data_ASU-19_rt

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_publ_author_name
'Plevert, Jacques'
'Gentz, Travis M.'
'Groy, Thomas L.'
'O'Keefe, Michael'
'Yaghi, Omar M.'

_publ_contact_author_name 'Jacques Plevert'
_publ_contact_author_address

;
Jacques Plevert
Department of Chemistry & Biochemistry
Physical Sciences D-121
Arizona State University
Tempe, AZ 85287-1604
USA
;

_publ_contact_author_email 'JPlevert@asu.edu'

_publ_section_title

Layered structures constructed from new linkages of Ge7(O,OH,F)19 clusters

_audit_creation_method SHELXL-97

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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^ > 2sigma(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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Ge8 Ge 0.83826(5) 0.26574(5) 0.04317(3) 0.02414(18) Uani 0.7908(13) 1 d P . .
F1A F 0.9946(2) 0.3837(2) 0.48561(14) 0.0300(7) Uani 1 1 d . . .
O1B O 0.6790(2) 0.1596(2) 0.23033(16) 0.0179(7) Uani 1 1 d . . .
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O1D O 0.9358(3) 0.1883(2) 0.44695(16) 0.0234(8) Uani 1 1 d . . .
O1E O 0.8926(2) 0.1250(2) 0.18630(15) 0.0177(7) Uani 1 1 d . . .
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O1O O 0.4953(2) 0.0731(2) 0.31513(18) 0.0251(8) Uani 1 1 d . . .
O1P O 0.6108(2) 0.2649(2) 0.36305(16) 0.0205(8) Uani 1 1 d . . .
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 O2C O 0.4381(2) 0.6548(2) 0.36220(16) 0.0220(8) Uani 1 1 d . . .
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 H3B1 H 0.8867 0.7997 0.2689 0.050 Uiso 0.586(5) 1 calc PR A -1
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 H3C2 H 0.9327 0.5659 0.2740 0.051 Uiso 0.586(5) 1 calc PR A -1
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 C3A' C 0.8898(6) 0.7255(6) 0.3682(4) 0.076(2) Uani 0.41 1 d PD A -2
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 H4A4 H 0.3969 0.4915 0.4507 0.058 Uiso 1 1 calc R . .
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 C4C C 0.2760(7) 0.2412(5) 0.4559(4) 0.079(3) Uani 1 1 d D . .
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 C4D C 0.2666(8) 0.1280(8) 0.4134(5) 0.132(4) Uani 0.633(7) 1 d PD B -3
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 H5AB H 0.4884 0.2764 0.1520 0.041 Uiso 1 1 calc R . . .
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 H5AD H 0.4779 0.3168 0.0244 0.043 Uiso 1 1 calc R . . .
 C5B C 0.5274(4) 0.4788(4) 0.0355(3) 0.0300(13) Uani 1 1 d . . .
 H5BA H 0.6095 0.4651 0.0287 0.036 Uiso 1 1 calc R . . .
 H5BB H 0.5232 0.5358 0.0734 0.036 Uiso 1 1 calc R . . .
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 H6AB H 0.7487 0.0264 0.1468 0.073 Uiso 1 1 calc R . . .
