Supplementary Information] Supplementary Information: Quantum-chemical study of stable, meta-stable and high-pressure
alumina polymorphs and aluminum hydroxides

1 Basis sets

The pob-DZVP basis sets used in this work are listed below in the CRYSTAL format:

1.1 Aluminum

```
13          8
 0          0           5       2       1
        5887.5727030    0.0013483347987
         885.61225996   0.0100715768090
         201.13604899   0.0451324540560
         56.284974674   0.1146126804300
         17.229551243   0.1015960894300
 0          0           3       2       1
         29.340249922   0.0693474542080
         3.0439630420   -0.4252811767900
         1.1285539518   -0.4144983221000
 0          0           1       2       1
         0.3614799900   1.0000000000000
 0          0           1       0       1
         0.1440019200   1.0000000000000
 0          2           5       6       1
         145.11918809   0.0063963373134
         33.717894833   0.0441893599650
         10.369863083   0.1558157599300
         3.5135616036   0.2863528695100
         1.1980050273   0.2292142324800
 0          2           1       1       1
         0.4200672400   1.0000000000000
 0          2           1       0       1
         0.2100336200   1.0000000000000
 0          3           1       0       1
         0.3030089300   1.0000000000000
```

1.2 Oxygen

```
8           6
 0          0           5       2       1
         2266.1767785   -0.005343180993
         340.87010191   -0.039890039230
         77.363135167   -0.178539119850
         21.479644940   -0.464276849590
         6.6589433124   -0.443097451720
 0          0           1       2       1
         0.8478937000   1.000000000000
 0          0           1       0       1
         0.2790534900   1.000000000000
 0          2           3       4       1
         17.721504317   0.043394573193
         3.8635505440   0.230941207650
         1.0480920883   0.513753110640
 0          2           1       0       1
         0.2623818000   1.000000000000
 0          3           1       0       1
         0.5000000000   1.000000000000
```

1.3 Hydrogen

1	3			
0	0	3	1	1
	24.62344998	0.01857031		
	3.640664800	0.14010862		
	0.773177290	0.55558583		
0	0	1	0	1
	0.136065500	1.00000000		
0	2	1	0	1
	0.184819860	1.00000000		

2 Monkhorst-Pack k-point-lattices

Table **??** shows the Monkhorst-Pack **k**-point-lattices that were applied in this work.

summary of the applied Monkhorst-Pack **k**-point-lattices

	k-point-lattice
α-Al_2O_3	12x12x12
κ-Al_2O_3	12x6x6
θ-Al_2O_3	12x12x12
γ-Spinell-Al_2O_3	6x6x2
γ-Paglia-Al_2O_3	6x12x3
η-E-Al_2O_3	12x12x4
η-ZS-Al_2O_3	4x12x12
δ-RH-Al_2O_3	12x12x3
δ-FE-Al_2O_3	12x12x4
ι-Al_2O_3	12x12x12
Rh_2O_3-Al_2O_3	8x12x12
$CaIrO_3$-Al_2O_3	12x12x12
Boehmite	12x12x12
Gibbsite	9x12x6
Bayerite	12x12x12
Tohdite	12x12x8

