



**Volume 56 (2023)**

**Supporting information for article:**

**BFIP: an online tool to calculate the best fitted idealized polyhedron**

**Zhen Song, Zhengxiao Li, Jiahao Zhang, Zeyao Chen, Leopoldo Suescun and Quanlin Liu**

KGaP2O7			
GaO6			
Input			
7			
86310; Picture 1			
Ga	-0.03684	3.94431	5.96151
O	-0.00273	3.89125	7.93436
O	0.85418	5.69651	6.01239
O	1.57816	2.80617	5.82288
O	-0.14372	4.04480	4.04209
O	-1.78271	4.87096	6.09567
O	-1.14910	2.33227	5.91285
Output			
14			
First 7 atoms fitted polyhedra/Last 7 atoms original polyhedra; Merit is 0.271555;Center-vertex distance is 1.9613			
X	0	0	0
L	-0.0807	0.0946	-1.9574
L	0.0807	-0.0946	1.9574
L	1.0158	1.6773	0.0392
L	-1.0158	-1.6773	-0.0392
L	1.6758	-1.0122	-0.1180
L	-1.6758	1.0122	0.1180
Ga	0	0	0
O	-0.1069	0.1005	-1.9194
O	0.0341	-0.0531	1.9729
O	0.8910	1.7522	0.0509
O	-1.1123	-1.6120	-0.0487
O	1.6150	-1.1381	-0.1386

O	-1.7459	0.9267	0.1342

KScP2O7			
ScO6			
Input			
7			
132289; Picture 1			
Sc	3.94689	1.03403	5.96286
O	2.26609	2.29194	6.10529
O	3.00295	-0.82689	5.88277
O	3.87279	1.15425	3.89383
O	5.79265	0.05016	5.78573
O	4.02328	0.95258	7.99424
O	5.09400	2.80625	6.02687
Output			
14			
First 7 atoms fitted polyhedra/Last 7 atoms original polyhedra; Merit is 0.30278;Center-vertex distance is 2.0818			
X	0	0	0
L	-0.0879	0.1213	-2.0764
L	0.0879	-0.1213	2.0764
L	1.0790	1.7794	0.0583
L	-1.0790	-1.7794	-0.0583
L	1.7782	-1.0737	-0.1380
L	-1.7782	1.0737	0.1380
Sc	0	0	0
O	-0.0741	0.1202	-2.0690

O	0.0764	-0.0815	2.0314
O	1.1471	1.7722	0.0640
O	-0.9439	-1.8609	-0.0801
O	1.8458	-0.9839	-0.1771
O	-1.6808	1.2579	0.1424

KInP2O7
---------

InO6
------

Input
-------

7
---

240260; Picture 1
-------------------

In	5.10594	9.37223	1.96464
O	3.36936	8.14126	2.14512
O	7.00285	10.34474	1.75303
O	6.27109	7.59372	2.05547
O	5.06462	9.28080	-0.16800
O	4.20999	11.27467	1.86682
O	5.22365	9.46945	4.05434

Output
--------

14
----

First 7 atoms fitted polyhedra/Last 7 atoms original polyhedra; Merit is 0.33205;Center-vertex distance is 2.1194
---

X	0	0	0
---	---	---	---

L	-1.0688	1.8290	-0.0666
L	1.0688	-1.8290	0.0666
L	-1.8274	-1.0622	0.1552
L	1.8274	1.0622	-0.1552
L	-0.1005	-0.1357	-2.1127
L	0.1005	0.1357	2.1127

In	0	0	0
O	-0.8960	1.9024	-0.0978
O	1.1652	-1.7785	0.0908
O	-1.7366	-1.2310	0.1805
O	1.8969	0.9725	-0.2116
O	-0.0413	-0.0914	-2.1326
O	0.1177	0.0972	2.0897

KLuP2O7
---------

LuO6
------

Input
-------

7
---

160191; Picture 1
-------------------

Lu	-0.08947	6.44213	6.15356
O	-1.29745	8.25032	6.03620
O	0.87310	4.42921	6.18547
O	-0.16399	6.44805	3.97082
O	0.01548	6.60734	8.28980
O	-2.03444	5.38235	6.39815
O	1.67652	7.79416	5.99077

Output
--------

14
----

First 7 atoms fitted polyhedra/Last 7 atoms original polyhedra; Merit is 0.405129; Center-vertex distance is 2.1935
---

X	0	0	0
---	---	---	---

L	-1.1408	1.8729	-0.0458
L	1.1408	-1.8729	0.0458
L	-1.8701	-1.1351	0.1603
L	1.8701	1.1351	-0.1603

L	-0.1132	-0.1224	-2.1872
L	0.1132	0.1224	2.1872
Lu	0	0	0
O	-1.2080	1.8082	-0.1174
O	0.9626	-2.0129	0.0319
O	-1.9450	-1.0598	0.2446
O	1.7660	1.3520	-0.1628
O	-0.0745	0.0059	-2.1827
O	0.1050	0.1652	2.1362