 C6A C 0.6097(6) 0.0352(5) 0.0748(4) 0.079(3) Uani 1 1 d . . .
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 O2W O 0.3274(4) 0.1957(4) 0.1614(3) 0.0710(15) Uani 1 1 d . . .
 O3W O 0.5239(6) 0.1460(7) 0.5047(3) 0.152(3) Uani 1 1 d . . .
 O4W O 0.1606(11) 0.1440(11) 0.0157(7) 0.135(5) Uani 0.50 1 d P . .
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 Ge5 0.0139(2) 0.0163(2) 0.0224(3) -0.0009(2) 0.0007(2) -0.00129(18)
 Ge6 0.0157(2) 0.0194(2) 0.0267(3) 0.0029(2) 0.0026(2) 0.00397(19)
 Ge7 0.0145(2) 0.0161(2) 0.0233(3) -0.0009(2) 0.0015(2) -0.00049(19)
 Ge8 0.0205(3) 0.0349(4) 0.0174(3) -0.0001(3) 0.0013(3) 0.0069(3)
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 O1G 0.0158(14) 0.0182(15) 0.0185(16) 0.0031(13) 0.0007(13) 0.0019(12)
 O1H 0.0197(15) 0.0185(15) 0.0233(17) 0.0011(14) 0.0024(14) 0.0040(13)
 O1I 0.0159(15) 0.0282(17) 0.0258(18) -0.0066(15) 0.0007(14) -0.0059(13)
 O1J 0.0244(16) 0.0189(16) 0.0276(18) 0.0014(14) 0.0073(14) 0.0063(13)
 O1K 0.0157(14) 0.0190(15) 0.0214(17) -0.0035(13) -0.0035(13) 0.0054(12)
 O1L 0.0184(15) 0.0221(16) 0.0330(19) 0.0075(15) 0.0009(14) 0.0000(13)
 O1M 0.0392(18) 0.0275(17) 0.0152(17) -0.0055(14) -0.0034(15) 0.0122(15)
 O1N 0.0177(15) 0.0194(16) 0.0312(18) -0.0021(14) 0.0082(14) -0.0070(13)
 O1O 0.0172(15) 0.0156(16) 0.042(2) -0.0083(15) 0.0005(15) -0.0016(13)
 O1P 0.0200(15) 0.0178(15) 0.0240(17) -0.0054(14) 0.0093(13) -0.0030(13)
 O1Q 0.0185(15) 0.0199(15) 0.0179(16) 0.0021(13) 0.0004(13) 0.0015(13)
 O1R 0.023(2) 0.127(5) 0.016(2) 0.008(3) 0.000(2) -0.022(3)
 O1S 0.133(5) 0.044(3) 0.022(3) -0.008(2) -0.008(3) 0.049(3)
 FlT 0.0496(18) 0.0429(18) 0.0452(19) 0.0116(15) 0.0051(16) 0.0068(15)
 GeA 0.0148(2) 0.0161(2) 0.0201(3) -0.0020(2) 0.0014(2) 0.00243(19)
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 GeG 0.0151(2) 0.0148(2) 0.0205(2) -0.0005(2) 0.0033(2) 0.00217(18)
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C3D 0.038(3) 0.062(4) 0.062(4) -0.011(3) 0.011(3) -0.012(3)
C3A' 0.066(4) 0.099(5) 0.061(4) -0.020(4) 0.023(4) -0.041(4)
C3D' 0.038(3) 0.062(4) 0.062(4) -0.011(3) 0.011(3) -0.012(3)
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C4D 0.141(8) 0.156(9) 0.101(7) -0.042(7) -0.001(6) 0.077(7)
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C4D' 0.141(8) 0.156(9) 0.101(7) -0.042(7) -0.001(6) 0.077(7)
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C6B 0.103(5) 0.049(4) 0.077(5) 0.012(4) -0.041(4) -0.023(4)
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O2W 0.056(3) 0.062(3) 0.099(3) 0.033(3) 0.029(3) 0.007(2)
O3W 0.132(5) 0.267(8) 0.051(4) -0.009(5) -0.015(4) -0.057(6)
O4W 0.139(9) 0.158(10) 0.111(9) -0.052(8) -0.006(8) 0.097(8)