3 Density of states

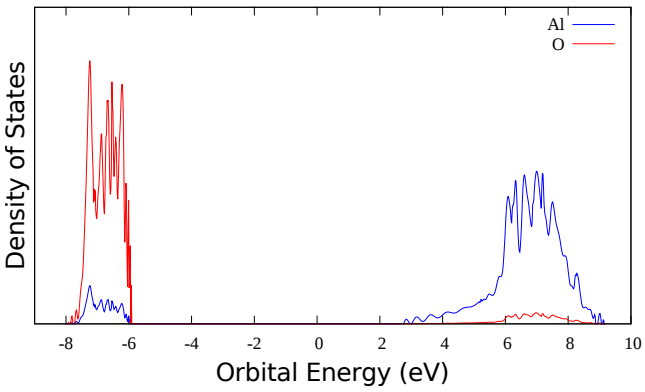


Figure 1: α-Al_2O_3, density of states

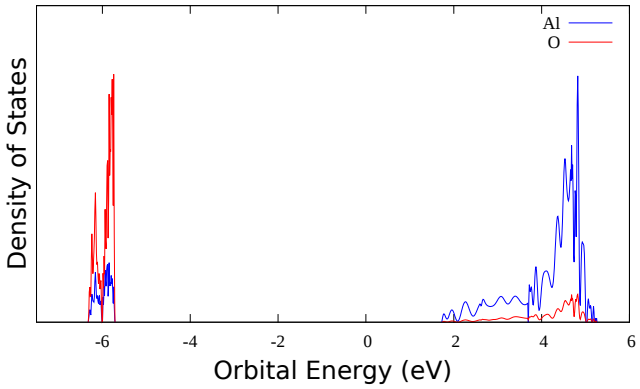


Figure 2: κ-Al_2O_3, density of states

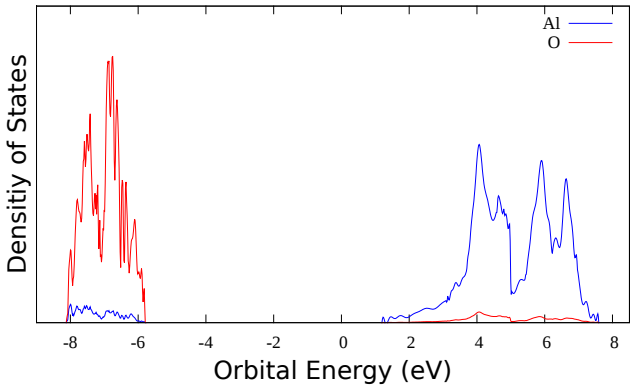
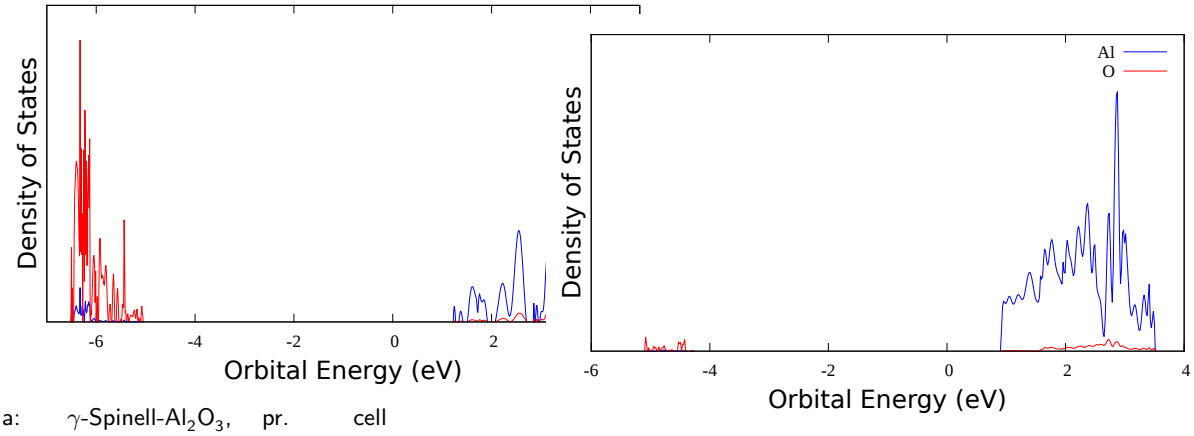


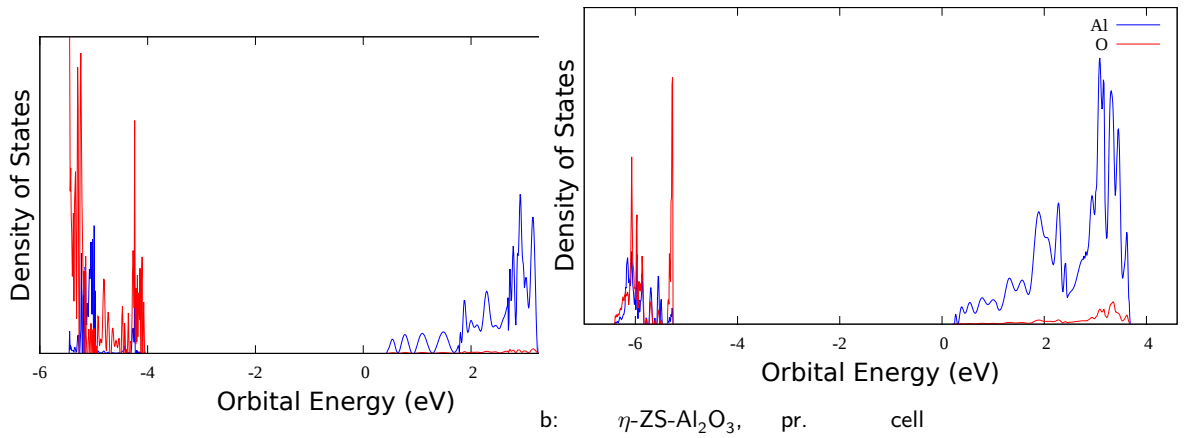
Figure 3: θ-Al_2O_3, density of states



a: γ-Spinell-Al_2O_3, pr. cell (α=β=γ=60°)

b: γ-Paglia-Al_2O_3

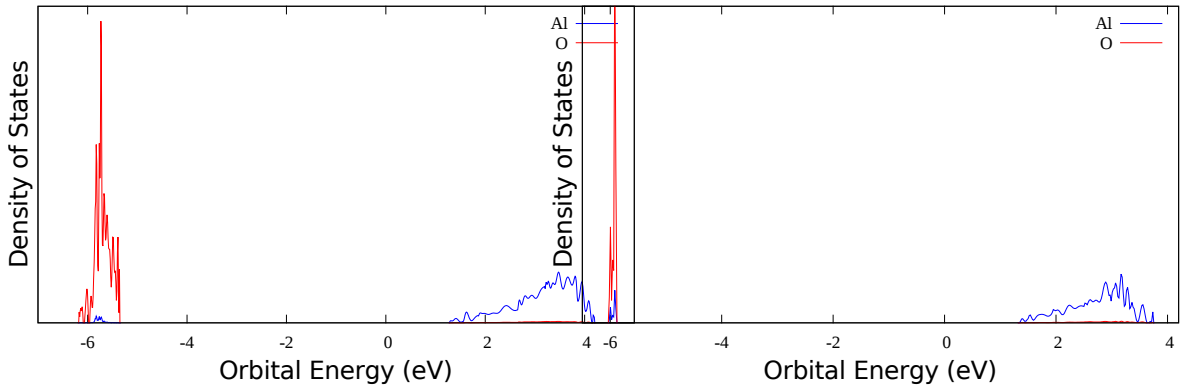
Figure 4: γ-Al_2O_3, density of states



a: η-E-Al_2O_3, pr. cell (α=β=γ=60°)

b: η-ZS-Al_2O_3, pr. cell (α=β=γ=60°)

