section 4. Figure S4.1 VT PXD and Figure S4.2 combined TGA/DTA data from BAF1125

Section 5 Figure S5.11. The structure of BAF845

Section 6 Comparison of Framework Densities for different zeotype topologies based on T = (AlSi), T = (BeSi), T = (BeP) and T = (BeAs).

1. Experimental

All of the samples were prepared from commercially available materials of reagent grade that did not require further purification. An example preparation is as follows: **Warning**. $Be(OH)_2$ is very toxic and may cause cancer by inhalation, H_3AsO_4 is very toxic and is regarded as a carcinogen by all routes of exposure and may be fatal if ingested; for both these materials ensure adequate control measures are in place and the authors recommend that $Be(OH)_2$ is handled in a glove box. $[\{H\text{-pyridine}\}_2]^{2+}\{Be_2[BeOH_2][AsO_4]_2[AsO_3OH]\}^{2-}$ (BAF1011) was synthesised *via* hydrothermal methods. To a stirred mixture of $Be(OH)_2$ (0.11 g, 2.56 mmoles), H_3AsO_4 (75% wt, 0.61 g, 4.34 mmol) and H_2O (3 mL), pyridine (4.11 g, 0.05 moles) was added and the solution left to stir for a further 60 minutes. The reaction mixture was transferred to a 23 mL Teflon^{TM}-lined Parr autoclave and heated at 160 °C for 7 days. The autoclave was allowed to cool slowly to room temperature over 4 h. and the solid product removed from the solution by vacuum filtration, washed with H_2O (40 mL) and EtOH (20 mL) and transfered to an oven to dry at 80 °C for 12 hours. Crystals of each product were isolated for study via single-crystal X-ray diffraction. Data were measured at 120 K on a Bruker Nonius KappaCCD diffractometer, using Mo-Kα (λ=0.71073 Å) radiation. Structures were solved using the WinGX package[22] by direct methods[23] using XPREP[24] and SHELXS-97[25] and refined using SHELXL-97. All of the non-hydrogen atoms were refined anisotropically using the F^2 least-squares method.

22 L. J. Farrugia, *J. Appl. Crystallogr.*, 1999, **32**, 837.
23 G. M. Sheldrick, *Acta Crystallogr., Sect. A:* 1990,**46**, 467.

24 XPREP Bruker AXS Inc., Madison, Wisconsin, USA

25 G. M. Sheldrick, University of Goettingen, Germany, 1997, *Release 97-2*, 1997.

Section 2 CIFs

BAF845

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As3 0.010(3) 0.010(3) 0.013(3) 0.001(2) -0.002(2) 0.002(2)
O13 0.005(12) 0.26(5) 0.035(15) 0.000 0.023(12) 0.000
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 and torsion angles; correlations between s.u.'s in cell parameters are only
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BAF847

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_diffrn_measurement_method        '\f & \w scans'
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_diffrn_standards_interval_count  23358
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_diffrn_reflns_limit_l_min        -21
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_computing_cell_refinement         'DENZO (Otwinowski & Minor, 1997)'
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 H atoms not present for OW1 & 2 due to high degree of disorder present.
;

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_refine_ls_extinction_coef        ?
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_refine_ls_R_factor_all           0.1175
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C1 C 0.8490(5) 0.2904(13) 0.4907(6) 0.031(3) Uiso 1 1 d . . .
H1A H 0.8140 0.2795 0.4690 0.037 Uiso 1 1 calc R . .
H1B H 0.8604 0.3822 0.4816 0.037 Uiso 1 1 calc R . .
C2 C 0.8856(5) 0.1944(13) 0.4562(6) 0.035(3) Uiso 1 1 d . . .
H2A H 0.8715 0.1038 0.4604 0.042 Uiso 1 1 calc R . .
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H2B H 0.9191 0.1965 0.4827 0.042 Uiso 1 1 calc R . .
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H4A H 0.8215 0.3327 0.5890 0.048 Uiso 1 1 calc R . .
H4B H 0.8340 0.1787 0.5790 0.048 Uiso 1 1 calc R . .
N1 N 0.8955(3) 0.2205(9) 0.3785(4) 0.0207(19) Uiso 1 1 d . . .
H5A H 0.9176 0.1583 0.3626 0.031 Uiso 1 1 calc R . .
H5B H 0.9097 0.3021 0.3738 0.031 Uiso 1 1 calc R . .
H5C H 0.8653 0.2165 0.3531 0.031 Uiso 1 1 calc R . .
CN1 N 0.8983(3) 0.2890(9) 0.6065(4) 0.0190(18) Uiso 1 1 d . . .
HN1A H 0.8954 0.2757 0.6533 0.028 Uiso 1 1 calc R . .
HN1B H 0.9095 0.3728 0.5989 0.028 Uiso 1 1 calc R . .
HN1C H 0.9212 0.2302 0.5896 0.028 Uiso 1 1 calc R . .
Be1 Be 0.8647(5) 0.4053(12) 0.8140(6) 0.012(2) Uiso 1 1 d . . .
Be2 Be 0.8649(4) -0.0868(12) 0.6713(6) 0.008(2) Uiso 1 1 d . . .
Be3 Be 0.9729(5) 0.6297(13) 0.5905(7) 0.016(3) Uiso 1 1 d . . .
Be4 Be 0.9748(4) 0.1351(11) 0.9097(6) 0.007(2) Uiso 1 1 d . . .
O1 O 0.8848(2) 0.5999(7) 0.3973(3) 0.0140(14) Uani 1 1 d . . .
O2 O 0.8890(2) -0.2119(6) 0.7193(3) 0.0128(13) Uani 1 1 d . . .
O3 O 0.8819(2) -0.0977(6) 0.5888(3) 0.0108(13) Uani 1 1 d . . .
O4 O 0.9395(2) -0.4298(7) 0.6591(3) 0.0128(13) Uani 1 1 d . . .
O5 O 0.9674(2) 0.0683(6) 0.5803(3) 0.0124(13) Uani 1 1 d . . .
O6 O 0.8939(3) 0.2878(6) 0.7675(3) 0.0142(14) Uani 1 1 d . . .
O7 O 0.8425(2) 0.0699(7) 0.8352(3) 0.0138(14) Uani 1 1 d . . .
O8 O 0.9475(2) 0.0729(7) 0.8324(3) 0.0127(13) Uani 1 1 d . . .
O9 O 0.9397(2) 0.5798(7) 0.5204(3) 0.0148(14) Uani 1 1 d . . .
O10 O 0.8333(3) -0.4216(8) 0.6465(3) 0.0202(15) Uani 1 1 d . . .
O11 O 0.9344(2) -0.1009(6) 0.4702(3) 0.0128(13) Uani 1 1 d . . .
O12 O 0.9830(3) -0.2059(7) 0.5957(3) 0.0138(14) Uani 1 1 d . . .
O13 O 0.8807(3) 0.5479(7) 0.7798(3) 0.0162(15) Uani 1 1 d . . .
O14 O 0.9861(2) 0.7042(6) 0.4015(3) 0.0128(13) Uani 1 1 d . . .
O15 O 0.6992(2) 0.4166(7) 0.8334(4) 0.0190(15) Uani 1 1 d . . .
O16 O 0.7491(3) 0.5562(7) 0.7269(4) 0.0191(15) Uani 1 1 d . . .
O17 O 0.7317(3) 0.2911(8) 0.7096(4) 0.0308(19) Uani 1 1 d . . .
O18 O 0.8025(2) 0.3727(7) 0.8176(4) 0.0216(16) Uani 1 1 d . . .
O19 O 0.9686(2) 0.4325(6) 0.4022(3) 0.0133(13) Uani 1 1 d . . .
O20 O 0.8916(3) 0.0479(7) 0.7047(3) 0.0138(14) Uani 1 1 d . . .
As1 As 0.94646(3) 0.58202(9) 0.43157(5) 0.0097(2) Uani 1 1 d . . .
As2 As 0.94340(3) -0.08609(9) 0.55941(5) 0.0087(2) Uani 1 1 d . . .
As3 As 0.88616(4) -0.37752(9) 0.70152(5) 0.0105(2) Uani 1 1 d . . .
As4 As 0.89441(3) 0.12143(9) 0.78439(5) 0.0102(2) Uani 1 1 d . . .
As5 As 0.74642(4) 0.41218(10) 0.77481(5) 0.0152(2) Uani 1 1 d . . .
OW1 O 0.0000 0.1150(12) 0.2500 0.030(3) Uani 1 2 d S . .
OW2 O 0.0000 0.5971(12) 0.2500 0.031(3) Uani 1 2 d S . .
N10A N 0.1696(4) 0.7958(11) 0.0324(5) 0.026(3) Uani 0.94(3) 1 d PD . .
C11A C 0.2272(9) 0.775(2) 0.0335(12) 0.026(5) Uani 0.50 1 d P . .
C12A C 0.2630(8) 0.836(3) 0.0227(12) 0.028(5) Uani 0.50 1 d P . .
C10A C 0.2099(9) 0.892(2) 0.0198(11) 0.028(5) Uani 0.50 1 d P . .

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O2 0.014(3) 0.006(3) 0.019(4) 0.000(3) -0.001(3) 0.002(3)
O3 0.010(3) 0.010(3) 0.012(3) -0.004(2) 0.001(2) -0.005(3)
O4 0.010(3) 0.014(3) 0.014(3) 0.003(3) 0.004(2) 0.004(3)
O5 0.010(3) 0.010(3) 0.017(3) -0.001(3) 0.000(2) 0.001(3)
O6 0.016(3) 0.005(3) 0.022(4) -0.004(3) 0.007(3) -0.001(3)
O7 0.013(3) 0.018(4) 0.011(3) 0.000(3) 0.002(2) -0.003(3)
O8 0.010(3) 0.018(4) 0.010(3) -0.004(3) 0.000(2) 0.004(3)
O9 0.013(3) 0.018(4) 0.014(3) -0.002(3) 0.001(3) 0.001(3)
O10 0.016(3) 0.029(4) 0.015(3) -0.005(3) -0.005(3) 0.001(3)
O11 0.014(3) 0.014(3) 0.011(3) -0.002(3) 0.002(2) 0.005(3)
O12 0.018(3) 0.015(4) 0.008(3) -0.002(3) -0.001(3) 0.002(3)
O13 0.024(4) 0.010(3) 0.016(3) 0.001(3) 0.007(3) -0.002(3)
O14 0.015(3) 0.009(3) 0.015(3) -0.004(3) 0.008(3) -0.004(3)
O15 0.010(3) 0.026(4) 0.021(4) -0.003(3) 0.004(3) 0.001(3)
O16 0.011(3) 0.012(4) 0.034(4) 0.005(3) 0.001(3) 0.000(3)
O17 0.048(5) 0.018(4) 0.027(4) -0.005(3) 0.005(4) 0.009(4)
O18 0.007(3) 0.025(4) 0.032(4) 0.010(3) -0.003(3) 0.001(3)
O19 0.014(3) 0.009(3) 0.017(3) -0.005(3) -0.001(3) 0.004(3)
O20 0.017(3) 0.013(3) 0.012(3) -0.004(3) 0.000(3) 0.000(3)
As1 0.0111(4) 0.0086(4) 0.0093(4) -0.0005(3) 0.0010(3) -0.0009(4)
As2 0.0099(4) 0.0072(4) 0.0091(4) -0.0001(3) 0.0006(3) -0.0005(3)
As3 0.0116(4) 0.0097(5) 0.0103(4) 0.0002(3) 0.0008(3) -0.0007(4)
As4 0.0102(4) 0.0106(5) 0.0096(4) 0.0002(3) -0.0003(3) 0.0000(4)
As5 0.0100(4) 0.0129(5) 0.0227(5) 0.0016(4) 0.0018(4) 0.0006(4)
OW1 0.025(6) 0.037(7) 0.028(6) 0.000 0.002(5) 0.000
OW2 0.035(6) 0.035(7) 0.024(6) 0.000 0.004(5) 0.000
N10A 0.017(5) 0.037(7) 0.024(6) 0.001(5) -0.003(4) 0.005(4)
C11A 0.024(12) 0.021(12) 0.033(13) -0.003(10) -0.006(9) -0.001(10)
C12A 0.019(11) 0.040(14) 0.025(12) -0.001(10) -0.007(9) -0.011(10)
C10A 0.035(12) 0.025(13) 0.023(11) 0.004(9) -0.003(9) -0.017(10)

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 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
;