Gd3Al5O12			
GdO8			
Input			
9			
192184; Picture 1			
Gd	1.51430	0.00000	3.02860
O	-0.41585	0.55795	1.80385
O	-0.41585	-0.55855	4.25275
O	1.22415	-2.47065	2.61275
O	1.80385	-0.41585	0.55795
O	1.80385	0.41524	5.49865
O	3.44384	-1.22475	3.58655
O	3.44384	1.22415	2.47005
O	1.22415	2.47005	3.44384
Output			
18			
First 9 atoms fitted polyhedra/Last 9 atoms original polyhedra; Merit is 1.15502;Center-vertex distance is 2.40425			
X	0	0	0

L	0.0000	2.3696	0.4066
L	1.9631	0.9815	-0.9815
L	0.0000	0.4066	2.3696
L	1.9631	-0.9815	0.9815
L	-1.9631	0.9815	-0.9815
L	0.0000	-0.4066	-2.3696
L	-1.9631	-0.9815	0.9815
L	0.0000	-2.3696	-0.4066
Gd	0	0	0
O	-0.2901	2.4701	0.4152
O	1.9295	1.2242	-0.5585
O	0.2896	0.4152	2.4701
O	1.9295	-1.2248	0.5580
O	-1.9302	0.5580	-1.2248
O	0.2896	-0.4159	-2.4707
O	-1.9302	-0.5586	1.2242
O	-0.2901	-2.4707	-0.4158
AlO6			
Input			
7			
192184; Picture 1			
Al	0.00000	0.00000	0.00000
O	-0.41585	0.55795	1.80385
O	1.80385	-0.41585	0.55795
O	0.55795	1.80385	-0.41585
O	0.41524	-0.55855	-1.80445
O	-1.80445	0.41524	-0.55855
O	-0.55855	-1.80445	0.41524
Output			

14

First 7 atoms fitted polyhedra/Last 7 atoms original polyhedra; Merit is 0.022823; Center-vertex distance is 1.9337

X 0 0 0

L 0.4236 -0.5536 -1.8037

L -0.4236 0.5536 1.8037

L 0.5536 1.8037 -0.4236

L -0.5536 -1.8037 0.4236

L 1.8037 -0.4236 0.5536

L -1.8037 0.4236 -0.5536

Al 0 0 0

O 0.4152 -0.5586 -1.8045

O -0.4159 0.5580 1.8039

O 0.5580 1.8039 -0.4159

O -0.5586 -1.8045 0.4152

O 1.8039 -0.4159 0.5580

O -1.8045 0.4152 -0.5586

AlO4

Input

5

192184; Picture 1

Al 4.54290 0.00000 3.02860

O 3.44384 -1.22475 3.58655

O 3.44384 1.22415 2.47005

O 5.64135 0.55795 4.25275

O 5.64135 -0.55855 1.80385

Output

10



First 5 atoms fitted polyhedra/Last 5 atoms original polyhedra; Merit is 0.240376;Center-vertex distance is 1.7331

X 0 0 0

L 1.0006 0.5870 1.2876

L -1.0006 -1.2876 0.5870

L 1.0006 -0.5870 -1.2876

L -1.0006 1.2876 -0.5870

Al 0 0 0

O 1.0985 0.5580 1.2242

O -1.0991 -1.2248 0.5580

O 1.0985 -0.5586 -1.2248

O -1.0991 1.2242 -0.5585

Y3Al5O12

YO8

Input

9

41145; Picture 1

Y 1.50025 0.00000 3.00050

O -0.36678 0.60750 1.79203

O 3.36773 1.20892 2.39345

O 3.36773 -1.20847 3.60800

O -0.36678 -0.60705 4.20942

O 1.20892 2.39345 3.36773

O 1.79203 0.36723 5.39395

O 1.79203 -0.36678 0.60750

O 1.20892 -2.39300 2.63372

Output

18

First 9 atoms fitted polyhedra/Last 9 atoms original polyhedra; Merit is 1.05938;Center-vertex distance is 2.3434