Figure 5: η-Al_2O_3, density of states



a: δ-RH-Al_2O_3 b: δ-FE-Al_2O_3

Figure 6: δ-Al_2O_3, density of states

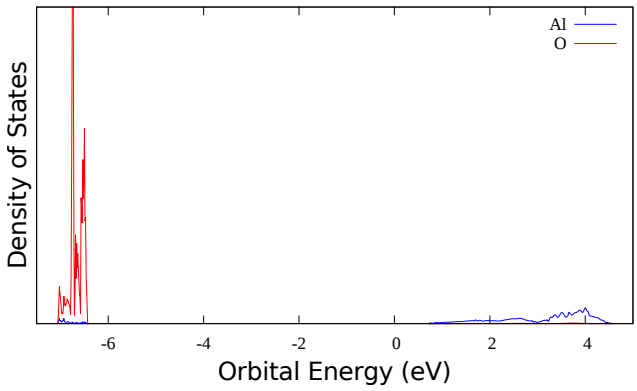
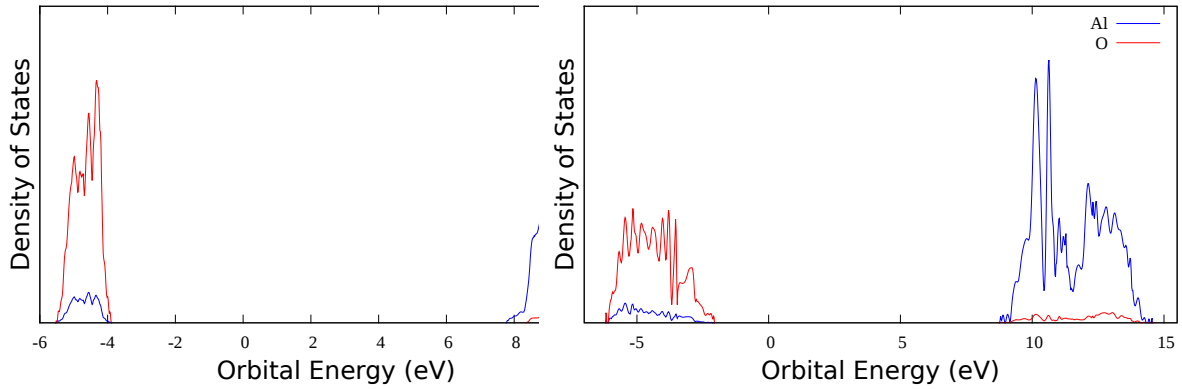


Figure 7: ι-Al_2O_3, density of states



a: Rh_2O_3-Al_2O_3 (113 GPa)

b: $CaIrO_3$-Al_2O_3 (150 GPa)

Figure 8: high pressure phases, density of states

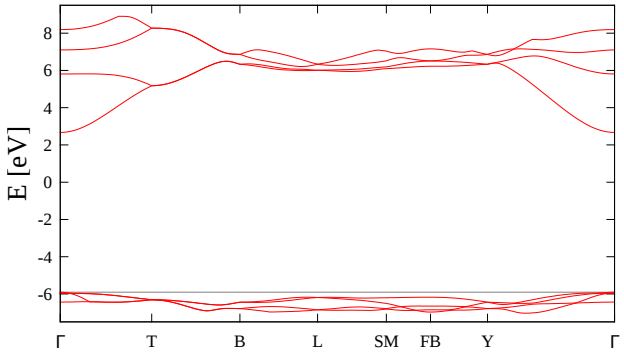


Figure 9: α-Al_2O_3, band structure

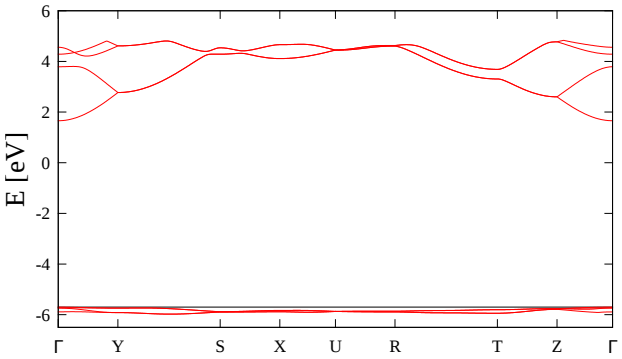


Figure 10: κ-Al_2O_3, band structure

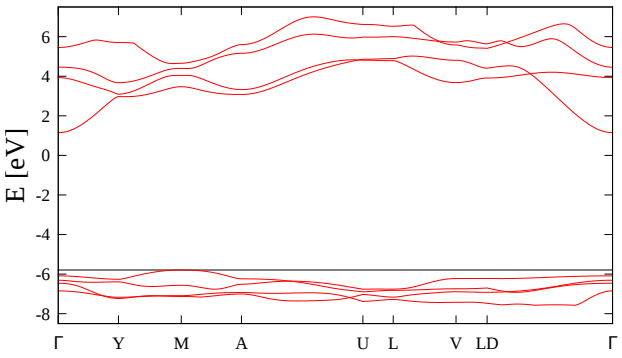
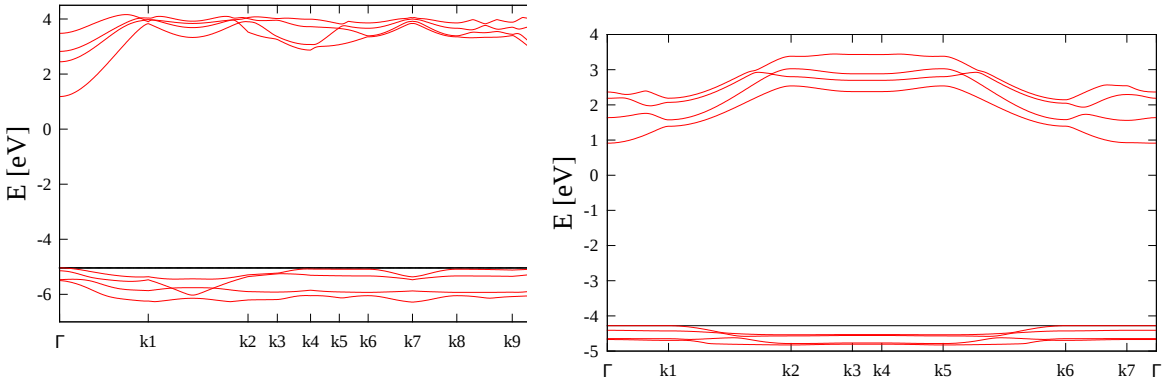