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C2 N1 1.508(14) . ?
C4 CN1 1.474(15) . ?
Be1 O13 1.608(14) . ?
Be1 O18 1.618(13) . ?
Be1 O1 1.622(13) 6_566 ?
Be1 O6 1.646(13) . ?
Be2 O20 1.611(13) . ?
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Be2 O3 1.622(12) . ?
Be2 O15 1.629(12) 4_646 ?
Be2 O2 1.634(13) . ?
Be3 O9 1.610(14) . ?
Be3 O19 1.612(14) 5_766 ?
Be3 O12 1.649(15) 1_565 ?
Be3 O4 1.673(14) 1_565 ?
Be4 O11 1.595(12) 6_556 ?
Be4 O5 1.616(12) 2_756 ?
Be4 O14 1.623(13) 6_566 ?
Be4 O8 1.698(12) . ?
O1 Be1 1.622(13) 6_565 ?
O1 As1 1.681(6) . ?
O2 As3 1.673(6) . ?
O3 As2 1.682(6) . ?
O4 Be3 1.673(14) 1_545 ?
O4 As3 1.678(6) . ?
O5 Be4 1.616(12) 2_756 ?
O5 As2 1.684(6) . ?
O6 As4 1.676(6) . ?
O7 As4 1.732(6) . ?
O8 As4 1.663(6) . ?
O9 As1 1.679(6) . ?
O10 As3 1.717(6) . ?
O11 Be4 1.595(12) 6 ?
O11 As2 1.682(6) . ?
O12 Be3 1.649(15) 1_545 ?
O12 As2 1.681(6) . ?
O13 As3 1.651(6) 1_565 ?
O14 Be4 1.623(13) 6_565 ?
O14 As1 1.684(6) . ?
O15 Be2 1.629(12) 4_656 ?
O15 As5 1.656(6) . ?
O16 As5 1.686(7) . ?
O17 As5 1.741(8) . ?
O18 As5 1.654(6) . ?
O19 Be3 1.612(14) 5_766 ?
O19 As1 1.683(6) . ?
O20 As4 1.658(6) . ?
As3 O13 1.651(6) 1_545 ?
N10A C10A 1.43(2) . ?
N10A C11A 1.48(2) . ?
C11A C12A 1.12(3) . ?
C11A C10A 1.26(3) . ?
C11A C12A 1.55(3) 7_565 ?
C11A C11A 1.81(5) 7_565 ?
C12A C10A 1.46(3) . ?
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C1 C2 N1 116.0(10) . . ?
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O13 Be1 O18 117.0(8) . . ?
O13 Be1 O1 109.6(8) . 6_566 ?
O18 Be1 O1 103.1(7) . 6_566 ?
O13 Be1 O6 106.4(7) . . ?
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O1 Be1 O6 110.7(8) 6_566 . ?
O20 Be2 O3 107.6(7) . . ?
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O3 Be2 O15 104.6(7) . 4_646 ?
O20 Be2 O2 105.6(7) . . ?
O3 Be2 O2 111.4(7) . . ?
O15 Be2 O2 113.4(7) 4_646 . ?
O9 Be3 O19 113.9(8) . 5_766 ?
O9 Be3 O12 115.2(8) . 1_565 ?
O19 Be3 O12 103.3(8) 5_766 1_565 ?
O9 Be3 O4 104.6(8) . 1_565 ?
O19 Be3 O4 107.1(8) 5_766 1_565 ?
O12 Be3 O4 112.6(8) 1_565 1_565 ?
O11 Be4 O5 116.0(7) 6_556 2_756 ?
O11 Be4 O14 113.3(7) 6_556 6_566 ?
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O11 Be4 O8 105.9(7) 6_556 . ?
O5 Be4 O8 106.9(7) 2_756 . ?
O14 Be4 O8 110.0(7) 6_566 . ?
Be1 O1 As1 128.2(6) 6_565 . ?
Be2 O2 As3 128.3(6) . . ?
Be2 O3 As2 126.2(5) . . ?
Be3 O4 As3 134.2(6) 1_545 . ?
Be4 O5 As2 135.8(6) 2_756 . ?
Be1 O6 As4 126.4(6) . . ?
As4 O8 Be4 130.7(5) . . ?
Be3 O9 As1 137.2(6) . . ?
Be4 O11 As2 130.9(6) 6 . ?
Be3 O12 As2 125.6(6) 1_545 . ?
Be1 O13 As3 141.0(6) . 1_565 ?
Be4 O14 As1 124.2(5) 6_565 . ?
Be2 O15 As5 135.4(6) 4_656 . ?
Be1 O18 As5 139.3(6) . . ?
Be3 O19 As1 128.8(6) 5_766 . ?
Be2 O20 As4 135.7(6) . . ?
O9 As1 O1 104.5(3) . . ?
O9 As1 O19 111.1(3) . . ?
O1 As1 O19 106.6(3) . . ?
O9 As1 O14 115.2(3) . . ?
O1 As1 O14 111.0(3) . . ?
O19 As1 O14 108.1(3) . . ?
O12 As2 O3 111.7(3) . . ?
O12 As2 O11 113.4(3) . . ?
O3 As2 O11 103.0(3) . . ?
O12 As2 O5 109.9(3) . . ?
O3 As2 O5 108.6(3) . . ?
O11 As2 O5 110.1(3) . . ?
O13 As3 O2 105.5(3) 1_545 . ?
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O13 As3 O4 112.2(3) 1_545 . ?
O2 As3 O4 111.5(3) . . ?
O13 As3 O10 109.2(3) 1_545 . ?
O2 As3 O10 113.2(3) . . ?
O4 As3 O10 105.4(3) . . ?
O20 As4 O8 111.4(3) . . ?
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O18 As5 O17 109.6(4) . . ?
O16 As5 O17 102.7(4) . . ?
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C12A C11A C10A 75(2) . . ?
C12A C11A N10A 137(2) . . ?
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C12A C11A C12A 96(2) . 7_565 ?
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C12A C11A C11A 58.3(18) . 7_565 ?
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BAF1011

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 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

_cell_length_a                    26.2341(6)
_cell_length_b                    4.91270(10)
_cell_length_c                    24.6048(5)
_cell_angle_alpha                 90.00
_cell_angle_beta                  118.7180(10)
_cell_angle_gamma                 90.00
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_cell_volume                        2781.01(10)
_cell_formula_units_Z               8
_cell_measurement_temperature       120(2)
_cell_measurement_reflns_used       16959
_cell_measurement_theta_min         2.91
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_exptl_crystal_density_method       'not measured'
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_exptl_special_details
;
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;