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_geom_special_details

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

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loop_

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Ge2 O1F 1.763(3) . ?
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Ge3 O1D 1.770(3) . ?
Ge3 F1T 1.812(3) . ?
Ge3 O1G 2.141(3) . ?
Ge3 Ge6 2.9079(7) . ?

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 Ge5 O1F 1.754(3) . ?
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 Ge6 O1I 1.776(3) . ?
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 Ge6 O1G 1.963(3) . ?
 Ge7 O1B 1.709(3) . ?
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 Ge7 O1L 1.755(3) . ?
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data_ASU-20-DAPe

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    'Plevert, Jacques'
    'Gentz, Travis M.'
    'Groy, Thomas L.'
    'O'Keefe, Michael'
    'Yaghi, Omar M.'

  _publ_contact_author_name      'Jacques Plevert'
  _publ_contact_author_address
    ;
    Jacques Plevert
    Department of Chemistry & Biochemistry
    Physical Sciences D-121
    Arizona State University
    Tempe, AZ 85287-1604
    USA
    ;

  _publ_contact_author_email      'JPlevert@asu.edu'

  _publ_section_title
    ;
    Layered structures constructed from new linkages of Ge7(O,OH,F)19 clusters
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  _cell_length_b                  16.6125(4)
  _cell_length_c                  17.8898(6)
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  _cell_angle_beta                99.6837(18)
  _cell_angle_gamma               90.0
  _cell_volume                    4780.5(3)
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    -x+1/2,+y+1/2,-z+1/2 -x+1/2,-y+1/2,-z +x+1/2,-y+1/2,+z+1/2

loop_
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ge2  0.2380(4)  -0.0053(4)  0.1788(4)  1.0  Uiso  0.0176(10)  8
ge3  0.0889(4)  0.0735(5)  0.2279(5)  1.0  Uiso  0.0176(10)  8
ge4  0.2470(5)  0.3052(4)  0.2855(4)  1.0  Uiso  0.0176(10)  8
ge5  0.3974(4)  0.2237(4)  0.2344(4)  1.0  Uiso  0.0176(10)  8
ge6  0.2800(5)  0.1458(4)  0.0986(4)  1.0  Uiso  0.0176(10)  8
ge7  0.1381(5)  0.2284(4)  0.1473(4)  1.0  Uiso  0.0176(10)  8
o1   0.2280(21)  0.1678(17)  0.2027(18)  1.0  Uiso  0.015(4)  8
o2   0.2789(21)  0.0411(9)  0.1066(14)  1.0  Uiso  0.015(4)  8
o3   0.0685(13)  0.1555(13)  0.1668(15)  1.0  Uiso  0.015(4)  8
o4   0.1621(14)  0.3067(12)  0.2117(13)  1.0  Uiso  0.015(4)  8
o5   0.3749(13)  0.1918(17)  0.1401(10)  1.0  Uiso  0.015(4)  8
o6   0.1910(12)  0.2032(15)  0.0757(10)  1.0  Uiso  0.007(12)  8
o7   0.1323(10)  0.0079(15)  0.1719(14)  1.0  Uiso  0.015(4)  8
o8   0.3311(13)  0.3017(12)  0.2411(15)  1.0  Uiso  0.015(4)  8
o9   0.2568(19)  -0.1060(8)  0.1661(13)  1.0  Uiso  0.013(13)  8
o10  0.0         0.0347(18)  0.25       1.0  Uiso  0.008(18)  4
o11  0.5         0.2465(23)  0.25       1.0  Uiso  0.009(17)  4
o12  0.2922(16)  0.0189(12)  0.2679(11)  1.0  Uiso  0.015(4)  8
o13  0.1594(9)   0.0894(17)  0.3088(11)  1.0  Uiso  0.015(4)  8
o14  0.2446(17)  0.2216(9)   0.3441(11)  1.0  Uiso  0.012(12)  8
o15  0.3752(11)  0.1573(15)  0.3023(13)  1.0  Uiso  0.015(4)  8
f1   0.2920(15)  0.0815(14)  0.3974(10)  1.0  Uiso  0.035(6)  8
f2   0.3090(15)  0.1438(15)  0.0056(9)   1.0  Uiso  0.035(6)  8
f3   0.0606(13)  0.2833(14)  0.0890(12)  1.0  Uiso  0.035(6)  8

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n1a	0.0029(21)	0.5658(16)	0.0806(19)	1.0	Uiso	0.022(6)	8
c1a	0.0422(22)	0.4912(20)	0.1207(18)	1.0	Uiso	0.022(6)	8
c2a	0.0112(25)	0.4357(16)	0.1763(10)	1.0	Uiso	0.022(6)	8
c3a	0.0	0.4673(24)	0.25	1.0	Uiso	0.022(6)	4
n1b	0.6967(18)	0.4313(20)	0.3959(23)	1.0	Uiso	0.022(6)	8
n2b	0.3882(21)	0.2963(24)	0.5883(16)	1.0	Uiso	0.022(6)	8
c1b	0.6186(21)	0.4478(20)	0.4263(25)	1.0	Uiso	0.022(6)	8
c2b	0.5491(20)	0.3889(23)	0.4186(20)	1.0	Uiso	0.022(6)	8
c3b	0.4866(22)	0.3826(19)	0.4699(20)	1.0	Uiso	0.022(6)	8
c4b	0.4308(23)	0.3092(19)	0.4586(18)	1.0	Uiso	0.022(6)	8
c5b	0.3614(17)	0.3042(24)	0.5036(17)	1.0	Uiso	0.022(6)	8
Ow	0.1344(19)	0.3770(18)	0.4613(18)	1.0	Uiso	0.040(14)	8