Figure 11: θ-Al_2O_3, band structure



a: γ-Spinell-Al_2O_3,pr. cell (α=β=γ=60°)*

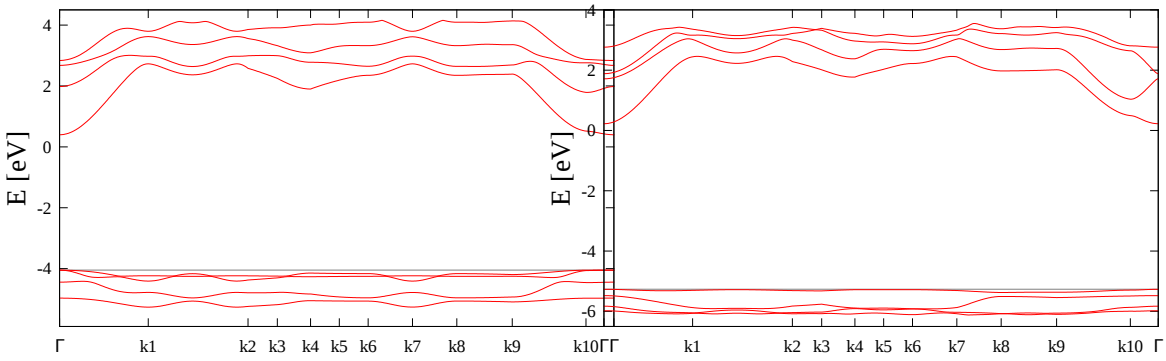
b: γ-Paglia-Al_2O_3**

Figure 12: γ-Al_2O_3, band structure

4 Band structure

* k1(1/3,-1/3,0); k2(u,v,1/8); k3(3/4,1/2,3/4); k4(5/8,5/8,3/4); k5(u,u,1/8); k6(1/2,1/2,1/2); k7(1/3,2/3,1/2); k8(0,1/2,0); k9(1/12,u,1/8); k10(u,u,7/12)

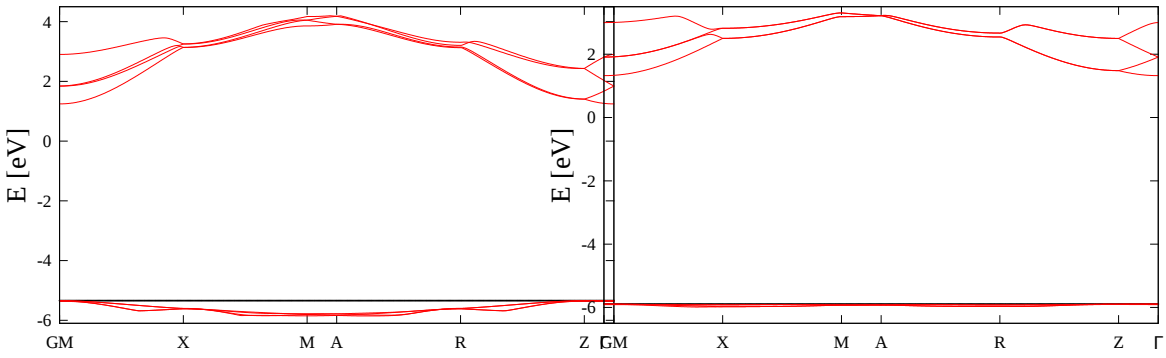
** k1(-1/2,0,0); k2(-1/2,-1/2,0); k3(0,-1/2,0); k4(0,-1/2,-1/2); k5(-1/2,-1/2,-1/2); k6(-1/2,0,-1/2); k7(0,0,-1/2)