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_diffrn_reflns_av_sigmaI/netI       0.0435
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_computing_data_reduction           'DENZO (Otwinowski & Minor, 1997)'
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_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0000P)^2^+42.3673P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_R_factor_all           0.0492
_refine_ls_R_factor_gt            0.0381
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_refine_ls_goodness_of_fit_ref    1.139
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As2 As 0.050636(19) 0.85473(9) 0.34221(2) 0.00650(11) Uani 1 1 d . . .
As3 As 0.261890(19) 0.97593(9) 0.56991(2) 0.00630(11) Uani 1 1 d . . .
Be1 Be 0.0691(3) 1.0009(13) 0.2379(3) 0.0112(12) Uani 1 1 d . . .
```

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Be2 Be 0.1749(2) 1.0171(12) 0.4338(3) 0.0085(11) Uani 1 1 d . . .
Be3 Be 0.2582(3) 1.1908(12) 0.6843(3) 0.0094(12) Uani 1 1 d . . .
O1 O 0.18458(13) 0.4753(6) 0.26578(14) 0.0080(6) Uani 1 1 d . . .
O2 O 0.20313(13) 0.8586(7) 0.19409(14) 0.0107(7) Uani 1 1 d . . .
O3 O 0.21855(13) 0.9874(6) 0.31022(14) 0.0083(6) Uani 1 1 d . . .
O4 O 0.10901(13) 0.8898(7) 0.21000(14) 0.0086(7) Uani 1 1 d . . .
O6 O 0.06560(13) 0.7693(6) 0.28537(14) 0.0084(6) Uani 1 1 d . . .
O7 O 0.02791(15) 0.5761(7) 0.36595(16) 0.0116(7) Uani 1 1 d D . .
H7 H 0.017(2) 0.439(8) 0.343(2) 0.023(17) Uiso 1 1 d D . .
O8 O -0.00367(13) 1.0825(7) 0.31602(14) 0.0086(7) Uani 1 1 d . . .
O9 O 0.10604(13) 0.9770(7) 0.40544(14) 0.0094(7) Uani 1 1 d . . .
O10 O 0.20408(13) 0.8304(6) 0.39756(14) 0.0082(6) Uani 1 1 d . . .
O11 O 0.18967(13) 1.3354(7) 0.43734(15) 0.0088(6) Uani 1 1 d . . .
O12 O 0.20297(13) 0.8878(7) 0.50376(14) 0.0089(7) Uani 1 1 d . . .
O13 O 0.23599(13) 1.1050(6) 0.61384(14) 0.0086(7) Uani 1 1 d . . .
N1 N 0.36866(18) 0.8905(9) 0.46413(19) 0.0151(9) Uani 1 1 d . . .
H6 H 0.3465 0.8063 0.4753 0.018 Uiso 1 1 calc R . .
C1 C 0.3712(2) 0.8032(10) 0.4138(2) 0.0160(11) Uani 1 1 d . . .
H1 H 0.3482 0.6577 0.3909 0.019 Uiso 1 1 calc R . .
C2 C 0.4076(2) 0.9285(11) 0.3961(2) 0.0167(11) Uani 1 1 d . . .
H2 H 0.4105 0.8653 0.3621 0.020 Uiso 1 1 calc R . .
C3 C 0.4399(2) 1.1492(11) 0.4295(2) 0.0171(11) Uani 1 1 d . . .
H3 H 0.4643 1.2384 0.4177 0.021 Uiso 1 1 calc R . .
C4 C 0.4356(2) 1.2382(11) 0.4812(2) 0.0170(11) Uani 1 1 d . . .
H4 H 0.4571 1.3870 0.5041 0.020 Uiso 1 1 calc R . .
C5 C 0.3994(2) 1.1033(11) 0.4975(2) 0.0160(11) Uani 1 1 d . . .
H5 H 0.3962 1.1598 0.5318 0.019 Uiso 1 1 calc R . .
O5 O 0.09870(14) 1.2758(7) 0.27762(16) 0.0104(7) Uani 1 1 d D . .
H5A H 0.127(2) 1.322(18) 0.273(4) 0.07(3) Uiso 1 1 d D . .
H5B H 0.082(2) 1.419(8) 0.280(3) 0.030(18) Uiso 1 1 d D . .

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 _atom_site_aniso_U_12
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As2 0.0063(2) 0.0071(2) 0.0063(2) -0.00044(18) 0.00314(18) -0.00002(17)
As3 0.0070(2) 0.0064(2) 0.0057(2) -0.00039(18) 0.00317(17) -0.00021(17)
Be1 0.009(3) 0.011(3) 0.015(3) 0.001(3) 0.007(2) 0.000(2)
Be2 0.008(3) 0.009(3) 0.009(3) 0.001(2) 0.005(2) -0.002(2)
Be3 0.011(3) 0.006(3) 0.011(3) -0.002(2) 0.005(2) -0.003(2)
O1 0.0070(14) 0.0075(15) 0.0081(15) 0.0033(13) 0.0025(12) -0.0002(12)
O2 0.0095(16) 0.0134(17) 0.0099(16) 0.0042(14) 0.0051(13) 0.0021(13)
O3 0.0108(15) 0.0067(15) 0.0077(15) -0.0014(13) 0.0047(13) -0.0030(13)
O4 0.0054(15) 0.0115(17) 0.0065(15) 0.0010(13) 0.0009(12) 0.0007(13)
O6 0.0109(16) 0.0066(15) 0.0084(15) 0.0007(13) 0.0054(13) 0.0004(13)
O7 0.0185(17) 0.0062(16) 0.0146(17) -0.0022(14) 0.0116(15) -0.0049(14)
O8 0.0047(14) 0.0098(16) 0.0098(16) -0.0002(13) 0.0022(12) 0.0013(12)
O9 0.0060(15) 0.0131(17) 0.0074(15) -0.0025(13) 0.0019(12) -0.0011(13)
O10 0.0105(15) 0.0083(15) 0.0079(15) -0.0002(13) 0.0061(13) 0.0024(13)
O11 0.0093(15) 0.0080(15) 0.0116(16) -0.0002(13) 0.0069(13) -0.0019(13)
O12 0.0054(14) 0.0140(17) 0.0052(15) -0.0015(13) 0.0008(12) -0.0027(13)
O13 0.0100(15) 0.0075(15) 0.0108(16) -0.0014(13) 0.0070(13) -0.0012(13)
```

```
N1 0.013(2) 0.021(2) 0.014(2) 0.0041(18) 0.0077(17) -0.0005(18)
C1 0.016(2) 0.011(2) 0.016(3) 0.003(2) 0.004(2) 0.002(2)
C2 0.020(3) 0.019(3) 0.011(2) 0.004(2) 0.007(2) 0.006(2)
C3 0.015(2) 0.017(3) 0.022(3) 0.003(2) 0.011(2) -0.003(2)
C4 0.016(2) 0.014(2) 0.018(3) -0.002(2) 0.006(2) -0.003(2)
C5 0.016(2) 0.020(3) 0.011(2) -0.001(2) 0.006(2) 0.005(2)
O5 0.0107(17) 0.0073(16) 0.0151(17) -0.0034(14) 0.0077(14) -0.0004(14)

_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
;

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As1 O4 1.661(3) . ?
As1 O1 1.677(3) . ?
As1 O3 1.721(3) . ?
As2 O9 1.649(3) . ?
As2 O6 1.677(3) . ?
As2 O8 1.678(3) . ?
As2 O7 1.705(3) . ?
As3 O11 1.650(3) 7_576 ?
As3 O13 1.655(3) . ?
As3 O12 1.676(3) . ?
As3 O10 1.737(3) 7_566 ?
Be1 O4 1.599(7) . ?
Be1 O5 1.629(7) . ?
Be1 O8 1.636(7) 2 ?
Be1 O6 1.664(7) . ?
Be2 O11 1.604(7) . ?
Be2 O9 1.605(6) . ?
Be2 O12 1.640(7) . ?
Be2 O10 1.696(7) . ?
Be3 O2 1.594(7) 6_576 ?
Be3 O13 1.597(7) . ?
Be3 O1 1.629(7) 7_566 ?
Be3 O3 1.676(7) 7_576 ?
O1 Be3 1.629(7) 7_566 ?
O2 Be3 1.594(7) 6_575 ?
O3 Be3 1.676(7) 7_576 ?
O8 Be1 1.636(7) 2 ?
O10 As3 1.737(3) 7_566 ?
O11 As3 1.650(3) 7_576 ?
N1 C5 1.334(7) . ?
N1 C1 1.343(7) . ?
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C1 C2 1.370(7) . ?
C2 C3 1.378(7) . ?
C3 C4 1.399(7) . ?
C4 C5 1.367(7) . ?

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O2 As1 O4 108.23(15) . . ?
O2 As1 O1 113.18(16) . . ?
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O2 As1 O3 109.84(16) . . ?
O4 As1 O3 110.88(15) . . ?
O1 As1 O3 106.16(15) . . ?
O9 As2 O6 115.11(15) . . ?
O9 As2 O8 108.67(16) . . ?
O6 As2 O8 110.02(15) . . ?
O9 As2 O7 105.32(16) . . ?
O6 As2 O7 110.19(16) . . ?
O8 As2 O7 107.17(16) . . ?
O11 As3 O13 115.77(16) 7_576 . ?
O11 As3 O12 116.04(16) 7_576 . ?
O13 As3 O12 104.89(16) . . ?
O11 As3 O10 106.53(15) 7_576 7_566 ?
O13 As3 O10 108.20(15) . 7_566 ?
O12 As3 O10 104.69(16) . 7_566 ?
O4 Be1 O5 108.6(4) . . ?
O4 Be1 O8 112.6(4) . 2 ?
O5 Be1 O8 107.2(4) . 2 ?
O4 Be1 O6 109.6(4) . . ?
O5 Be1 O6 108.5(4) . . ?
O8 Be1 O6 110.3(4) 2 . ?
O11 Be2 O9 109.6(4) . . ?
O11 Be2 O12 110.2(4) . . ?
O9 Be2 O12 104.6(4) . . ?
O11 Be2 O10 113.4(4) . . ?
O9 Be2 O10 113.8(4) . . ?
O12 Be2 O10 104.7(4) . . ?
O2 Be3 O13 103.8(4) 6_576 . ?
O2 Be3 O1 112.5(4) 6_576 7_566 ?
O13 Be3 O1 114.2(4) . 7_566 ?
O2 Be3 O3 116.9(4) 6_576 7_576 ?
O13 Be3 O3 105.4(4) . 7_576 ?
O1 Be3 O3 104.1(4) 7_566 7_576 ?
Be3 O1 As1 129.2(3) 7_566 . ?
Be3 O2 As1 142.0(3) 6_575 . ?
Be3 O3 As1 127.4(3) 7_576 . ?
Be1 O4 As1 131.7(3) . . ?
Be1 O6 As2 121.8(3) . . ?
Be1 O8 As2 120.9(3) 2 . ?
Be2 O9 As2 138.8(3) . . ?
Be2 O10 As3 119.2(3) . 7_566 ?
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Be2 O11 As3 136.1(3) . 7_576 ?
Be2 O12 As3 131.2(3) . . ?
Be3 O13 As3 139.4(3) . . ?
C5 N1 C1 122.3(5) . . ?
N1 C1 C2 120.0(5) . . ?
C1 C2 C3 119.1(5) . . ?
C2 C3 C4 119.5(5) . . ?
C5 C4 C3 119.0(5) . . ?
N1 C5 C4 119.9(5) . . ?

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N1 H6 O12  0.86 1.87 2.730(5) 177.3 7_566
O5 H5A O1  0.85(2) 1.76(3) 2.598(5) 170(9) 1_565
O5 H5B O6  0.85(2) 1.79(3) 2.613(5) 162(6) 1_565

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BAF1013

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 'O'  'O'   0.0106   0.0060
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 'As'  'As'   0.0499   2.0058
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 'H'  'H'   0.0000   0.0000
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_symmetry_space_group_name_H-M    'P 1 21/c 1'

loop_
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 'x, y, z'
 '-x, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y-1/2, z-1/2'

_cell_length_a                    5.0833(2)
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_cell_angle_gamma                 90.00
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;
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;

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goniostat'
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COLLECT (Hooft, R.W.W., 1998)'
_computing_data_reduction         'DENZO (Otwinowski & Minor, 1997) &
COLLECT (Hooft, R.W.W., 1998)'
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_computing_structure_refinement   'SHELXL-97 (Sheldrick, 2008)'
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_computing_publication_material   ?

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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O2 O -0.2528(5) 0.0913(4) 0.4643(3) 0.0106(6) Uani 1 1 d . . .
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OW1 O 1.0000 0.5000 0.5000 0.012 Uiso 0.137(10) 2 d SP . .
H1 H 0.834(10) 0.448(7) 0.593(3) 0.026(15) Uiso 1 1 d D . .
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O4 0.0106(13) 0.0107(14) 0.0079(14) 0.0009(11) -0.0028(11) -0.0004(11)
O2 0.0101(14) 0.0096(14) 0.0120(15) -0.0004(11) -0.0009(11) 0.0016(12)
O3 0.0116(14) 0.0097(14) 0.0151(16) 0.0012(12) 0.0041(12) -0.0025(12)
O5 0.0112(14) 0.0101(14) 0.0088(15) -0.0011(11) 0.0017(11) 0.0001(12)
Sr1 0.00795(18) 0.00807(19) 0.0088(2) 0.00027(13) 0.00109(14) 0.00091(14)
As1 0.0081(2) 0.0061(2) 0.0075(2) -0.00043(14) 0.00043(15) -0.00026(15)

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 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
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O4 Sr1 2.730(3) . ?
O4 Sr1 2.749(3) 2_556 ?
O2 As1 1.658(3) 1_455 ?
O2 Sr1 2.509(3) . ?
O2 Sr1 2.508(3) 3_556 ?
O3 Be1 1.647(6) . ?
O3 As1 1.699(3) 3_666 ?
O3 Sr1 2.543(3) 2_556 ?
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Sr1 O2 2.508(3) 3_556 ?
Sr1 O3 2.543(3) 2_546 ?
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Sr1 O4 2.749(3) 2_546 ?
Sr1 Be1 3.331(6) 2_546 ?
Sr1 Be1 3.614(6) 2_646 ?
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As1 O3 1.699(3) 3_666 ?
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Sr1 O4 Sr1 103.03(9) . 2_556 ?
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Sr1 O2 Sr1 105.49(10) . 3_556 ?
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BAF1074

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 '-x, -y, -z'
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 'x+1/2, -y+1/2, z-1/2'

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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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Be1 0.010(2) 0.013(2) 0.011(2) 0.000 -0.0019(16) 0.000
Be2 0.0110(15) 0.0042(15) 0.0085(14) 0.0017(10) 0.0004(12) 0.0000(11)
O5 0.0156(10) 0.0139(11) 0.0186(10) 0.0033(8) 0.0063(8) 0.0030(8)
As1 0.00665(15) 0.00554(16) 0.00569(14) 0.00038(8) -0.00074(9) -0.00031(8)
O2 0.0079(8) 0.0100(9) 0.0047(8) 0.0012(6) 0.0001(6) 0.0000(6)
O4 0.0103(8) 0.0058(8) 0.0124(9) -0.0003(7) 0.0026(7) -0.0004(7)
O1 0.0101(9) 0.0136(9) 0.0194(10) 0.0063(8) -0.0091(7) -0.0039(7)
O3 0.0115(8) 0.0070(8) 0.0051(8) 0.0001(6) 0.0014(6) 0.0012(7)

_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
;

loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
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 _geom_bond_site_symmetry_2
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Be1 O1 1.594(4) . ?
Be1 O5 1.661(4) 2 ?
Be1 O5 1.661(4) . ?
Be2 O4 1.586(4) . ?
Be2 O2 1.623(4) 7_556 ?
Be2 O3 1.657(3) 1_565 ?
Be2 O3 1.662(3) 4 ?
As1 O4 1.6629(18) . ?
As1 O1 1.6635(18) . ?
As1 O2 1.6667(16) . ?
As1 O3 1.7207(17) . ?
O2 Be2 1.623(4) 7_556 ?
O3 Be2 1.657(3) 1_545 ?
O3 Be2 1.662(3) 4_545 ?

loop_
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 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
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 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
O1 Be1 O1 103.2(3) 2 . ?
O1 Be1 O5 114.42(10) 2 2 ?
O1 Be1 O5 112.06(11) . 2 ?
O1 Be1 O5 112.06(11) 2 . ?
O1 Be1 O5 114.42(10) . . ?
O5 Be1 O5 101.1(3) 2 . ?
O4 Be2 O2 115.9(2) . 7_556 ?
O4 Be2 O3 107.0(2) . 1_565 ?
O2 Be2 O3 106.99(19) 7_556 1_565 ?
O4 Be2 O3 109.6(2) . 4 ?
O2 Be2 O3 108.2(2) 7_556 4 ?
O3 Be2 O3 108.94(18) 1_565 4 ?
O4 As1 O1 112.13(9) . . ?
O4 As1 O2 110.70(9) . . ?
O1 As1 O2 109.31(9) . . ?
O4 As1 O3 106.24(8) . . ?
O1 As1 O3 108.14(9) . . ?
O2 As1 O3 110.26(8) . . ?
Be2 O2 As1 125.13(15) 7_556 . ?
Be2 O4 As1 128.08(16) . . ?
Be1 O1 As1 127.52(17) . . ?
Be2 O3 Be2 123.27(15) 1_545 4_545 ?
Be2 O3 As1 118.01(15) 1_545 . ?
Be2 O3 As1 118.11(15) 4_545 . ?

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_diffrn_measured_fraction_theta_full   0.993