X 0 0 0

L 0.0000 2.3096 0.3963

L 1.9134 0.9567 -0.9567

L 0.0000 0.3963 2.3096

L 1.9134 -0.9567 0.9567

L -1.9134 0.9567 -0.9567

L 0.0000 -0.3963 -2.3096

L -1.9134 -0.9567 0.9567

L 0.0000 -2.3096 -0.3963

Y 0 0 0

O -0.2913 2.3935 0.3672

O 1.8675 1.2089 -0.6071

O 0.2918 0.3672 2.3935

O 1.8675 -1.2085 0.6075

O -1.8670 0.6075 -1.2085

O 0.2918 -0.3668 -2.3930

O -1.8670 -0.6071 1.2089

O -0.2913 -2.3930 -0.3668

AlO6

Input

7

41145; Picture 1

Al 0.00000 0.00000 0.00000

O 0.36723 -0.60705 -1.79158

O -1.79158 0.36723 -0.60705

O -0.60705 -1.79158 0.36723

O -0.36678 0.60750 1.79203

O	1.79203	-0.36678	0.60750
O	0.60750	1.79203	-0.36678
Output			
14			
First 7 atoms fitted polyhedra/Last 7 atoms original polyhedra; Merit is 0.18422;Center-vertex distance is 1.9257			
X	0	0	0
L	0.4321	-0.5698	-1.7880
L	-0.4321	0.5698	1.7880
L	0.5698	1.7880	-0.4321
L	-0.5698	-1.7880	0.4321
L	1.7880	-0.4321	0.5698
L	-1.7880	0.4321	-0.5698
Al	0	0	0
O	0.3672	-0.6071	-1.7916
O	-0.3668	0.6075	1.7920
O	0.6075	1.7920	-0.3668
O	-0.6071	-1.7916	0.3672
O	1.7920	-0.3668	0.6075
O	-1.7916	0.3672	-0.6071
AlO4			
Input			
5			
41145; Picture 1			
Al	4.50075	0.00000	3.00050
O	5.63422	0.60750	4.20942
O	5.63422	-0.60705	1.79203
O	3.36773	1.20892	2.39345
O	3.36773	-1.20847	3.60800

Output
10
First 5 atoms fitted polyhedra/Last 5 atoms original polyhedra; Merit is 0.288649;Center-vertex distance is 1.7588
X 0 0 0
L 1.0154 0.6447 1.2832
L -1.0154 -1.2832 0.6447
L 1.0154 -0.6447 -1.2832
L -1.0154 1.2832 -0.6447
Al 0 0 0
O 1.1335 0.6075 1.2089
O -1.1330 -1.2085 0.6075
O 1.1335 -0.6071 -1.2085
O -1.1330 1.2089 -0.6071
Lu3Al5O12
LuO8
Input
9
23846; Picture 1
Lu 1.48825 0.00000 2.97650
O -0.35002 0.63972 1.79660
O -0.35002 -0.63924 4.15688
O 1.18038 -2.33678 2.62648
O 1.79660 -0.35002 0.63972
O 1.79660 0.35050 5.31376
O 3.32700 -1.17990 3.61622
O 3.32700 1.18038 2.33726
O 1.18038 2.33726 3.32700
Output

18

First 9 atoms fitted polyhedra/Last 9 atoms original polyhedra; Merit is 1.00148; Center-vertex distance is 2.3033

X 0 0 0

L 1.8806 0.9403 -0.9403

L 1.8806 -0.9403 0.9403

L 0.0000 2.2701 0.3895

L 0.0000 0.3895 2.2701

L 0.0000 -0.3895 -2.2701

L 0.0000 -2.2701 -0.3895

L -1.8806 0.9403 -0.9403

L -1.8806 -0.9403 0.9403

Lu 0 0 0

O 1.8388 1.1804 -0.6392

O 1.8388 -1.1799 0.6397

O -0.3079 2.3373 0.3505

O 0.3083 0.3505 2.3373

O 0.3083 -0.3500 -2.3368

O -0.3079 -2.3368 -0.3500

O -1.8383 0.6397 -1.1799

O -1.8383 -0.6392 1.1804

AlO6

Input

7

23846; Picture 1

Al 0.00000 0.00000 0.00000

O -0.35002 0.63972 1.79660

O 1.79660 -0.35002 0.63972

O 0.63972 1.79660 -0.35002

O	0.35050	-0.63924	-1.79612
O	-1.79612	0.35050	-0.63924
O	-0.63924	-1.79612	0.35050
Output			
14			
First 7 atoms fitted polyhedra/Last 7 atoms original polyhedra; Merit is 0.259434; Center-vertex distance is 1.9358			
X	0	0	0
L	0.4423	-0.5873	-1.7907
L	-0.4423	0.5873	1.7907
L	0.5873	1.7907	-0.4423
L	-0.5873	-1.7907	0.4423
L	1.7907	-0.4423	0.5873
L	-1.7907	0.4423	-0.5873
Al	0	0	0
O	0.3505	-0.6392	-1.7961
O	-0.3500	0.6397	1.7966
O	0.6397	1.7966	-0.3500
O	-0.6392	-1.7961	0.3505
O	1.7966	-0.3500	0.6397
O	-1.7961	0.3505	-0.6392
AlO4			
Input			
5			
23846; Picture 1			
Al	4.46475	0.00000	2.97650
O	3.32700	-1.17990	3.61622
O	3.32700	1.18038	2.33726
O	5.60298	0.63972	4.15688

O	5.60298	-0.63924	1.79660
Output			
10			
First 5 atoms fitted polyhedra/Last 5 atoms original polyhedra; Merit is 0.308421;Center-vertex distance is 1.753			
X	0	0	0
L	1.0121	0.6819	1.2584
L	-1.0121	-1.2584	0.6819
L	1.0121	-0.6819	-1.2584
L	-1.0121	1.2584	-0.6819
Al	0	0	0
O	1.1382	0.6397	1.1804
O	-1.1378	-1.1799	0.6397
O	1.1382	-0.6392	-1.1799
O	-1.1378	1.1804	-0.6392