a: η-E-Al_2O_3, pr. cell (α=β=γ=60°)*

b: η-ZS-Al_2O_3, pr. cell (α=β=γ=60°)*

Figure 13: η-Al_2O_3, band structure



a: δ-RH-Al_2O_3

b: δ-FE-Al_2O_3

Figure 14: δ-Al_2O_3, band structure

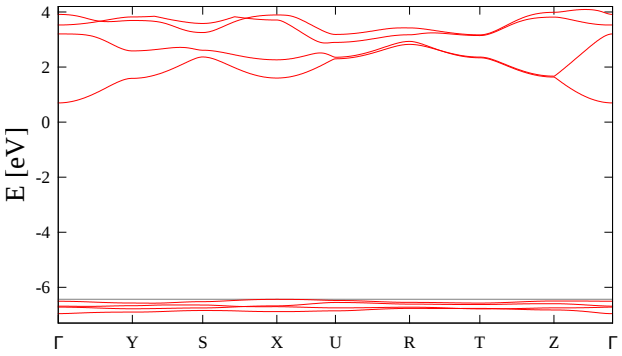
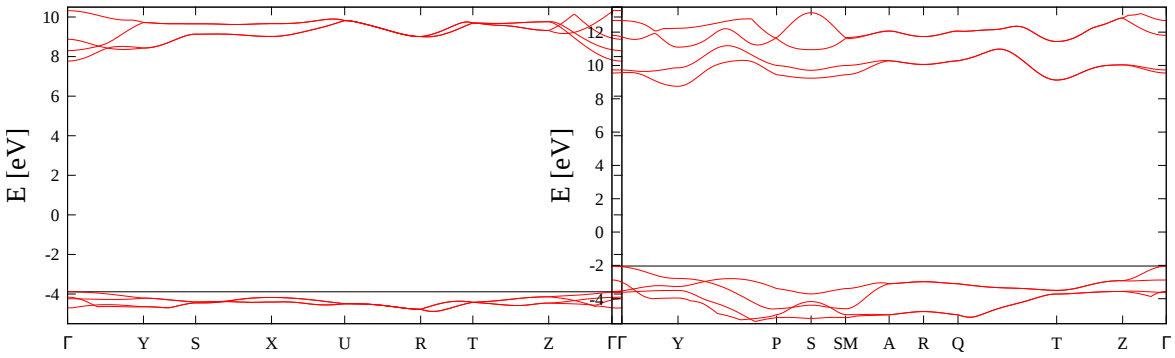


Figure 15: ι-Al_2O_3, band structure



a: Rh_2O_3-Al_2O_3 (113 GPa)

b: $CaIrO_3$-Al_2O_3 (150 GPa)

Figure 16: high pressure phases, band structure

5 Atomic positions

The atomic positions of the relaxed structures are given below:

5.1 α-Al_2O_3

Conventional cell with the space group $R\overline{3}c$ (no. 167) and the lattice constants:
a = 4.788 Å, b = 4.788 Å, c = 13.032 Å, $\alpha = 90.0°$, $\beta = 90.0°$, $\gamma = 120.0°$
atoms in the asymmetric unit: 2

		x/a	y/b	z/c
1	AL	3.33333E-01	-3.33333E-01	1.86064E-02
2	O	-3.61026E-01	-3.33333E-01	-8.33333E-02

5.2 κ-Al_2O_3

Primitive cell with the space group $Pna2_1$ (no. 33) and the lattice constants:
a = 4.870 Å, b = 8.355 Å, c = 8.968 Å, $\alpha = 90.0°$, $\beta = 90.0°$, $\gamma = 90.0°$
atoms in the asymmetric unit: 10

		x/a	y/b	z/c
1	AL	-3.16834E-01	-1.61042E-01	4.53033E-03
2	AL	1.85678E-01	3.45864E-01	-2.16909E-01
3	AL	-1.78532E-01	-3.48677E-01	-3.05444E-01
4	AL	-3.26911E-01	4.70679E-01	-5.07909E-03
5	O	3.42572E-01	-1.61097E-01	-1.05299E-01
6	O	2.18512E-02	4.86871E-01	-3.70028E-01
7	O	4.79161E-01	-3.31758E-01	-3.64114E-01
8	O	-4.80268E-01	-3.24726E-01	1.23847E-01
9	O	-1.56460E-01	3.31523E-01	-1.30602E-01
10	O	3.42949E-01	-4.99914E-01	-1.00200E-01

5.3 θ-Al_2O_3

Conventional cell with the space group $C2/m$ (no. 12) and the lattice constants:
a = 11.803 Å, b = 2.932 Å, c = 5.650 Å, $\alpha = 90.0°$, $\beta = 103.9°$, $\gamma = 90.0°$
atoms in the asymmetric unit: 5

		x/a	y/b	z/c
1	AL	9.16622E-02	-1.20229E-17	-2.02707E-01
2	AL	-1.58498E-01	5.00000E-01	-3.17427E-01
3	O	1.63995E-01	6.42347E-19	1.10240E-01
4	O	-4.91736E-03	5.00000E-01	2.54787E-01
5	O	-1.72741E-01	2.15009E-17	4.36309E-01

5.4 γ-Spinell-Al_2O_3

Primitive cell (3×1×1-supercell) with the space group $Fd\bar{3}m$ (no. 227) and the lattice constants:

a = 5.607 Å, b = 5.607 Å, c = 16.821 Å, $\alpha = 60.0°$, $\beta = 60.0°$, $\gamma = 60.0°$