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BAF1025

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;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety
'2(As O4), 2(H4 N), 2(H O), 3(Be)'
_chemical_formula_sum
 'As2 Be3 H10 N2 O10'
_chemical_formula_weight          374.97

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 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
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 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'As'  'As'   0.0499   2.0058
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    'P 1 21/n 1'

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

_cell_length_a                    9.9140(3)
_cell_length_b                    8.5660(3)
_cell_length_c                    11.1562(4)
_cell_angle_alpha                 90.00
_cell_angle_beta                  100.050(2)
_cell_angle_gamma                 90.00
_cell_volume                      932.88(5)
_cell_formula_units_Z             4
_cell_measurement_temperature     120(2)
_cell_measurement_reflns_used     10226
_cell_measurement_theta_min       2.91
_cell_measurement_theta_max       27.48
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_exptl_crystal_size_mid           0.01
_exptl_crystal_size_min           0.01
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     2.670
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              728.0
_exptl_absorpt_coefficient_mu     7.164
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_exptl_absorpt_correction_T_min   ?
_exptl_absorpt_correction_T_max   ?
_exptl_absorpt_process_details    ?

_exptl_special_details
;

;

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_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   '10cm confocal mirrors'
_diffrn_measurement_device_type   'Bruker-Nonius APEX II CCD camera'
_diffrn_measurement_method        '\f & \w scans'
_diffrn_detector_area_resol_mean  '4096x4096pixels / 62x62mm'
_diffrn_standards_number          2279
_diffrn_standards_interval_count  9095
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         ?
_diffrn_reflns_number             12090
_diffrn_reflns_av_R_equivalents   0.0437
_diffrn_reflns_av_sigmaI/netI     0.0375
_diffrn_reflns_limit_h_min        -12
_diffrn_reflns_limit_h_max        12
_diffrn_reflns_limit_k_min        -11
_diffrn_reflns_limit_k_max        11
_diffrn_reflns_limit_l_min        -14
_diffrn_reflns_limit_l_max        14
_diffrn_reflns_theta_min          3.02
_diffrn_reflns_theta_max          27.55
_reflns_number_total              2133
_reflns_number_gt                 1710
_reflns_threshold_expression      >2\s(I)

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_computing_cell_refinement        'DENZO (Otwinowski & Minor, 1997) &
COLLECT (Hooft, R.W.W., 1998)'
_computing_data_reduction         'DENZO (Otwinowski & Minor, 1997) &
COLLECT (Hooft, R.W.W., 1998)'
_computing_structure_solution     ?
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics     ?
_computing_publication_material   ?
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_refine_special_details
;
Refinement has been attempted in suggested spg P2(1)/2 - leads to
unacceptable bond distances
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0000P)^2^+7.1150P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          2133
_refine_ls_number_parameters      194
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0547
_refine_ls_R_factor_gt            0.0385
_refine_ls_wR_factor_ref          0.0772
_refine_ls_wR_factor_gt           0.0700
_refine_ls_goodness_of_fit_ref    1.105
_refine_ls_restrained_S_all       1.105
_refine_ls_shift/su_max           0.064
_refine_ls_shift/su_mean          0.007

loop_
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 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
N2 N 0.4168(4) 0.1502(5) 0.5483(4) 0.0101(8) Uani 1 1 d . . .
N1 N 0.4194(4) 0.6570(5) 0.0473(4) 0.0118(8) Uani 1 1 d . . .
Be2 Be 0.3989(6) 0.0675(7) 0.1644(5) 0.0088(12) Uani 1 1 d . . .
Be3 Be 0.0891(6) 0.0647(7) -0.1855(5) 0.0097(12) Uani 1 1 d . . .
H1 H 0.383(6) 0.238(8) 0.580(6) 0.026(17) Uiso 1 1 d . . .
H2 H 0.363(6) 0.615(7) -0.017(6) 0.019(15) Uiso 1 1 d . . .
H3 H 0.437(8) 0.587(10) 0.116(8) 0.06(2) Uiso 1 1 d . . .
H4 H 0.367(7) 0.062(9) 0.558(6) 0.04(2) Uiso 1 1 d . . .
H6 H 0.504(7) 0.128(7) 0.584(6) 0.028(17) Uiso 1 1 d . . .
H5 H 0.406(6) 0.159(7) 0.470(6) 0.016(14) Uiso 1 1 d . . .
H7 H 0.488(7) 0.692(7) 0.030(5) 0.019(16) Uiso 1 1 d . . .
H9 H 0.113(6) 0.088(8) -0.003(6) 0.022(19) Uiso 1 1 d . . .
H10 H 0.374(8) 0.736(11) 0.065(8) 0.06(3) Uiso 1 1 d . . .
```

```
H8 H 0.378(7) 0.115(8) -0.009(6) 0.02(2) Uiso 1 1 d . . .
As1 As 0.68971(4) 0.13389(5) 0.24184(4) 0.00601(13) Uani 1 1 d . . .
As2 As 0.20042(4) -0.13923(5) 0.25115(4) 0.00620(13) Uani 1 1 d . . .
O8 O 0.1030(3) 0.1453(4) -0.0515(3) 0.0081(6) Uani 1 1 d . . .
O9 O 0.3688(3) 0.1619(4) 0.0335(3) 0.0093(7) Uani 1 1 d . . .
O6 O 0.2037(3) 0.3694(4) 0.1094(3) 0.0092(6) Uani 1 1 d . . .
O5 O 0.2996(3) -0.0908(4) 0.1487(3) 0.0103(7) Uani 1 1 d . . .
O1 O 0.2409(3) 0.3953(4) -0.1076(3) 0.0098(7) Uani 1 1 d . . .
O7 O 0.0694(3) -0.0128(4) 0.2391(3) 0.0099(7) Uani 1 1 d . . .
O2 O 0.5591(3) 0.0123(4) 0.1887(3) 0.0105(7) Uani 1 1 d . . .
O3 O 0.8209(3) 0.0979(4) 0.1694(3) 0.0091(7) Uani 1 1 d . . .
O10 O 0.3598(3) 0.1775(4) 0.2750(3) 0.0080(6) Uani 1 1 d . . .
O4 O 0.6462(3) 0.3221(4) 0.2182(3) 0.0089(6) Uani 1 1 d . . .
Be1 Be 0.2289(6) 0.2626(7) -0.0055(5) 0.0105(12) Uani 1 1 d . . .

loop_
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 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
N2 0.0097(19) 0.012(2) 0.0082(19) 0.0004(17) 0.0007(16) 0.0009(17)
N1 0.0092(19) 0.012(2) 0.015(2) -0.0001(18) 0.0025(17) -0.0005(17)
Be2 0.013(3) 0.002(3) 0.009(3) 0.000(2) -0.004(2) 0.001(2)
Be3 0.009(3) 0.010(3) 0.011(3) 0.000(2) 0.003(2) -0.001(2)
As1 0.0064(2) 0.0058(2) 0.0058(2) -0.00026(17) 0.00103(16) 0.00046(17)
As2 0.0058(2) 0.0065(2) 0.0063(2) -0.00049(18) 0.00118(16) -0.00064(17)
O8 0.0110(15) 0.0070(17) 0.0062(15) 0.0002(14) 0.0010(12) -0.0023(12)
O9 0.0109(16) 0.0110(18) 0.0066(16) -0.0023(15) 0.0029(13) 0.0006(13)
O6 0.0100(15) 0.0112(17) 0.0055(14) -0.0013(13) -0.0011(12) 0.0014(13)
O5 0.0128(15) 0.0126(17) 0.0063(15) -0.0009(13) 0.0042(12) -0.0018(13)
O1 0.0135(15) 0.0087(17) 0.0071(15) 0.0021(13) 0.0015(12) -0.0004(13)
O7 0.0067(14) 0.0088(17) 0.0137(16) -0.0018(13) 0.0009(12) 0.0010(12)
O2 0.0078(15) 0.0061(16) 0.0171(17) -0.0005(13) 0.0010(13) 0.0009(12)
O3 0.0100(15) 0.0090(17) 0.0101(15) -0.0007(13) 0.0064(12) 0.0019(12)
O10 0.0090(14) 0.0063(16) 0.0088(15) -0.0013(12) 0.0018(12) -0.0015(12)
O4 0.0082(14) 0.0068(16) 0.0108(15) 0.0008(13) -0.0006(12) 0.0003(12)
Be1 0.014(3) 0.008(3) 0.009(3) 0.000(2) 0.000(2) 0.003(2)

_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
;

loop_
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 _geom_bond_site_symmetry_2
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 _geom_bond_publ_flag
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Be2 O10 1.652(7) . ?
Be2 O9 1.650(7) . ?
Be2 O5 1.667(7) . ?
Be3 O4 1.621(7) 4_565 ?
Be3 O8 1.631(7) . ?
Be3 O7 1.642(6) 3 ?
Be3 O3 1.647(7) 3_655 ?
As1 O3 1.675(3) . ?
As1 O4 1.678(3) . ?
As1 O2 1.687(3) . ?
As1 O1 1.687(3) 4_666 ?
As2 O6 1.677(3) 2_545 ?
As2 O7 1.678(3) . ?
As2 O5 1.684(3) . ?
As2 O10 1.687(3) 2_545 ?
O8 Be1 1.615(7) . ?
O9 Be1 1.627(7) . ?
O6 Be1 1.629(7) . ?
O6 As2 1.677(3) 2 ?
O1 Be1 1.628(7) . ?
O1 As1 1.687(3) 4_565 ?
O7 Be3 1.642(6) 3 ?
O3 Be3 1.647(7) 3_655 ?
O10 As2 1.687(3) 2 ?
O4 Be3 1.621(7) 4_666 ?

loop_
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 _geom_angle_atom_site_label_3
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 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
O2 Be2 O10 112.9(4) . . ?
O2 Be2 O9 108.0(4) . . ?
O10 Be2 O9 110.6(4) . . ?
O2 Be2 O5 108.7(4) . . ?
O10 Be2 O5 109.3(4) . . ?
O9 Be2 O5 107.1(3) . . ?
O4 Be3 O8 111.8(4) 4_565 . ?
O4 Be3 O7 110.1(4) 4_565 3 ?
O8 Be3 O7 111.8(4) . 3 ?
O4 Be3 O3 109.4(4) 4_565 3_655 ?
O8 Be3 O3 107.5(4) . 3_655 ?
O7 Be3 O3 106.0(4) 3 3_655 ?
O3 As1 O4 107.49(16) . . ?
O3 As1 O2 109.28(15) . . ?
O4 As1 O2 112.18(15) . . ?
O3 As1 O1 109.22(15) . 4_666 ?
O4 As1 O1 108.89(16) . 4_666 ?
O2 As1 O1 109.71(16) . 4_666 ?
O6 As2 O7 110.57(16) 2_545 . ?
O6 As2 O5 108.36(15) 2_545 . ?
O7 As2 O5 108.75(16) . . ?
```

```
O6 As2 O10 109.13(16) 2_545 2_545 ?
O7 As2 O10 109.96(15) . 2_545 ?
O5 As2 O10 110.03(15) . 2_545 ?
Be1 O8 Be3 119.4(4) . . ?
Be1 O9 Be2 120.7(4) . . ?
Be1 O6 As2 124.4(3) . 2 ?
Be2 O5 As2 122.2(3) . . ?
Be1 O1 As1 123.2(3) . 4_565 ?
Be3 O7 As2 122.2(3) 3 . ?
Be2 O2 As1 122.9(3) . . ?
Be3 O3 As1 123.7(3) 3_655 . ?
Be2 O10 As2 121.6(3) . 2 ?
Be3 O4 As1 125.5(3) 4_666 . ?
O8 Be1 O6 112.5(4) . . ?
O8 Be1 O1 111.0(4) . . ?
O6 Be1 O1 101.4(4) . . ?
O8 Be1 O9 109.3(4) . . ?
O6 Be1 O9 109.2(4) . . ?
O1 Be1 O9 113.3(4) . . ?

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_diffrn_measured_fraction_theta_full   0.993
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_refine_diff_density_rms    0.161
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BAF1152

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data_BAF1152

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;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety
'2(As4 Be4 H2 O17), 0.72(C2), 5(N), 3.62(C0.50), 0.84(C)'
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 'C4.90 H4 As8 Be8 N5 O34'
_chemical_formula_weight          1348.37

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 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
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 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'As'  'As'   0.0499   2.0058
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    C2/c

loop_
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 '-x, y, -z+1/2'
 'x+1/2, y+1/2, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y, z-1/2'
 '-x+1/2, -y+1/2, -z'
 'x+1/2, -y+1/2, z-1/2'

_cell_length_a                    12.9639(6)
_cell_length_b                    14.0423(6)
_cell_length_c                    18.6966(9)
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.160(4)
_cell_angle_gamma                 90.00
_cell_volume                      3403.6(3)
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_cell_formula_units_Z            4
_cell_measurement_temperature    120(2)
_cell_measurement_reflns_used    ?
_cell_measurement_theta_min      ?
_cell_measurement_theta_max      ?

_exptl_crystal_description       Plate
_exptl_crystal_colour            Colourless
_exptl_crystal_size_max          0.01
_exptl_crystal_size_mid          0.01
_exptl_crystal_size_min          0.01
_exptl_crystal_density_meas      ?
_exptl_crystal_density_diffrn    2.642
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_exptl_crystal_F_000             2564
_exptl_absorpt_coefficient_mu    7.881
_exptl_absorpt_correction_type   none
_exptl_absorpt_correction_T_min  ?
_exptl_absorpt_correction_T_max  ?
_exptl_absorpt_process_details   ?

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature      120(2)
_diffrn_radiation_wavelength     0.71073
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_diffrn_measurement_device_type  'Bruker-Nonius APEX II CCD camera'
_diffrn_measurement_method       '\f & \w scans'
_diffrn_detector_area_resol_mean '4096x4096pixels / 62x62mm'
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_diffrn_reflns_av_sigmaI/netI    0.0560
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_computing_data_collection       'COLLECT (Hooft, R.W.W., 1998)'
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_computing_publication_material   ?

_refine_special_details
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Refinement attempted in Cmca but has proven to be unconclusive
High degree of disorder of templating organic materal
;

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_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
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_atom_sites_solution_secondary    difmap
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C1 C 0.2565(11) 0.1320(10) 0.2164(8) 0.053(5) Uiso 0.81(4) 1 d P . .
N3 N 0.5000 0.8937(7) 0.7500 0.029(2) Uani 1 2 d S . .
N4 N 0.7500 0.7500 0.5000 0.025(2) Uani 1 2 d S . .
N2 N 0.0000 0.1024(7) 0.2500 0.035(3) Uani 1 2 d S . .