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      O 120.0
      F 24.0
      N 24.0
      C 60.0

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_pd_meas_2theta_range_min     7.0
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ge1 o14 1.887(13) . ?
ge1 o15 1.860(13) . ?
ge1 f1 1.788(13) . ?
ge2 o2 1.732(13) . ?
ge2 o7 1.722(13) . ?
ge2 o9 1.723(13) . ?
ge2 o12 1.736(14) . ?
ge3 o3 1.744(13) . ?
ge3 o7 1.713(13) . ?
ge3 o10 1.693(11) . ?
ge3 o13 1.711(13) . ?
ge4 o4 1.746(13) . ?
ge4 o8 1.699(13) . ?
ge4 o9 1.716(13) . ?
ge4 o14 1.744(13) . ?
ge5 o5 1.746(13) . ?
ge5 o8 1.706(13) . ?
ge5 o11 1.693(9) . ?
ge5 o15 1.724(13) . ?
ge6 o1 2.205(30) . ?
ge6 o2 1.745(13) . ?
ge6 o5 1.775(13) . ?
ge6 o6 1.728(13) . ?
ge6 f2 1.805(13) . ?
ge7 o1 1.913(31) . ?
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loop_
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o1_ge1_o13 89.5(11) . . ?
o1_ge1_o14 87.0(11) . . ?
o1_ge1_o15 91.6(12) . . ?
o1_ge1_f1 173.3(14) . . ?
o12_ge1_o13 91.2(12) . . ?
o12_ge1_o14 177.0(10) . . ?
o12_ge1_o15 91.9(13) . . ?
o12_ge1_f1 87.7(10) . . ?
o13_ge1_o14 88.7(12) . . ?
o13_ge1_o15 176.5(14) . . ?
o13_ge1_f1 84.8(10) . . ?
o14_ge1_o15 88.1(13) . . ?
o14_ge1_f1 89.3(10) . . ?
o15_ge1_f1 93.8(10) . . ?
o2_ge2_o7 113.4(15) . . ?
o2_ge2_o9 103.6(10) . . ?
o2_ge2_o12 112.4(15) . . ?
o7_ge2_o9 108.3(13) . . ?
o7_ge2_o12 112.7(12) . . ?
o9_ge2_o12 105.7(11) . . ?
o3_ge3_o7 100.5(15) . . ?
o3_ge3_o10 111.3(12) . . ?
o3_ge3_o13 116.1(13) . . ?
o7_ge3_o10 110.4(12) . . ?
o7_ge3_o13 107.9(12) . . ?
o10_ge3_o13 110.0(8) . . ?
o4_ge4_o8 104.3(14) . . ?
o4_ge4_o9 106.2(13) . . ?
o4_ge4_o14 111.8(14) . . ?
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o8_ge4_o14 110.8(12) . . ?
o9_ge4_o14 112.0(10) . . ?
o5_ge5_o8 105.4(13) . . ?
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o5_ge5_o15 116.8(14) . . ?
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o8_ge5_o15 103.1(12) . . ?
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ge5_o5_ge6 124.2(12) . . ?

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ge6_o6_ge7  117.9(11) . . ?
ge2_o7_ge3  123.2(12) . . ?
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#===END
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'Gentz, Travis M.'
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'Groy, Thomas L.'
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'O'Keefe, Michael'
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'Yaghi, Omar M.'
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```
_publ_contact_author_name      'Jacques Plevert'
```