atoms in the asymmetric unit: 31

		x/a	y/b	z/c			x/a	y/b	z/c
1	AL	-3.70845E-01	-3.81301E-01	2.14708E-01	17	O	4.03176E-01	3.67775E-01	-4.62423E-02
2	AL	-3.78345E-01	-3.68852E-01	-4.64679E-01	18	O	3.87217E-01	3.75748E-01	2.87095E-01
3	AL	-3.75466E-01	-3.74792E-01	-1.25001E-01	19	O	3.75860E-01	3.87274E-01	-3.83469E-01
4	AL	-3.44432E-01	-3.82533E-01	3.64998E-02	20	O	-1.39911E-01	3.77728E-01	1.28151E-01
5	AL	-4.06010E-01	-3.67268E-01	-2.86484E-01	21	O	-1.44063E-01	3.68948E-01	4.68721E-01
6	AL	1.21859E-01	-3.81272E-01	2.13561E-01	22	O	-1.45804E-01	3.85368E-01	-2.08311E-01
7	AL	1.28864E-01	-3.69075E-01	-4.63571E-01	23	O	-1.09876E-01	-1.21214E-01	2.81382E-01
8	AL	2.67863E-01	2.44069E-01	8.13325E-02	24	O	-1.42009E-01	-1.31773E-01	-3.79276E-01
9	AL	2.40861E-01	2.46894E-01	4.21783E-01	25	O	-1.52469E-01	-1.18842E-01	-3.86742E-02
10	AL	2.53328E-01	2.44996E-01	-2.47773E-01	26	O	-1.25556E-01	-1.37403E-01	1.33454E-01
11	AL	-3.97869E-03	5.39950E-03	-2.27343E-03	27	O	-1.36612E-01	-1.26021E-01	4.62885E-01
12	AL	9.59061E-03	2.89603E-03	3.28205E-01	28	O	-1.54084E-01	-1.17305E-01	-2.03768E-01
13	AL	-1.80054E-02	5.99987E-03	-3.31331E-01	29	O	3.95034E-01	-1.34989E-01	-4.16852E-02
14	O	3.92136E-01	3.81577E-01	1.29295E-01	30	O	3.94499E-01	-1.19216E-01	2.81311E-01
15	O	3.60414E-01	3.70851E-01	4.68632E-01	31	O	3.89943E-01	-1.27716E-01	-3.78170E-01
16	O	4.01640E-01	3.69352E-01	-2.11348E-01					

5.5 γ-Paglia-Al_2O_3

Primitive cell (2×1×4-supercell) with the space group P1 (no. 1) (originally SG $I4_1/amd$) and the lattice constants:

a = 5.661 Å, b = 5.661 Å, c = 7.840 Å, $\alpha = 90.0°$, $\beta = 90.0°$, $\gamma = 90.0°$

atoms in the asymmetric unit: 160

		x/a	y/b	z/c			x/a	y/b	z/c
1	AL	3.19988E-01	4.12891E-02	1.74664E-01	41	AL	-3.21652E-01	3.08975E-01	-2.37877E-01
2	AL	1.80010E-01	-2.07861E-01	9.21882E-02	42	AL	-1.93214E-01	-4.48765E-01	-3.31154E-01
3	AL	1.71091E-01	2.98319E-01	2.56861E-01	43	AL	-5.61254E-02	3.04158E-01	-2.42615E-01
4	AL	3.20331E-01	-4.50435E-01	1.73601E-01	44	AL	3.21602E-01	-1.88208E-01	4.64566E-01
5	AL	4.39569E-01	2.98139E-01	2.62767E-01	45	AL	3.14525E-01	2.98376E-01	-4.48757E-01
6	AL	-1.82419E-01	5.15790E-02	1.76132E-01	46	AL	6.01065E-02	2.96022E-01	-3.72763E-01
7	AL	-3.12951E-01	2.98016E-01	2.60413E-01	47	AL	-1.85359E-01	-2.12567E-01	4.61220E-01
8	AL	-1.81840E-01	-4.60223E-01	1.72594E-01	48	AL	-1.81869E-01	2.98759E-01	-4.52067E-01
9	AL	-4.36353E-01	-4.56624E-01	1.32204E-02	49	AL	-4.45164E-01	2.99044E-01	-3.70205E-01
10	AL	-5.80945E-02	-2.00065E-01	8.75142E-02	50	AL	5.55170E-02	-1.97982E-01	-2.83089E-01
11	AL	7.58157E-02	6.03656E-03	3.44182E-01	51	AL	-4.29085E-01	-1.91706E-01	-2.86404E-01
12	AL	-4.44107E-01	4.01634E-02	3.47805E-01	52	AL	-1.87033E-01	-1.93993E-01	-2.10001E-01
13	AL	-4.39398E-01	-4.36712E-01	3.47822E-01	53	AL	-4.34731E-01	2.93778E-01	1.35128E-01
14	AL	2.97846E-01	2.33795E-02	-1.67493E-01	54	AL	6.38561E-02	-1.98098E-01	2.14167E-01
15	AL	1.90426E-01	2.88791E-01	-6.93419E-02	55	AL	3.18400E-01	-1.94902E-01	3.01362E-01
16	AL	4.39401E-01	2.84186E-01	-7.50725E-02	56	AL	3.05640E-01	2.83442E-01	-2.92056E-01
17	AL	-3.13905E-01	3.02392E-01	-8.25619E-02	57	AL	-4.37770E-01	-2.05910E-01	1.33817E-01
18	AL	-6.27157E-02	2.90629E-01	-6.89169E-02	58	AL	3.11294E-01	-2.15204E-01	-2.88989E-01
19	AL	3.31129E-01	4.28486E-02	1.56776E-02	59	AL	6.81719E-02	-2.10251E-01	-3.07084E-02
20	AL	1.77790E-01	2.93469E-01	9.39614E-02	60	AL	-1.93782E-01	-1.87925E-01	-1.02230E-01
21	AL	3.16488E-01	-4.62665E-01	1.29701E-02	61	AL	-2.94512E-01	4.21704E-02	3.91112E-02
22	AL	-3.30378E-01	-2.00780E-01	2.56684E-01	62	AL	-6.72564E-02	-4.69694E-01	2.99695E-01
23	AL	-1.86403E-01	-4.47461E-01	1.01871E-02	63	AL	1.85436E-01	4.98487E-01	3.84890E-01
24	AL	-6.05069E-02	2.94923E-01	8.70169E-02	64	AL	4.40806E-01	-4.83231E-01	-1.96948E-01
25	AL	7.42295E-02	4.83986E-02	4.97341E-01	65	O	-7.33400E-02	-1.99151E-01	-3.29095E-01
26	AL	1.94415E-01	-2.00588E-01	-4.08436E-01	66	O	-3.79933E-02	3.04518E-01	-1.52895E-01
27	AL	7.11820E-02	-4.58824E-01	-4.96701E-01	67	O	-1.87652E-01	-4.74166E-01	-2.45043E-01
28	AL	4.22688E-01	2.92683E-01	4.26599E-01	68	O	-4.48413E-01	-4.76177E-01	-6.86157E-02
29	AL	4.42155E-01	-2.01717E-01	-4.07125E-01	69	O	-7.05689E-02	-1.93312E-01	-1.52604E-01
30	AL	-4.29667E-01	3.90569E-02	-4.91495E-01	70	O	-7.24384E-02	3.03381E-01	-3.23877E-01
31	AL	-1.81093E-01	1.68928E-02	3.38457E-01	71	O	-4.31786E-01	-4.45335E-01	-2.39111E-01
32	AL	-3.06227E-01	3.00114E-01	4.24732E-01	72	O	-1.88134E-01	-4.71250E-01	-7.01450E-02
33	AL	-4.29768E-01	-4.44144E-01	-4.91086E-01	73	O	-3.31973E-01	2.82224E-01	-1.57954E-01
34	AL	-5.92227E-02	3.04354E-01	4.20437E-01	74	O	-2.93504E-01	-1.98053E-01	-3.21269E-01
35	AL	-6.69795E-02	-1.98487E-01	-4.14237E-01	75	O	-4.47329E-01	4.48809E-02	-8.04096E-02
36	AL	5.46120E-02	3.43023E-02	-1.58182E-01	76	O	-1.86863E-01	8.43274E-02	-2.45766E-01
37	AL	8.37903E-02	-4.58778E-01	-1.60175E-01	77	O	-3.05766E-01	3.03130E-01	-3.24113E-01
38	AL	4.40597E-01	-2.18887E-01	-7.52693E-02	78	O	-3.01219E-01	-1.94047E-01	-1.56476E-01
39	AL	-4.28286E-01	1.81993E-02	-1.61564E-01	79	O	-1.92082E-01	8.78882E-02	-7.06423E-02
40	AL	-1.92808E-01	5.35020E-02	-3.30209E-01	80	O	-4.23896E-01	4.73612E-02	-2.37494E-01