N1 N 0.7564(5) 0.5069(4) 0.1025(3) 0.0189(13) Uani 1 1 d . . .
C4 C 0.2488(9) 0.2522(9) 0.0394(6) 0.032(4) Uiso 0.72(3) 1 d P . .
C2 C 0.3062(14) 0.1878(13) 0.1090(10) 0.037(6) Uiso 0.50(4) 1 d P . .
C6 C 0.203(3) 0.187(3) 0.110(2) 0.043(15) Uiso 0.23(4) 1 d P . .
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C7 C 0.118(3) 0.125(3) 0.154(2) 0.025(13) Uiso 0.19(3) 1 d P . .
H1 H 0.382(5) 0.190(4) 0.378(3) 0.007(17) Uiso 1 1 d D . .
H2 H -0.113(5) 0.186(4) 0.129(3) 0.010(18) Uiso 1 1 d D . .
As1 As 0.00178(5) 0.35983(4) 0.00905(3) 0.00795(17) Uani 1 1 d . . .
As2 As 0.13545(5) 0.38092(4) 0.20225(3) 0.00860(17) Uani 1 1 d . . .
As3 As 0.36538(5) 0.51121(4) 0.07496(3) 0.00791(17) Uani 1 1 d . . .
As4 As 0.43302(5) 0.33203(4) 0.34456(3) 0.00908(17) Uani 1 1 d . . .
O1 O 0.3767(3) 0.4051(3) 0.2869(2) 0.0133(9) Uani 1 1 d . . .
O2 O 0.4440(3) 0.6076(3) 0.0655(2) 0.0090(8) Uani 1 1 d . . .
O3 O -0.0864(3) 0.3676(3) 0.0745(2) 0.0127(9) Uani 1 1 d . . .
O4 O 0.2471(3) 0.5535(3) 0.0587(2) 0.0113(9) Uani 1 1 d . . .
O5 O 0.4218(4) 0.3790(3) 0.4266(2) 0.0147(10) Uani 1 1 d . . .
O6 O 0.1070(3) 0.4258(3) 0.0233(2) 0.0124(9) Uani 1 1 d . . .
O7 O 0.3910(3) 0.4238(3) 0.0172(2) 0.0127(9) Uani 1 1 d . . .
O8 O 0.3815(3) 0.4799(3) 0.1609(2) 0.0127(9) Uani 1 1 d . . .
O9 O 0.3588(3) 0.2293(3) 0.3457(3) 0.0137(9) Uani 1 1 d D . .
O10 O 0.0494(3) 0.3013(3) 0.1716(2) 0.0123(9) Uani 1 1 d . . .
O11 O 0.2509(3) 0.3324(3) 0.1853(2) 0.0113(9) Uani 1 1 d . . .
O12 O 0.1199(3) 0.4026(3) 0.2894(2) 0.0120(9) Uani 1 1 d . . .
O13 O -0.1332(3) 0.2250(3) 0.1602(3) 0.0145(9) Uani 1 1 d D . .
O14 O 0.5416(4) 0.7482(3) -0.0021(2) 0.0159(9) Uani 1 1 d . . .
O15 O 0.0551(3) 0.6058(3) 0.0679(2) 0.0106(9) Uani 1 1 d . . .
O16 O 0.1216(3) 0.4874(3) 0.1625(2) 0.0118(9) Uani 1 1 d . . .
O19 O 0.4466(3) 0.2986(3) 0.1766(2) 0.0124(9) Uani 1 1 d . . .
Be2 Be 0.1325(6) 0.5129(6) 0.0772(5) 0.0105(15) Uiso 1 1 d . . .
Be4 Be 0.5048(6) 0.6374(6) -0.0082(5) 0.0137(17) Uiso 1 1 d . . .

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N2 0.031(5) 0.030(5) 0.044(6) 0.000 -0.026(5) 0.000
N1 0.022(3) 0.022(3) 0.013(3) 0.001(2) 0.003(2) 0.001(2)
As1 0.0080(3) 0.0096(3) 0.0062(3) -0.0005(2) 0.0016(2) -0.0004(2)
As2 0.0081(3) 0.0119(3) 0.0058(3) 0.0003(2) 0.0014(2) -0.0004(2)
As3 0.0082(3) 0.0092(3) 0.0063(3) 0.0006(2) 0.0014(2) -0.0003(2)
As4 0.0093(3) 0.0121(3) 0.0059(3) 0.0006(2) 0.0013(2) -0.0008(2)
O1 0.017(2) 0.014(2) 0.009(2) 0.0043(17) -0.0014(18) 0.0040(18)
O2 0.0040(19) 0.014(2) 0.009(2) 0.0007(17) 0.0018(16) -0.0039(16)
O3 0.010(2) 0.021(2) 0.008(2) 0.0027(17) 0.0031(17) 0.0015(17)
O4 0.010(2) 0.014(2) 0.010(2) -0.0005(17) 0.0032(17) -0.0014(17)
O5 0.012(2) 0.024(2) 0.008(2) -0.0020(18) 0.0015(18) 0.0025(18)
O6 0.011(2) 0.013(2) 0.014(2) -0.0054(17) 0.0038(17) -0.0007(17)
O7 0.017(2) 0.010(2) 0.011(2) -0.0041(17) 0.0041(17) 0.0000(17)
O8 0.017(2) 0.015(2) 0.007(2) 0.0019(17) 0.0016(18) -0.0068(18)
O9 0.007(2) 0.013(2) 0.020(2) 0.0067(19) -0.0041(18) 0.0000(17)
O10 0.010(2) 0.016(2) 0.011(2) -0.0022(17) 0.0000(17) -0.0012(17)
O11 0.008(2) 0.014(2) 0.012(2) 0.0002(17) 0.0012(17) 0.0033(16)
O12 0.016(2) 0.013(2) 0.007(2) 0.0016(17) 0.0022(17) -0.0019(17)
O13 0.013(2) 0.015(2) 0.016(2) -0.0054(18) 0.0057(18) 0.0014(18)
O14 0.018(2) 0.015(2) 0.014(2) 0.0017(18) 0.0057(18) 0.0008(18)
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O15 0.012(2) 0.012(2) 0.007(2) 0.0001(16) -0.0010(17) 0.0053(17)
O16 0.012(2) 0.014(2) 0.009(2) 0.0011(17) 0.0036(17) 0.0023(17)
O19 0.013(2) 0.014(2) 0.010(2) -0.0007(17) -0.0005(17) -0.0033(17)

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;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
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Be3 O8 1.623(9) . ?
Be3 O1 1.650(9) . ?
Be3 O19 1.656(9) . ?
Be1 O12 1.593(9) 2 ?
Be1 O3 1.617(9) . ?
Be1 O10 1.622(9) . ?
Be1 O13 1.689(9) . ?
C4 C4 1.47(2) 7 ?
C4 C6 1.72(5) . ?
C4 C2 1.75(2) . ?
C2 C6 1.34(5) . ?
C6 C7 1.61(6) . ?
As1 O14 1.663(5) 3_445 ?
As1 O6 1.670(4) . ?
As1 O3 1.682(4) . ?
As1 O15 1.686(4) 5_565 ?
As2 O12 1.670(4) . ?
As2 O11 1.676(4) . ?
As2 O16 1.679(4) . ?
As2 O10 1.679(4) . ?
As3 O7 1.669(4) . ?
As3 O4 1.672(4) . ?
As3 O8 1.678(4) . ?
As3 O2 1.704(4) . ?
As4 O1 1.657(4) . ?
As4 O5 1.677(5) . ?
As4 O19 1.677(4) 2_655 ?
As4 O9 1.734(4) . ?
O2 Be4 1.644(10) . ?
O4 Be2 1.630(9) . ?
O5 Be4 1.640(9) 6_566 ?
O6 Be2 1.618(9) . ?
O7 Be4 1.610(9) 5_665 ?
O12 Be1 1.593(9) 2 ?
O14 Be4 1.631(9) . ?
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O14 As1 1.663(5) 3 ?
O15 Be2 1.654(9) . ?
O15 As1 1.686(4) 5_565 ?
O16 Be2 1.640(9) . ?
O19 As4 1.677(4) 2_655 ?
Be4 O7 1.610(9) 5_665 ?
Be4 O5 1.640(9) 6_565 ?

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O11 Be3 O1 112.3(5) . . ?
O8 Be3 O1 104.1(5) . . ?
O11 Be3 O19 105.2(5) . . ?
O8 Be3 O19 110.8(5) . . ?
O1 Be3 O19 109.9(5) . . ?
O12 Be1 O3 109.9(5) 2 . ?
O12 Be1 O10 115.3(6) 2 . ?
O3 Be1 O10 112.4(5) . . ?
O12 Be1 O13 108.9(5) 2 . ?
O3 Be1 O13 105.7(5) . . ?
O10 Be1 O13 103.9(5) . . ?
C4 C4 C6 139.3(19) 7 . ?
C4 C4 C2 135.4(14) 7 . ?
C6 C4 C2 45.4(16) . . ?
C6 C2 C4 66(2) . . ?
C2 C6 C7 134(4) . . ?
C2 C6 C4 68(2) . . ?
C7 C6 C4 155(3) . . ?
O14 As1 O6 106.8(2) 3_445 . ?
O14 As1 O3 111.4(2) 3_445 . ?
O6 As1 O3 113.9(2) . . ?
O14 As1 O15 107.3(2) 3_445 5_565 ?
O6 As1 O15 109.4(2) . 5_565 ?
O3 As1 O15 107.8(2) . 5_565 ?
O12 As2 O11 111.7(2) . . ?
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O11 As2 O16 111.8(2) . . ?
O12 As2 O10 111.8(2) . . ?
O11 As2 O10 104.9(2) . . ?
O16 As2 O10 111.9(2) . . ?
O7 As3 O4 109.1(2) . . ?
O7 As3 O8 113.7(2) . . ?
O4 As3 O8 112.3(2) . . ?
O7 As3 O2 113.4(2) . . ?
O4 As3 O2 104.3(2) . . ?
O8 As3 O2 103.5(2) . . ?
O1 As4 O5 108.2(2) . . ?
O1 As4 O19 115.4(2) . 2_655 ?
O5 As4 O19 114.1(2) . 2_655 ?
O1 As4 O9 106.3(2) . . ?
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O5 As4 O9 105.5(2) . . ?
O19 As4 O9 106.6(2) 2_655 . ?
Be3 O1 As4 123.3(4) . . ?
Be4 O2 As3 125.3(4) . . ?
Be1 O3 As1 124.7(4) . . ?
Be2 O4 As3 132.3(4) . . ?
Be4 O5 As4 124.5(4) 6_566 . ?
Be2 O6 As1 133.2(4) . . ?
Be4 O7 As3 129.0(4) 5_665 . ?
Be3 O8 As3 130.9(4) . . ?
Be1 O10 As2 122.0(4) . . ?
Be3 O11 As2 126.4(4) . . ?
Be1 O12 As2 124.4(4) 2 . ?
Be4 O14 As1 144.8(4) . 3 ?
Be2 O15 As1 125.4(4) . 5_565 ?
Be2 O16 As2 128.0(4) . . ?
Be3 O19 As4 119.9(4) . 2_655 ?
O6 Be2 O4 108.4(5) . . ?
O6 Be2 O16 115.0(5) . . ?
O4 Be2 O16 111.3(5) . . ?
O6 Be2 O15 114.1(5) . . ?
O4 Be2 O15 104.8(5) . . ?
O16 Be2 O15 102.8(5) . . ?
O7 Be4 O14 105.7(5) 5_665 . ?
O7 Be4 O5 113.3(6) 5_665 6_565 ?
O14 Be4 O5 112.1(5) . 6_565 ?
O7 Be4 O2 110.8(5) 5_665 . ?
O14 Be4 O2 109.0(5) . . ?
O5 Be4 O2 105.8(5) 6_565 . ?

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BAF2021

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 'As Be2 H5 O7'
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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Be'  'Be'   0.0005   0.0002
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 'N'  'N'   0.0061   0.0033
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 'O'  'O'   0.0106   0.0060
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 'As'  'As'   0.0499   2.0058
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    'P 21/n'

loop_
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 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

_cell_length_a                    6.4806(2)
_cell_length_b                    11.0971(4)
_cell_length_c                    8.4133(2)
_cell_angle_alpha                 90.00
_cell_angle_beta                  105.881(2)
_cell_angle_gamma                 90.00
_cell_volume                      581.96(3)
_cell_formula_units_Z             4
_cell_measurement_temperature     120(2)
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_exptl_special_details
;
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;

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_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
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goniostat'
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_computing_cell_refinement        'DENZO (Otwinowski & Minor, 1997) &
COLLECT (Hooft, R.W.W., 1998)'
_computing_data_reduction         'DENZO (Otwinowski & Minor, 1997) &
COLLECT (Hooft, R.W.W., 1998)'
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_computing_publication_material   ?

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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 'calc w=1/[\s^2^(Fo^2^)+(0.0231P)^2^+2.1223P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
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_refine_ls_wR_factor_gt           0.0486
_refine_ls_goodness_of_fit_ref    0.835
_refine_ls_restrained_S_all       0.835
_refine_ls_shift/su_max           0.031
_refine_ls_shift/su_mean          0.005

loop_
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 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
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 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
O7 O 0.5780(3) 0.90359(17) 0.6656(2) 0.0108(3) Uani 1 1 d . . .
O6 O 0.7668(3) 0.60025(16) 0.5330(2) 0.0108(3) Uani 1 1 d . . .
O5 O 0.9501(3) 0.80366(15) 0.6726(2) 0.0090(3) Uani 1 1 d . . .
Be1 Be 0.9723(5) 0.6962(3) 0.5524(3) 0.0084(5) Uani 1 1 d . . .
Be2 Be 0.8085(4) 0.9236(3) 0.6250(4) 0.0085(5) Uani 1 1 d . . .
```

```
H2 H 0.479(5) 0.952(3) 0.638(4) 0.021(8) Uiso 1 1 d . . .
H1 H 0.555(5) 0.857(3) 0.727(4) 0.023(9) Uiso 1 1 d . . .
H3 H 1.025(6) 0.812(3) 0.749(5) 0.027(10) Uiso 1 1 d . . .
H4 H 0.720(6) 0.591(3) 0.605(5) 0.026(9) Uiso 1 1 d . . .
H5 H 0.781(6) 0.530(4) 0.493(5) 0.041(11) Uiso 1 1 d . . .
As1 As 1.12926(3) 1.116449(19) 0.70462(3) 0.00570(9) Uani 1 1 d . . .
O3 O 1.1926(3) 0.61910(13) 0.60813(19) 0.0082(3) Uani 1 1 d . . .
O2 O 0.9418(3) 0.74315(14) 0.36251(19) 0.0093(3) Uani 1 1 d . . .
O1 O 0.9171(2) 1.04075(14) 0.73050(19) 0.0089(3) Uani 1 1 d . . .
O4 O 0.7586(2) 0.95244(14) 0.42872(19) 0.0089(3) Uani 1 1 d . . .

loop_
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 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
O7 0.0075(8) 0.0115(8) 0.0145(8) 0.0067(7) 0.0049(7) 0.0023(7)
O6 0.0119(8) 0.0112(8) 0.0114(8) -0.0017(6) 0.0069(7) -0.0025(6)
O5 0.0101(8) 0.0099(8) 0.0049(7) -0.0014(6) -0.0012(6) 0.0002(6)
Be1 0.0084(13) 0.0081(13) 0.0081(13) -0.0005(10) 0.0013(10) -0.0013(10)
Be2 0.0062(13) 0.0098(13) 0.0094(13) 0.0013(10) 0.0018(10) 0.0007(10)
As1 0.00594(13) 0.00559(13) 0.00539(13) 0.00019(7) 0.00125(9) -0.00018(7)
O3 0.0081(7) 0.0090(8) 0.0059(7) -0.0020(5) -0.0007(6) 0.0017(6)
O2 0.0149(8) 0.0053(7) 0.0076(7) 0.0012(6) 0.0032(6) 0.0018(6)
O1 0.0067(7) 0.0106(8) 0.0094(7) -0.0014(6) 0.0023(6) -0.0027(6)
O4 0.0084(7) 0.0109(8) 0.0076(7) 0.0006(6) 0.0026(6) 0.0025(6)

_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
;

loop_
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 _geom_bond_atom_site_label_2
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 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
O7 Be2 1.636(3) . ?
O6 Be1 1.678(3) . ?
O5 Be1 1.595(3) . ?
O5 Be2 1.604(3) . ?
Be1 O3 1.620(3) . ?
Be1 O2 1.640(3) . ?
Be2 O1 1.622(3) . ?
Be2 O4 1.625(3) . ?
As1 O1 1.6754(15) . ?
As1 O2 1.6781(15) 3_776 ?
```

```
As1 O3 1.6794(16) 2_756 ?
As1 O4 1.6784(15) 3_776 ?
O3 As1 1.6794(15) 2_746 ?
O2 As1 1.6781(15) 3_776 ?
O4 As1 1.6784(15) 3_776 ?

loop_
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 _geom_angle_atom_site_label_3
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 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
Be1 O5 Be2 127.32(18) . . ?
O5 Be1 O3 115.87(19) . . ?
O5 Be1 O2 111.89(19) . . ?
O3 Be1 O2 108.14(18) . . ?
O5 Be1 O6 109.22(18) . . ?
O3 Be1 O6 107.80(18) . . ?
O2 Be1 O6 103.08(17) . . ?
O5 Be2 O1 113.30(19) . . ?
O5 Be2 O4 111.00(19) . . ?
O1 Be2 O4 109.52(19) . . ?
O5 Be2 O7 109.13(19) . . ?
O1 Be2 O7 106.19(18) . . ?
O4 Be2 O7 107.44(18) . . ?
O1 As1 O2 110.48(8) . 3_776 ?
O1 As1 O3 105.36(8) . 2_756 ?
O2 As1 O3 110.75(8) 3_776 2_756 ?
O1 As1 O4 112.29(8) . 3_776 ?
O2 As1 O4 109.09(8) 3_776 3_776 ?
O3 As1 O4 108.83(8) 2_756 3_776 ?
Be1 O3 As1 127.30(14) . 2_746 ?
Be1 O2 As1 124.85(14) . 3_776 ?
Be2 O1 As1 125.41(14) . . ?
Be2 O4 As1 125.97(14) . 3_776 ?

_diffrn_measured_fraction_theta_max    0.999
_diffrn_reflns_theta_full              27.48
_diffrn_measured_fraction_theta_full   0.999
_refine_diff_density_max    0.362
_refine_diff_density_min   -0.463
_refine_diff_density_rms    0.095
```