```
_publ_contact_author_address
```

```
;
```

```
Jacques Plevert
```

```
Department of Chemistry & Biochemistry
```

```
Physical Sciences D-121
```

```
Arizona State University
```

```
Tempe, AZ 85287-1604
```

```
USA
```

```
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```

```
_publ_contact_author_email      'JPlevert@asu.edu'
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Layered structures constructed from new linkages of Ge7(O,OH,F)19 clusters
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'H' 'H' 0.0000 0.0000
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'Ge' 'Ge' 0.1547 1.8001
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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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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'

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_cell_length_b              17.5476(12)
_cell_length_c              19.0027(13)
_cell_angle_alpha           90.00
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_cell_angle_gamma           90.00
_cell_volume                 5015.9(6)
_cell_formula_units_Z       8
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_cell_measurement_reflns_used 5370
_cell_measurement_theta_min  2.34
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_diffn_measurement_device_type 'Bruker SMART APEX'
_diffn_measurement_method     '\w scan'
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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^ > 2sigma(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^)+(0.0473P)^2+51.5578P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary  difmap
_atom_sites_solution_hydrogens  geom
_refine_ls_hydrogen_treatment  mixed
_refine_ls_extinction_method     SHELXL
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_refine_ls_extinction_expression Fc^*=kFc[1+0.001xFc^2^l^3^/sin(2\q)]^-1/4^
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loop_

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_atom_site_fract_y
_atom_site_fract_z
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_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
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Ge2 Ge 0.60454(3) 0.42190(3) 0.26374(3) 0.00940(12) Uani 1 1 d . . .
Ge3 Ge 0.72279(3) 0.53380(3) 0.38000(3) 0.01318(13) Uani 1 1 d . . .
Ge4 Ge 0.77175(3) 0.34505(3) 0.25729(3) 0.00987(12) Uani 1 1 d . . .
Ge5 Ge 0.88196(4) 0.46059(3) 0.37380(3) 0.01383(13) Uani 1 1 d . . .
Ge6 Ge 0.90781(3) 0.58141(3) 0.26594(3) 0.01164(13) Uani 1 1 d . . .
Ge7 Ge 0.72335(3) 0.50705(3) 0.18854(3) 0.00801(12) Uani 1 1 d . . .
O1 O 0.7699(2) 0.50211(19) 0.29770(18) 0.0099(7) Uani 1 1 d . . .
F2 F 0.6814(2) 0.51429(19) 0.08869(17) 0.0224(7) Uani 1 1 d . . .
O3 O 0.7610(2) 0.40607(19) 0.1831(2) 0.0133(7) Uani 1 1 d . . .
O4 O 0.8358(2) 0.5405(2) 0.1859(2) 0.0127(7) Uani 1 1 d . . .

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O5 O 0.6863(2) 0.60778(19) 0.1950(2) 0.0120(7) Uani 1 1 d . . .