		x/a	y/b	z/c			x/a	y/b	z/c
81	O	4.42576E-01	-2.04853E-01	-3.27518E-01	121	O	1.77363E-01	2.96263E-01	-4.88526E-01
82	O	4.25692E-01	2.53998E-01	-1.54762E-01	122	O	1.88190E-01	-2.32717E-01	3.40780E-01
83	O	3.16791E-01	-4.63917E-01	-2.42568E-01	123	O	6.16250E-02	2.21823E-02	-4.15119E-01
84	O	7.02377E-02	-4.75971E-01	-7.38105E-02	124	O	3.20852E-01	6.17237E-02	4.24494E-01
85	O	4.32394E-01	-2.04849E-01	-1.54083E-01	125	O	1.74221E-01	2.73768E-01	3.33624E-01
86	O	4.39963E-01	2.88273E-01	-3.23984E-01	126	O	1.79564E-01	-2.04307E-01	-4.94406E-01
87	O	4.77207E-02	-4.46632E-01	-2.35667E-01	127	O	3.14337E-01	1.84532E-02	-4.14352E-01
88	O	3.21180E-01	-4.81898E-01	-6.76091E-02	128	O	4.91329E-02	6.19505E-02	4.20183E-01
89	O	1.86118E-01	2.65529E-01	-1.48276E-01	129	O	-6.35230E-02	-2.16785E-01	1.00527E-02
90	O	1.80145E-01	-2.08427E-01	-3.27867E-01	130	O	-8.11824E-02	2.92598E-01	1.65858E-01
91	O	6.24472E-02	6.15022E-02	-7.06856E-02	131	O	-1.69577E-01	-4.45116E-01	9.10000E-02
92	O	3.07075E-01	3.28547E-02	-2.42993E-01	132	O	-4.28648E-01	-4.69434E-01	2.63355E-01
93	O	1.75644E-01	2.91729E-01	-3.27570E-01	133	O	-7.21469E-02	-1.99961E-01	1.70552E-01
94	O	1.72996E-01	-1.88169E-01	-1.55074E-01	134	O	-7.44700E-02	3.17115E-01	1.01615E-02
95	O	3.23232E-01	4.62259E-02	-6.74072E-02	135	O	-4.37932E-01	-4.58524E-01	9.17852E-02
96	O	4.18924E-02	4.70287E-02	-2.35927E-01	136	O	-2.00507E-01	-4.55815E-01	2.53498E-01
97	O	-6.21070E-02	-1.93339E-01	3.33434E-01	137	O	-3.04598E-01	2.98186E-01	1.77465E-01
98	O	-5.16898E-02	2.91697E-01	-4.97469E-01	138	O	-3.12482E-01	-2.37835E-01	9.62074E-03
99	O	-1.85510E-01	-4.85343E-01	4.23734E-01	139	O	-4.34300E-01	7.05297E-02	2.60904E-01
100	O	-4.43402E-01	-4.45500E-01	-4.13456E-01	140	O	-1.75814E-01	3.99197E-02	9.14461E-02
101	O	-5.26290E-02	-2.04245E-01	-4.94047E-01	141	O	-3.16316E-01	3.18041E-01	4.72892E-03
102	O	-7.07649E-02	2.66070E-01	3.39605E-01	142	O	-3.04751E-01	-2.07699E-01	1.76819E-01
103	O	-4.33665E-01	-4.84606E-01	4.23685E-01	143	O	-2.10516E-01	4.02699E-02	2.55887E-01
104	O	-1.72833E-01	-4.48900E-01	-4.08328E-01	144	O	-4.18144E-01	4.59443E-02	9.13352E-02
105	O	-3.15390E-01	2.95200E-01	-4.95046E-01	145	O	4.32647E-01	-2.25328E-01	6.29437E-03
106	O	-3.21903E-01	-1.89637E-01	3.35498E-01	146	O	4.35306E-01	2.96501E-01	1.77549E-01
107	O	-4.43719E-01	4.29492E-02	-4.13789E-01	147	O	2.91706E-01	-4.58201E-01	9.25874E-02
108	O	-1.89364E-01	5.74298E-02	4.18026E-01	148	O	5.60704E-02	-4.67696E-01	2.51277E-01
109	O	-3.15114E-01	2.75010E-01	3.40919E-01	149	O	4.27583E-01	-2.02799E-01	1.70245E-01
110	O	-3.18481E-01	-2.03143E-01	-4.99765E-01	150	O	4.36286E-01	3.02764E-01	9.26086E-03
111	O	-1.72878E-01	4.99828E-02	-4.07430E-01	151	O	6.44977E-02	-4.53509E-01	9.26930E-02
112	O	-4.33705E-01	8.26340E-02	4.24584E-01	152	O	3.16291E-01	-4.68790E-01	2.54188E-01
113	O	4.53291E-01	-2.01840E-01	3.37858E-01	153	O	2.10153E-01	2.94347E-01	1.74475E-01
114	O	4.51256E-01	3.02078E-01	-4.95019E-01	154	O	2.02323E-01	-2.08528E-01	1.28055E-02
115	O	3.17405E-01	-4.57470E-01	4.24268E-01	155	O	7.70147E-02	3.94785E-02	2.59160E-01
116	O	6.08738E-02	-4.28903E-01	-4.14835E-01	156	O	2.93262E-01	4.30366E-02	9.31588E-02
117	O	4.55031E-01	-2.03045E-01	-4.92215E-01	157	O	2.09615E-01	2.84901E-01	1.12206E-02
118	O	4.55676E-01	3.03731E-01	3.40882E-01	158	O	1.99566E-01	-2.04788E-01	1.71647E-01
119	O	5.68221E-02	-4.70603E-01	4.25479E-01	159	O	3.19778E-01	6.45472E-02	2.54215E-01
120	O	3.13709E-01	-4.22716E-01	-4.13839E-01	160	O	6.21327E-02	4.27807E-02	9.10739E-02