Section 3. BAF1125 Output from "TOTOPOL", version 1.68, 20 May 2010). Written by Mike Treacy, with input from Srinivasen Srivilliputhur, Martin Foster, Keith Randall.

Report for the framework in file "temp.cif"

There are 20 T-atoms per unit cell
There are 37 O-atoms per unit cell

Framework density = 21.44 T-atoms per nm^3
Material density = 2.313 grams per cm^3 (excluding extra-framework material)

Cell volume = 932.9 Angstrom^3
Available Volume = 527.8 +/- 1.5 Angstrom^3
Occupiable Volume = 31.8 +/- 0.5 Angstrom^3
Available Area = 719.3 +/- 1.5 Angstrom^2
Occupiable Area = 162.3 +/- 2.4 Angstrom^2

---------- T-O Analysis ----------

[As] Ideal TO distance = 1.671 Angstroms
T1 -- O2 = 1.6878 Angstrom
T1 -- O11 = 1.6751 Angstrom
T1 -- O13 = 1.6779 Angstrom
T1 -- O16 = 1.6866 Angstrom
mean = 1.6818 Angstrom
t1 = 0.011486
t2 = 0.006330

[As] Ideal TO distance = 1.671 Angstroms
T2 -- O6 = 1.6878 Angstrom
T2 -- O9 = 1.6779 Angstrom
T2 -- O12 = 1.6866 Angstrom
T2 -- O15 = 1.6751 Angstrom
mean = 1.6818 Angstrom
t1 = 0.011486
t2 = 0.006680

[As] Ideal TO distance = 1.671 Angstroms
T3 -- O3 = 1.6751 Angstrom
T3 -- O5 = 1.6779 Angstrom
T3 -- O8 = 1.6866 Angstrom
T3 -- O10 = 1.6878 Angstrom
mean = 1.6818 Angstrom
t1 = 0.011486
t2 = 0.006098

[As] Ideal TO distance = 1.671 Angstroms
T4 -- O1 = 1.6779 Angstrom
T4 -- O4 = 1.6866 Angstrom
T4 -- O7 = 1.6751 Angstrom
T4 -- O14 = 1.6878 Angstrom
mean = 1.6818 Angstrom
t1 = 0.011486
t2 = 0.011211

[As] Ideal TO distance = 1.671 Angstroms
T5 -- O17 = 1.6769 Angstrom
T5 -- O18 = 1.6780 Angstrom
T5 -- O20 = 1.6870 Angstrom
T5 -- O23 = 1.6843 Angstrom
mean = 1.6816 Angstrom
t1 = 0.008147
t2 = 0.003455

[As] Ideal TO distance = 1.671 Angstroms
T6 -- O19 = 1.6843 Angstrom
T6 -- O21 = 1.6769 Angstrom
T6 -- O22 = 1.6780 Angstrom
T6 -- O24 = 1.6870 Angstrom
mean = 1.6816 Angstrom
t1 = 0.008147
t2 = 0.004537

[As] Ideal TO distance = 1.671 Angstroms
T7 -- O25 = 1.6769 Angstrom
T7 -- O26 = 1.6780 Angstrom
T7 -- O28 = 1.6870 Angstrom
T7 -- O31 = 1.6843 Angstrom
mean = 1.6816 Angstrom
t1 = 0.008147
t2 = 0.003455

[As] Ideal TO distance = 1.671 Angstroms
T8 -- O27 = 1.6843 Angstrom
T8 -- O29 = 1.6769 Angstrom
T8 -- O30 = 1.6780 Angstrom
T8 -- O32 = 1.6870 Angstrom
mean = 1.6816 Angstrom
t1 = 0.008146
t2 = 0.004537

[Be] Ideal TO distance = 1.634 Angstroms
T9 -- O2 = 1.6270 Angstrom
T9 -- O34 = 1.6154 Angstrom
T9 -- O17 = 1.6295 Angstrom
mean = 1.6240 Angstrom

[Be] Ideal TO distance = 1.634 Angstroms
T10 -- O6 = 1.6270 Angstrom
T10 -- O21 = 1.6295 Angstrom
T10 -- O35 = 1.6154 Angstrom
mean = 1.6240 Angstrom

[Be] Ideal TO distance = 1.634 Angstroms
T11 -- O10 = 1.6270 Angstrom
T11 -- O36 = 1.6154 Angstrom
T11 -- O25 = 1.6295 Angstrom
mean = 1.6240 Angstrom

[Be] Ideal TO distance = 1.634 Angstroms
T12 -- O14 = 1.6270 Angstrom
T12 -- O29 = 1.6295 Angstrom
T12 -- O33 = 1.6256 Angstrom
T12 -- O37 = 1.6154 Angstrom
mean = 1.6244 Angstrom
t1 = 0.024766
t2 = 0.022086

[Be] Ideal TO distance = 1.634 Angstroms
T13 -- O1 = 1.6209 Angstrom
T13 -- O3 = 1.6475 Angstrom
T13 -- O18 = 1.6408 Angstrom
T13 -- O37 = 1.6304 Angstrom
mean = 1.6349 Angstrom
t1 = 0.010226
t2 = 0.006590

[Be] Ideal TO distance = 1.634 Angstroms
T14 -- O5 = 1.6209 Angstrom
T14 -- O36 = 1.6304 Angstrom
T14 -- O7 = 1.6475 Angstrom
T14 -- O22 = 1.6408 Angstrom
mean = 1.6349 Angstrom
t1 = 0.010225
t2 = 0.006468

[Be] Ideal TO distance = 1.634 Angstroms

T15 -- O9 = 1.6209 Angstrom
T15 -- O11 = 1.6475 Angstrom
T15 -- O26 = 1.6408 Angstrom
T15 -- O35 = 1.6304 Angstrom
mean = 1.6349 Angstrom
t1 = 0.010226
t2 = 0.006590

[Be] Ideal TO distance = 1.634 Angstroms
T16 -- O13 = 1.6209 Angstrom
T16 -- O34 = 1.6304 Angstrom
T16 -- O30 = 1.6408 Angstrom
T16 -- O15 = 1.6475 Angstrom
mean = 1.6349 Angstrom
t1 = 0.010225
t2 = 0.006590

[Be] Ideal TO distance = 1.634 Angstroms
T17 -- O4 = 1.6338 Angstrom
T17 -- O20 = 1.6515 Angstrom
T17 -- O19 = 1.6662 Angstrom
mean = 1.6505 Angstrom

[Be] Ideal TO distance = 1.634 Angstroms
T18 -- O23 = 1.6662 Angstrom
T18 -- O24 = 1.6515 Angstrom
T18 -- O8 = 1.6338 Angstrom
mean = 1.6505 Angstrom

[Be] Ideal TO distance = 1.634 Angstroms
T19 -- O12 = 1.6338 Angstrom
T19 -- O28 = 1.6515 Angstrom
T19 -- O27 = 1.6662 Angstrom
mean = 1.6505 Angstrom

[Be] Ideal TO distance = 1.634 Angstroms
T20 -- O31 = 1.6662 Angstrom
T20 -- O32 = 1.6515 Angstrom
T20 -- O33 = 1.6499 Angstrom
T20 -- O16 = 1.6338 Angstrom
mean = 1.6503 Angstrom
t1 = 0.014317
t2 = 0.009278

T-O SUMMARY
Range = 1.6154 A <--> 1.6878 A

Mean = 1.6560 A
StdDev = 0.0253 A

---------- O-T-O Analysis ----------

O2 -- T1 -- O11 = 109.250 degrees ; O2 -- O11 = 2.7420 Angstrom
O2 -- T1 -- O13 = 108.846 degrees ; O2 -- O13 = 2.7374 Angstrom
O2 -- T1 -- O16 = 109.690 degrees ; O2 -- O16 = 2.7589 Angstrom
O11 -- T1 -- O13 = 107.557 degrees ; O11 -- O13 = 2.7050 Angstrom
O11 -- T1 -- O16 = 109.272 degrees ; O11 -- O16 = 2.7415 Angstrom
O13 -- T1 -- O16 = 112.167 degrees ; O13 -- O16 = 2.7921 Angstrom

O6 -- T2 -- O9 = 108.846 degrees ; O6 -- O9 = 2.7374 Angstrom
O6 -- T2 -- O12 = 109.690 degrees ; O6 -- O12 = 2.7589 Angstrom
O6 -- T2 -- O15 = 109.250 degrees ; O6 -- O15 = 2.7420 Angstrom
O9 -- T2 -- O12 = 112.167 degrees ; O9 -- O12 = 2.7921 Angstrom
O9 -- T2 -- O15 = 107.557 degrees ; O9 -- O15 = 2.7050 Angstrom
O12 -- T2 -- O15 = 109.272 degrees ; O12 -- O15 = 2.7415 Angstrom

O3 -- T3 -- O5 = 107.557 degrees ; O3 -- O5 = 2.7050 Angstrom
O3 -- T3 -- O8 = 109.272 degrees ; O3 -- O8 = 2.7415 Angstrom
O3 -- T3 -- O10 = 109.250 degrees ; O3 -- O10 = 2.7420 Angstrom
O5 -- T3 -- O8 = 112.167 degrees ; O5 -- O8 = 2.7921 Angstrom
O5 -- T3 -- O10 = 108.846 degrees ; O5 -- O10 = 2.7374 Angstrom
O8 -- T3 -- O10 = 109.690 degrees ; O8 -- O10 = 2.7589 Angstrom

O1 -- T4 -- O4 = 112.167 degrees ; O1 -- O4 = 2.7921 Angstrom
O1 -- T4 -- O7 = 107.557 degrees ; O1 -- O7 = 2.7050 Angstrom
O1 -- T4 -- O14 = 108.846 degrees ; O1 -- O14 = 2.7374 Angstrom
O4 -- T4 -- O7 = 109.272 degrees ; O4 -- O7 = 2.7415 Angstrom
O4 -- T4 -- O14 = 109.690 degrees ; O4 -- O14 = 2.7589 Angstrom
O7 -- T4 -- O14 = 109.250 degrees ; O7 -- O14 = 2.7420 Angstrom

O17 -- T5 -- O18 = 110.669 degrees ; O17 -- O18 = 2.7593 Angstrom
O17 -- T5 -- O20 = 109.133 degrees ; O17 -- O20 = 2.7409 Angstrom
O17 -- T5 -- O23 = 108.332 degrees ; O17 -- O23 = 2.7250 Angstrom
O18 -- T5 -- O20 = 109.939 degrees ; O18 -- O20 = 2.7555 Angstrom
O18 -- T5 -- O23 = 108.698 degrees ; O18 -- O23 = 2.7322 Angstrom
O20 -- T5 -- O23 = 110.050 degrees ; O20 -- O23 = 2.7625 Angstrom

O19 -- T6 -- O21 = 108.332 degrees ; O19 -- O21 = 2.7250 Angstrom
O19 -- T6 -- O22 = 108.698 degrees ; O19 -- O22 = 2.7322 Angstrom
O19 -- T6 -- O24 = 110.050 degrees ; O19 -- O24 = 2.7625 Angstrom
O21 -- T6 -- O22 = 110.669 degrees ; O21 -- O22 = 2.7593 Angstrom
O21 -- T6 -- O24 = 109.133 degrees ; O21 -- O24 = 2.7409 Angstrom

O22 -- T6 -- O24 = 109.939 degrees ; O22 -- O24 = 2.7555 Angstrom

O25 -- T7 -- O26 = 110.669 degrees ; O25 -- O26 = 2.7593 Angstrom
O25 -- T7 -- O28 = 109.133 degrees ; O25 -- O28 = 2.7409 Angstrom
O25 -- T7 -- O31 = 108.332 degrees ; O25 -- O31 = 2.7250 Angstrom
O26 -- T7 -- O28 = 109.939 degrees ; O26 -- O28 = 2.7555 Angstrom
O26 -- T7 -- O31 = 108.698 degrees ; O26 -- O31 = 2.7322 Angstrom
O28 -- T7 -- O31 = 110.050 degrees ; O28 -- O31 = 2.7625 Angstrom

O27 -- T8 -- O29 = 108.332 degrees ; O27 -- O29 = 2.7250 Angstrom
O27 -- T8 -- O30 = 108.698 degrees ; O27 -- O30 = 2.7322 Angstrom
O27 -- T8 -- O32 = 110.050 degrees ; O27 -- O32 = 2.7625 Angstrom
O29 -- T8 -- O30 = 110.669 degrees ; O29 -- O30 = 2.7593 Angstrom
O29 -- T8 -- O32 = 109.133 degrees ; O29 -- O32 = 2.7409 Angstrom
O30 -- T8 -- O32 = 109.939 degrees ; O30 -- O32 = 2.7555 Angstrom

O2 -- T9 -- O34 = 111.000 degrees ; O2 -- O34 = 2.6722 Angstrom
O2 -- T9 -- O17 = 101.401 degrees ; O2 -- O17 = 2.5200 Angstrom
O34 -- T9 -- O17 = 112.486 degrees ; O34 -- O17 = 2.6978 Angstrom

O6 -- T10 -- O21 = 101.401 degrees ; O6 -- O21 = 2.5200 Angstrom
O6 -- T10 -- O35 = 111.000 degrees ; O6 -- O35 = 2.6722 Angstrom
O21 -- T10 -- O35 = 112.486 degrees ; O21 -- O35 = 2.6978 Angstrom

O10 -- T11 -- O36 = 111.000 degrees ; O10 -- O36 = 2.6722 Angstrom
O10 -- T11 -- O25 = 101.401 degrees ; O10 -- O25 = 2.5200 Angstrom
O36 -- T11 -- O25 = 112.486 degrees ; O36 -- O25 = 2.6978 Angstrom