 O6 O 0.7177(2) 0.6302(2) 0.3533(2) 0.0147(7) Uani 1 1 d . . .
 O7 O 0.6260(2) 0.4770(2) 0.3449(2) 0.0182(8) Uani 1 1 d . . .
 O8 O 0.6102(2) 0.47320(19) 0.1880(2) 0.0126(7) Uani 1 1 d . . .
 F9 F 0.9754(2) 0.4299(2) 0.4524(2) 0.0341(9) Uani 1 1 d . . .
 O10 O 0.8570(2) 0.6610(2) 0.2921(2) 0.0162(8) Uani 1 1 d . . .
 O11 O 0.8622(2) 0.3681(2) 0.3360(2) 0.0179(8) Uani 1 1 d . . .
 O12 O 0.8256(2) 0.4924(2) 0.4350(2) 0.0175(8) Uani 1 1 d . . .
 O13 O 0.5000 0.3812(3) 0.2500 0.0174(11) Uani 1 2 d S . .
 F14 F 0.6932(3) 0.5591(2) 0.4614(2) 0.0331(9) Uani 1 1 d . . .
 O15 O 0.6743(2) 0.34201(19) 0.2812(2) 0.0159(8) Uani 1 1 d . . .
 O16 O 1.0000 0.6214(3) 0.2500 0.0224(13) Uani 1 2 d S . .
 O17 O 0.9513(2) 0.5196(2) 0.3414(2) 0.0186(8) Uani 1 1 d . . .
 O18 O 0.7028(3) 0.75386(19) 0.2655(2) 0.0190(8) Uani 1 1 d . . .
 N1 N 0.6494(4) 0.8981(3) 0.4208(3) 0.0313(12) Uani 1 1 d . . .
 H1B H 0.6160 0.9260 0.3853 0.038 Uiso 1 1 calc R . .
 H1C H 0.6918 0.9185 0.4564 0.038 Uiso 1 1 calc R . .
 N2 N 0.4929(4) 0.6060(4) 0.4216(3) 0.0442(16) Uani 1 1 d . . .
 H2C H 0.4924 0.5789 0.3837 0.053 Uiso 1 1 calc R . .
 H2D H 0.4820 0.5851 0.4585 0.053 Uiso 1 1 calc R . .
 C1 C 0.6336(4) 0.8143(4) 0.4207(3) 0.0242(13) Uani 1 1 d . . .
 H1A H 0.6866 0.7876 0.4185 0.029 Uiso 1 1 calc R . .
 C2 C 0.5554(4) 0.7938(4) 0.3521(3) 0.0246(13) Uani 1 1 d . . .
 H2A H 0.5049 0.8255 0.3504 0.030 Uiso 1 1 calc R . .
 H2B H 0.5707 0.8044 0.3077 0.030 Uiso 1 1 calc R . .
 C3 C 0.5292(4) 0.7106(4) 0.3516(3) 0.0257(13) Uani 1 1 d . . .
 H3A H 0.4758 0.7011 0.3096 0.031 Uiso 1 1 calc R . .
 H3B H 0.5763 0.6787 0.3460 0.031 Uiso 1 1 calc R . .
 C4 C 0.5130(4) 0.6902(4) 0.4231(4) 0.0275(13) Uani 1 1 d . . .
 H4A H 0.4615 0.7188 0.4260 0.033 Uiso 1 1 calc R . .
 C5 C 0.5932(5) 0.7080(4) 0.4919(4) 0.0304(14) Uani 1 1 d . . .
 H5A H 0.6434 0.6770 0.4914 0.036 Uiso 1 1 calc R . .
 H5B H 0.5795 0.6957 0.5367 0.036 Uiso 1 1 calc R . .
 C6 C 0.6178(4) 0.7925(4) 0.4929(3) 0.0281(13) Uani 1 1 d . . .
 H6A H 0.5700 0.8234 0.4988 0.034 Uiso 1 1 calc R . .
 H6B H 0.6710 0.8025 0.5351 0.034 Uiso 1 1 calc R . .
 N1' N 0.3635(4) 0.8757(3) 0.5641(3) 0.0401(15) Uani 1 1 d . . .
 H1'C H 0.3784 0.8771 0.6119 0.048 Uiso 1 1 calc R . .
 H1'D H 0.3915 0.9032 0.5417 0.048 Uiso 1 1 calc R . .
 C1' C 0.2892(5) 0.8253(4) 0.5198(4) 0.0330(15) Uani 1 1 d . . .
 H1'A H 0.2422 0.8570 0.4863 0.040 Uiso 1 1 calc R . .
 C2' C 0.3222(5) 0.7702(4) 0.4734(4) 0.0352(16) Uani 1 1 d . . .
 H2'A H 0.3708 0.7403 0.5060 0.042 Uiso 1 1 calc R . .
 H2'B H 0.3447 0.7988 0.4398 0.042 Uiso 1 1 calc R . .
 C3' C 0.2481(5) 0.7166(4) 0.4279(4) 0.0321(15) Uani 1 1 d . . .
 H3'A H 0.2015 0.7457 0.3920 0.039 Uiso 1 1 calc R . .
 H3'B H 0.2717 0.6804 0.4007 0.039 Uiso 1 1 calc R . .
 O1W O 0.5071(4) 0.2473(3) 0.3670(4) 0.0634(18) Uani 1 1 d . . .
 O2W O 0.5260(4) 0.4248(5) 0.4381(4) 0.079(2) Uani 1 1 d . . .

loop_

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 Ge3 0.0094(3) 0.0107(3) 0.0191(3) -0.0005(2) 0.0044(2) -0.00070(19)
 Ge4 0.0055(2) 0.0069(2) 0.0197(3) 0.00084(19) 0.0075(2) 0.00080(17)