O14 -- T12 -- O29 = 101.401 degrees ; O14 -- O29 = 2.5200 Angstrom
O14 -- T12 -- O33 = 113.353 degrees ; O14 -- O33 = 2.7179 Angstrom
O14 -- T12 -- O37 = 111.000 degrees ; O14 -- O37 = 2.6722 Angstrom
O29 -- T12 -- O33 = 109.182 degrees ; O29 -- O33 = 2.6530 Angstrom
O29 -- T12 -- O37 = 112.486 degrees ; O29 -- O37 = 2.6978 Angstrom
O33 -- T12 -- O37 = 109.275 degrees ; O33 -- O37 = 2.6431 Angstrom

O1 -- T13 -- O3 = 109.427 degrees ; O1 -- O3 = 2.6679 Angstrom
O1 -- T13 -- O18 = 110.138 degrees ; O1 -- O18 = 2.6740 Angstrom
O1 -- T13 -- O37 = 111.759 degrees ; O1 -- O37 = 2.6916 Angstrom
O3 -- T13 -- O18 = 106.074 degrees ; O3 -- O18 = 2.6274 Angstrom
O3 -- T13 -- O37 = 107.473 degrees ; O3 -- O37 = 2.6430 Angstrom
O18 -- T13 -- O37 = 111.752 degrees ; O18 -- O37 = 2.7080 Angstrom

O5 -- T14 -- O36 = 111.759 degrees ; O5 -- O36 = 2.6916 Angstrom
O5 -- T14 -- O7 = 109.427 degrees ; O5 -- O7 = 2.6679 Angstrom
O5 -- T14 -- O22 = 110.138 degrees ; O5 -- O22 = 2.6740 Angstrom
O36 -- T14 -- O7 = 107.473 degrees ; O36 -- O7 = 2.6430 Angstrom

O36 -- T14 -- O22 = 111.752 degrees ; O36 -- O22 = 2.7080 Angstrom
O7 -- T14 -- O22 = 106.074 degrees ; O7 -- O22 = 2.6274 Angstrom

O9 -- T15 -- O11 = 109.427 degrees ; O9 -- O11 = 2.6679 Angstrom
O9 -- T15 -- O26 = 110.138 degrees ; O9 -- O26 = 2.6740 Angstrom
O9 -- T15 -- O35 = 111.759 degrees ; O9 -- O35 = 2.6916 Angstrom
O11 -- T15 -- O26 = 106.074 degrees ; O11 -- O26 = 2.6274 Angstrom
O11 -- T15 -- O35 = 107.473 degrees ; O11 -- O35 = 2.6430 Angstrom
O26 -- T15 -- O35 = 111.752 degrees ; O26 -- O35 = 2.7080 Angstrom

O13 -- T16 -- O34 = 111.759 degrees ; O13 -- O34 = 2.6916 Angstrom
O13 -- T16 -- O30 = 110.138 degrees ; O13 -- O30 = 2.6740 Angstrom
O13 -- T16 -- O15 = 109.427 degrees ; O13 -- O15 = 2.6679 Angstrom
O34 -- T16 -- O30 = 111.752 degrees ; O34 -- O30 = 2.7080 Angstrom
O34 -- T16 -- O15 = 107.473 degrees ; O34 -- O15 = 2.6430 Angstrom
O30 -- T16 -- O15 = 106.074 degrees ; O30 -- O15 = 2.6274 Angstrom

O4 -- T17 -- O20 = 112.909 degrees ; O4 -- O20 = 2.7381 Angstrom
O4 -- T17 -- O19 = 108.753 degrees ; O4 -- O19 = 2.6825 Angstrom
O20 -- T17 -- O19 = 109.308 degrees ; O20 -- O19 = 2.7061 Angstrom

O23 -- T18 -- O24 = 109.308 degrees ; O23 -- O24 = 2.7061 Angstrom
O23 -- T18 -- O8 = 108.753 degrees ; O23 -- O8 = 2.6825 Angstrom
O24 -- T18 -- O8 = 112.909 degrees ; O24 -- O8 = 2.7381 Angstrom

O12 -- T19 -- O28 = 112.909 degrees ; O12 -- O28 = 2.7381 Angstrom
O12 -- T19 -- O27 = 108.753 degrees ; O12 -- O27 = 2.6825 Angstrom
O28 -- T19 -- O27 = 109.308 degrees ; O28 -- O27 = 2.7061 Angstrom

O31 -- T20 -- O32 = 109.308 degrees ; O31 -- O32 = 2.7061 Angstrom
O31 -- T20 -- O33 = 107.044 degrees ; O31 -- O33 = 2.6664 Angstrom
O31 -- T20 -- O16 = 108.753 degrees ; O31 -- O16 = 2.6825 Angstrom
O32 -- T20 -- O33 = 110.607 degrees ; O32 -- O33 = 2.7143 Angstrom
O32 -- T20 -- O16 = 112.909 degrees ; O32 -- O16 = 2.7381 Angstrom
O33 -- T20 -- O16 = 108.033 degrees ; O33 -- O16 = 2.6571 Angstrom

O-T-O SUMMARY
Range = 101.4008 deg <--> 113.3528 deg
Mean = 109.4296 deg
StdDev = 2.3281 deg

O--O SUMMARY
Range = 2.5200 A <--> 2.7921 A
Mean = 2.7056 A
StdDev = 0.0554 A

---------- T-T-T Analysis ----------

---------- T-O-T Analysis ----------

T4 -- O1 -- T13 = 125.520 degrees ; T4 -- T13 = 2.9330 Angstrom

T1 -- O2 -- T9 = 123.192 degrees ; T1 -- T9 = 2.9159 Angstrom

T3 -- O3 -- T13 = 123.706 degrees ; T3 -- T13 = 2.9297 Angstrom

T4 -- O4 -- T17 = 122.956 degrees ; T4 -- T17 = 2.9175 Angstrom

T3 -- O5 -- T14 = 125.520 degrees ; T3 -- T14 = 2.9330 Angstrom

T2 -- O6 -- T10 = 123.192 degrees ; T2 -- T10 = 2.9159 Angstrom

T4 -- O7 -- T14 = 123.706 degrees ; T4 -- T14 = 2.9297 Angstrom

T3 -- O8 -- T18 = 122.956 degrees ; T3 -- T18 = 2.9175 Angstrom

T2 -- O9 -- T15 = 125.520 degrees ; T2 -- T15 = 2.9330 Angstrom

T3 -- O10 -- T11 = 123.192 degrees ; T3 -- T11 = 2.9159 Angstrom

T1 -- O11 -- T15 = 123.706 degrees ; T1 -- T15 = 2.9297 Angstrom

T2 -- O12 -- T19 = 122.956 degrees ; T2 -- T19 = 2.9175 Angstrom

T1 -- O13 -- T16 = 125.520 degrees ; T1 -- T16 = 2.9330 Angstrom

T4 -- O14 -- T12 = 123.192 degrees ; T4 -- T12 = 2.9159 Angstrom

T2 -- O15 -- T16 = 123.706 degrees ; T2 -- T16 = 2.9297 Angstrom

T1 -- O16 -- T20 = 122.956 degrees ; T1 -- T20 = 2.9175 Angstrom

T5 -- O17 -- T9 = 124.382 degrees ; T5 -- T9 = 2.9246 Angstrom

T5 -- O18 -- T13 = 122.204 degrees ; T5 -- T13 = 2.9056 Angstrom

T6 -- O19 -- T17 = 122.280 degrees ; T6 -- T17 = 2.9344 Angstrom

T5 -- O20 -- T17 = 121.576 degrees ; T5 -- T17 = 2.9140 Angstrom

T6 -- O21 -- T10 = 124.382 degrees ; T6 -- T10 = 2.9246 Angstrom

T6 -- O22 -- T14 = 122.204 degrees ; T6 -- T14 = 2.9056 Angstrom

T5 -- O23 -- T18 = 122.280 degrees ; T5 -- T18 = 2.9344 Angstrom

T6 -- O24 -- T18 = 121.576 degrees ; T6 -- T18 = 2.9140 Angstrom

T7 -- O25 -- T11 = 124.382 degrees ; T7 -- T11 = 2.9246 Angstrom

T7 -- O26 -- T15 = 122.204 degrees ; T7 -- T15 = 2.9056 Angstrom

T8 -- O27 -- T19 = 122.280 degrees ; T8 -- T19 = 2.9344 Angstrom

T7 -- O28 -- T19 = 121.576 degrees ; T7 -- T19 = 2.9140 Angstrom

T8 -- O29 -- T12 = 124.382 degrees ; T8 -- T12 = 2.9246 Angstrom

T8 -- O30 -- T16 = 122.204 degrees ; T8 -- T16 = 2.9056 Angstrom

T7 -- O31 -- T20 = 122.280 degrees ; T7 -- T20 = 2.9344 Angstrom

T8 -- O32 -- T20 = 121.576 degrees ; T8 -- T20 = 2.9140 Angstrom

T12 -- O33 -- T20 = 120.762 degrees ; T12 -- T20 = 2.8476 Angstrom

T9 -- O34 -- T16 = 119.475 degrees ; T9 -- T16 = 2.8036 Angstrom

T10 -- O35 -- T15 = 119.475 degrees ; T10 -- T15 = 2.8036 Angstrom

T11 -- O36 -- T14 = 119.475 degrees ; T11 -- T14 = 2.8036 Angstrom

T12 -- O37 -- T13 = 119.475 degrees ; T12 -- T13 = 2.8036 Angstrom

T-O-T SUMMARY
Range = 119.4748 deg <--> 125.5201 deg
Mean = 122.7547 deg
StdDev = 1.6700 deg

T--T SUMMARY
Range = 2.8036 A <--> 2.9344 A
Mean = 2.9070 A
StdDev = 0.0395 A

---------- Topological Analysis ----------

T1: multiplicity = 1
Coordination Sequence =
1 4 8 17 30 50 66 96 116 152 198 222 277 324 364 424 508
TD10 = 738
Circuit symbol = 3.8.4.8.5.8
Weight = 20
Vertex symbol = 3.8.4.8.8.8
Weight = 23

T2: multiplicity = 1
Coordination Sequence =
1 4 7 16 29 47 62 95 118 146 189 228 264 318 378 418 481
TD10 = 714
Circuit symbol = 3.8.4.8.5.8
Weight = 20
Vertex symbol = 3.8.4.8.8.8
Weight = 23

T3: multiplicity = 1
Coordination Sequence =
1 4 7 17 30 50 66 95 114 157 195 223 272 333 355 436 499
TD10 = 736
Circuit symbol = 3.8.4.8.5.8
Weight = 20
Vertex symbol = 3.8.4.8.8.8
Weight = 23

T4: multiplicity = 1
Coordination Sequence =
1 4 8 17 29 51 64 98 122 155 187 240 264 327 377 437 473
TD10 = 736
Circuit symbol = 3.8.4.8.5.8
Weight = 20
Vertex symbol = 3.8.4.8.8.8
Weight = 23

T5: multiplicity = 1
Coordination Sequence =
1 4 8 18 31 47 64 94 118 151 188 230 268 321 367 434 478
TD10 = 724
Circuit symbol = 4.8.8.8.8.10_{4}
Weight = 34
Vertex symbol = 4.8.8.8.8.10_{3}
Weight = 34

T6: multiplicity = 1
Coordination Sequence =
1 4 8 17 32 48 65 94 120 155 190 226 269 335 357 433 490
TD10 = 734
Circuit symbol = 4.8.8.8.8.9_{2}
Weight = 31
Vertex symbol = 4.8.8.8.8.9_{2}
Weight = 31

T7: multiplicity = 1
Coordination Sequence =
1 4 9 18 33 52 67 96 127 152 195 235 278 317 386 426 495
TD10 = 754
Circuit symbol = 4.8.8.8.8.10_{4}
Weight = 34
Vertex symbol = 4.8.8.8.8.10_{3}
Weight = 34

T8: multiplicity = 1
Coordination Sequence =
1 4 8 17 31 46 65 96 117 154 194 223 277 329 365 427 502
TD10 = 733
Circuit symbol = 3.8.4.8.5.8
Weight = 20
Vertex symbol = 3.8.4.8.8.8
Weight = 23

T9: multiplicity = 1
Coordination Sequence =
1 3 7 15 28 48 63 90 116 151 182 236 264 318 364 428 483
TD10 = 704
Circuit symbol = 3.8_{2}.9_{3}
Weight = 15
Vertex symbol = 3.8_{2}.10_{5}
Weight = 28

T10: multiplicity = 1
Coordination Sequence =
1 3 7 15 29 45 61 90 119 142 179 230 257 309 375 413 466
TD10 = 691
Circuit symbol = 3.8_{2}.9_{6}
Weight = 25
Vertex symbol = 3.8_{2}.9_{3}
Weight = 25

T11: multiplicity = 1
Coordination Sequence =
1 3 7 16 30 51 67 96 118 158 187 246 258 334 367 439 476
TD10 = 734
Circuit symbol = 3.8_{2}.9_{3}
Weight = 15
Vertex symbol = 3.8_{2}.10_{5}
Weight = 28

T12: multiplicity = 1
Coordination Sequence =
1 4 8 17 32 48 68 97 128 147 195 236 271 321 395 417 487
TD10 = 745
Circuit symbol = 3.3.8_{2}.9_{3}.9_{3}.9_{3}
Weight = 28
Vertex symbol = 3.3.8_{2}.9_{3}.*.*
Weight = 28

T13: multiplicity = 1
Coordination Sequence =
1 4 9 16 33 46 68 97 121 150 198 224 274 330 375 423 503
TD10 = 743
Circuit symbol = 3.8_{2}.4.9_{3}.5.8
Weight = 26
Vertex symbol = 3.8_{2}.4.9_{2}.8.9
Weight = 29

T14: multiplicity = 1
Coordination Sequence =
1 4 8 16 34 47 69 94 124 152 199 225 280 321 376 425 507
TD10 = 748
Circuit symbol = 3.8_{2}.4.9.5.8
Weight = 21
Vertex symbol = 3.8_{2}.4.10_{4}.8.10
Weight = 31

T15: multiplicity = 1
Coordination Sequence =
1 4 8 17 33 45 69 96 118 152 195 226 270 331 362 435 488
TD10 = 738
Circuit symbol = 3.8_{2}.4.9_{3}.5.8
Weight = 27
Vertex symbol = 3.8_{2}.4.9_{2}.8.9
Weight = 30

T16: multiplicity = 1

Coordination Sequence =
1 4 8 15 31 47 64 91 120 148 190 229 266 322 367 423 489
TD10 = 719
Circuit symbol = 3.8_{2}.4.9.5.8
Weight = 21
Vertex symbol = 3.8_{2}.4.10_{4}.8.10
Weight = 31

T17: multiplicity = 1
Coordination Sequence =
1 3 8 16 30 46 66 93 121 149 195 220 273 323 370 418 505
TD10 = 728
Circuit symbol = 4.8.8_{2}
Weight = 20
Vertex symbol = 4.8.8_{2}
Weight = 20

T18: multiplicity = 1
Coordination Sequence =
1 3 8 15 31 46 64 90 119 143 192 225 262 315 380 405 491
TD10 = 712
Circuit symbol = 4.8.8_{2}
Weight = 20
Vertex symbol = 4.8.8_{2}
Weight = 20

T19: multiplicity = 1
Coordination Sequence =
1 3 8 16 30 45 66 92 120 151 195 222 269 338 357 424 504
TD10 = 727
Circuit symbol = 4.8.8_{2}
Weight = 20
Vertex symbol = 4.8.8_{2}
Weight = 20

T20: multiplicity = 1
Coordination Sequence =
1 4 9 17 34 49 70 96 124 155 193 234 275 332 369 439 483
TD10 = 752
Circuit symbol = 3.8_{2}.4.9_{2}.5.8
Weight = 26
Vertex symbol = 3.8_{2}.4.9.8.9_{2}
Weight = 31

<TD10> = 730.500
Average ring size = 6.4219

Section 4. VT PXD and combined TGA/DTA data from BAF1125

Figure S4.1 Variable temperature (25- 450°C) powder X-ray diffraction data (Bruker D8 $Cu_{K\alpha 1}$) from BAF1125; material shows main crystal reflections until >350°C.

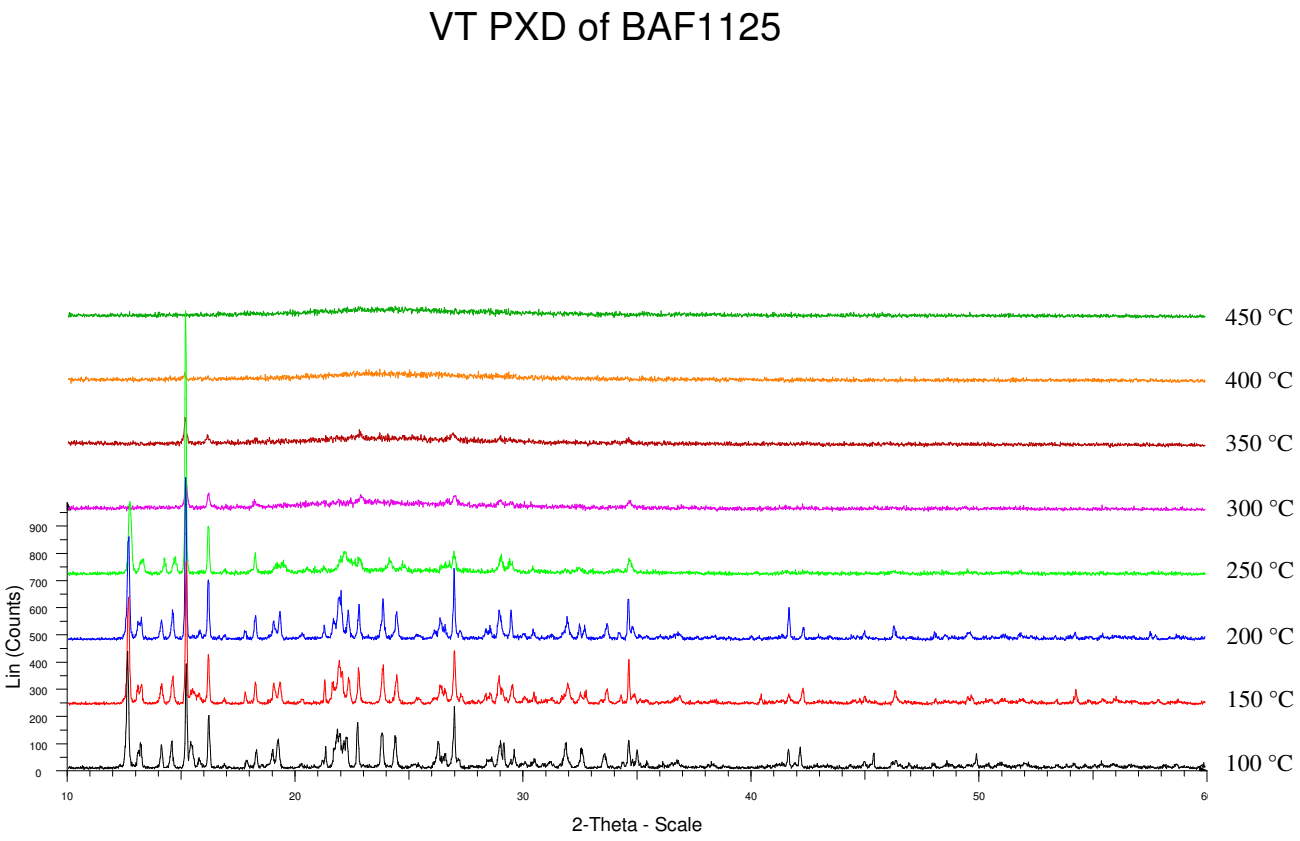
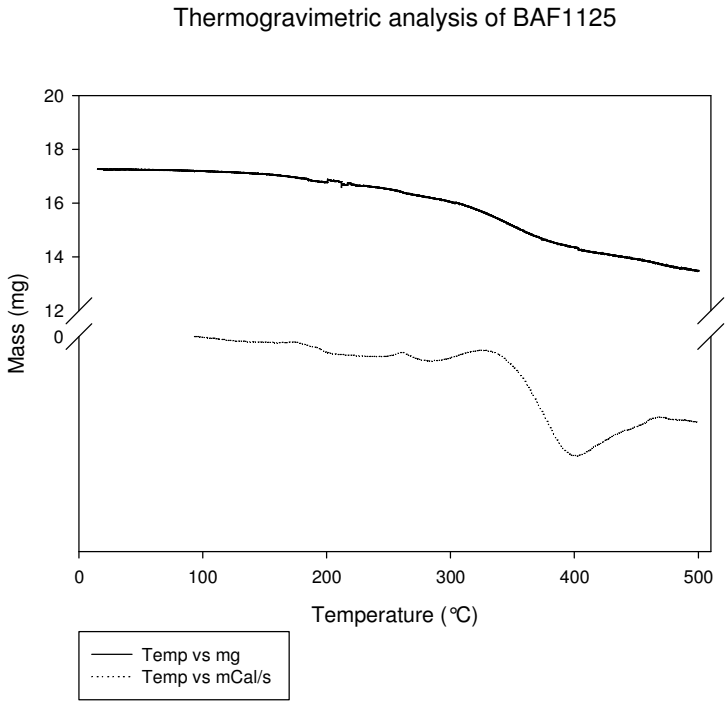
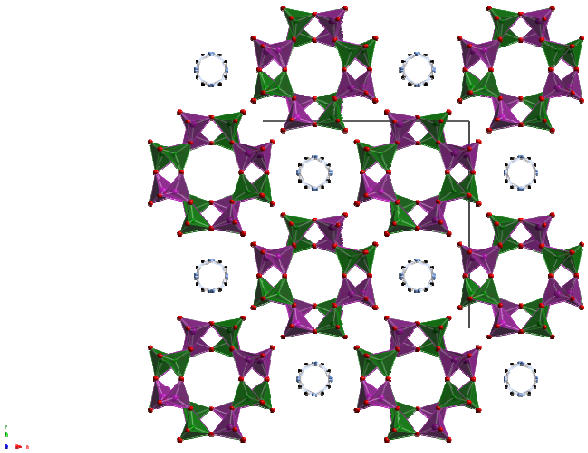


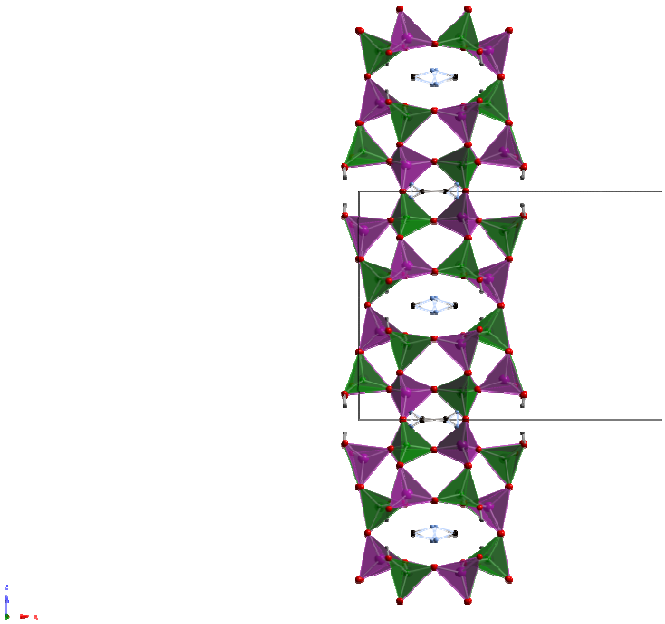
Figure S4.2. Combined TGA/DTA trace for BAF1125 (Stanton-Redcroft 1500 thermobalance) showing evolution of ammonia starting at 300°C .



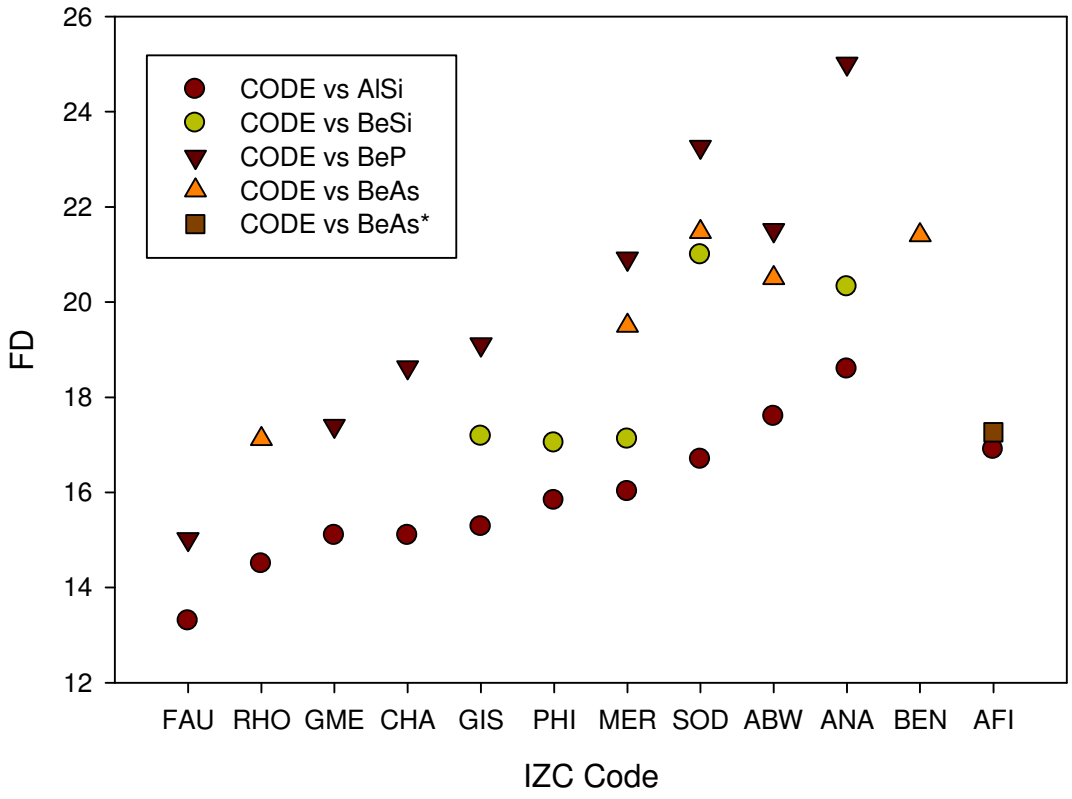
Section 5. The structure of BAF845.

Figure S5.1. The structure of BAF845 $[\{H\text{-pyridine}\}_{0.5}]^{0.5+}$ $[As_2(As_{0.25}Be_{0.75})_2O_7(OH)_2]^{0.5-}\bullet(H_2O)_{0.65}$ showing the linked $Be(O,OH)_4$ and $As(O,OH)_4$ tetrahedra in green and purple respectively; pyridine molecules are shown, carbon-black, nitrogen-pale blue, and hydrogen as small grey spheres. Upper diagram is viewed down c and lower diagram perpendicular to c





Section 6 Comparison of Framework Densities for different zeotype topologies based on T = (AlSi), T = (BeSi), T = (BeP) and T = (BeAs).



Framework densities (FD) of aluminosilicate zeolites as known as beryllium containing zeotype analogues; IZA code is plotted as a function of increasing FD for FAU to ANA. BEN represents the **BAF1125**, $[NH_4^+]_2[As_2Be_3O_8(OH)_2]^{2-}$ topology showing a value similar to other small pore zeotypes MER, SOD, ABW and ANA. The values of AFI-SiAl and the structurally related BAF1011and also shown for comparison.