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 Ge6 0.0046(2) 0.0105(3) 0.0236(3) -0.0005(2) 0.0096(2) -0.00034(18)
 Ge7 0.0067(2) 0.0079(2) 0.0112(2) 0.00020(18) 0.00539(19) 0.00030(18)
 O1 0.0082(16) 0.0127(17) 0.0100(17) -0.0020(13) 0.0045(13) 0.0030(13)
 F2 0.0272(18) 0.0275(17) 0.0134(16) -0.0003(13) 0.0081(14) 0.0020(14)
 O3 0.0139(17) 0.0096(16) 0.0215(19) -0.0010(14) 0.0127(15) 0.0031(13)
 O4 0.0108(17) 0.0151(17) 0.0177(18) 0.0001(14) 0.0122(15) -0.0021(13)
 O5 0.0094(16) 0.0106(16) 0.0171(18) 0.0020(14) 0.0057(14) 0.0041(13)
 O6 0.0170(18) 0.0109(17) 0.0210(19) -0.0007(14) 0.0129(15) 0.0025(14)
 O7 0.0128(18) 0.026(2) 0.023(2) -0.0069(16) 0.0154(16) -0.0058(15)

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O8 0.0082(16) 0.0142(17) 0.0153(18) 0.0018(14) 0.0036(14) -0.0020(13)
F9 0.0252(19) 0.034(2) 0.035(2) 0.0033(17) -0.0003(17) 0.0059(16)
O10 0.0050(16) 0.0143(18) 0.032(2) -0.0097(15) 0.0100(15) -0.0031(13)
O11 0.0101(17) 0.0126(17) 0.029(2) 0.0001(15) 0.0036(16) 0.0032(14)
O12 0.0130(18) 0.0216(19) 0.0178(19) 0.0010(15) 0.0050(15) 0.0016(15)
O13 0.006(2) 0.010(2) 0.038(3) 0.000 0.009(2) 0.000
F14 0.040(2) 0.032(2) 0.032(2) 0.0007(16) 0.0192(18) -0.0014(17)
O15 0.0099(17) 0.0124(17) 0.030(2) 0.0046(15) 0.0132(16) 0.0017(13)
O16 0.015(3) 0.014(3) 0.049(4) 0.000 0.025(3) 0.000
O17 0.0050(16) 0.0215(19) 0.029(2) 0.0057(16) 0.0056(15) -0.0014(14)
O18 0.0156(19) 0.0051(16) 0.041(2) 0.0028(16) 0.0160(18) -0.0002(13)
N1 0.037(3) 0.039(3) 0.017(3) -0.004(2) 0.007(2) -0.010(3)
N2 0.055(4) 0.048(4) 0.031(3) -0.010(3) 0.017(3) -0.028(3)
C1 0.013(3) 0.039(3) 0.022(3) -0.005(3) 0.007(2) 0.002(2)
C2 0.017(3) 0.043(4) 0.016(3) -0.007(3) 0.007(2) 0.002(2)
C3 0.011(3) 0.049(4) 0.016(3) -0.012(3) 0.004(2) -0.001(2)
C4 0.019(3) 0.038(4) 0.027(3) -0.005(3) 0.011(3) 0.002(3)
C5 0.034(4) 0.033(3) 0.023(3) -0.001(3) 0.008(3) 0.002(3)
C6 0.029(3) 0.034(3) 0.021(3) -0.003(3) 0.008(3) 0.001(3)
N1' 0.063(4) 0.040(3) 0.026(3) -0.008(3) 0.027(3) -0.021(3)
C1' 0.050(4) 0.019(3) 0.035(4) -0.002(3) 0.021(3) -0.001(3)
C2' 0.050(4) 0.035(4) 0.031(4) -0.007(3) 0.028(3) -0.011(3)
C3' 0.050(4) 0.028(3) 0.029(3) -0.006(3) 0.027(3) -0.004(3)
O1W 0.045(4) 0.055(4) 0.077(5) -0.018(3) 0.004(3) -0.006(3)
O2W 0.047(4) 0.139(7) 0.052(4) 0.040(4) 0.021(3) -0.009(4)

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_geom_special_details

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

loop_

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Ge2 O8 1.725(4) . ?
Ge2 O15 1.752(3) . ?
Ge2 O13 1.752(2) . ?
Ge2 O7 1.755(4) . ?
Ge3 O6 1.760(4) . ?
Ge3 O7 1.771(4) . ?
Ge3 O12 1.780(4) . ?
Ge3 F14 1.817(4) . ?
Ge3 O1 2.025(3) . ?
Ge3 Ge5 2.8829(8) . ?
Ge4 O3 1.732(4) . ?
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Ge4 O11 1.745(4) . ?
Ge4 O15 1.759(3) . ?
Ge5 O11 1.761(4) . ?
Ge5 O17 1.769(4) . ?
Ge5 O12 1.780(4) . ?
Ge5 F9 1.807(4) . ?
Ge5 O1 2.024(3) . ?
Ge6 O4 1.728(4) . ?
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Ge6 O10 1.768(3) . ?

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