5.6 η-E-Al_2O_3

Primitive cell (1×1×3-supercell) with the space group $Fd\bar{3}m$ (no. 227) and the lattice constants:

a = 5.630 Å, b = 5.630 Å, c = 16.891 Å, $\alpha = 60.0°$, $\beta = 60.0°$, $\gamma = 60.0°$

atoms in the asymmetric unit: 40

		x/a	y/b	z/c			x/a	y/b	z/c
1	AL	1.02699E-01	1.05950E-01	-1.12185E-01	21	O	3.48763E-01	4.01264E-01	2.92244E-01
2	AL	1.18925E-01	1.02860E-01	2.11596E-01	22	O	3.49016E-01	3.90032E-01	-3.70731E-01
3	AL	1.15859E-01	1.21181E-01	-4.58934E-01	23	O	-1.28597E-01	3.81687E-01	1.29196E-01
4	AL	1.23651E-01	-3.66079E-01	3.64934E-01	24	O	-1.39915E-01	3.70885E-01	4.69111E-01
5	AL	1.06940E-01	-3.81308E-01	-2.85483E-01	25	O	-1.29059E-01	3.83378E-01	-2.03452E-01
6	AL	1.13026E-01	-3.75393E-01	4.16324E-02	26	O	3.49030E-01	-1.40720E-01	1.39353E-01
7	AL	4.84558E-01	-3.84368E-03	-3.29668E-01	27	O	3.37715E-01	-1.51218E-01	4.83877E-01
8	AL	-2.71142E-01	2.39356E-01	9.28326E-02	28	O	3.57686E-01	-1.29654E-01	-2.03267E-01
9	AL	-2.54768E-01	2.55865E-01	4.09945E-01	29	O	-1.08917E-01	-1.41045E-01	2.92224E-01
10	AL	-2.76657E-01	2.35581E-01	-2.35475E-01	30	O	-1.21475E-01	-1.39608E-01	-3.70723E-01
11	AL	-4.07463E-01	-3.70855E-01	2.11620E-01	31	O	-1.00901E-01	-1.36224E-01	-4.64843E-02
12	AL	-3.89811E-01	-3.73126E-01	-4.58963E-01	32	O	-1.28712E-01	-1.54595E-01	1.29219E-01
13	AL	-4.06947E-01	-3.83555E-01	-1.12377E-01	33	O	-1.39675E-01	-1.51561E-01	4.68963E-01
14	AL	1.18908E-01	-3.70929E-01	2.11654E-01	34	O	-1.28972E-01	-1.55845E-01	-2.03479E-01
15	AL	1.15667E-01	-3.73259E-01	-4.58859E-01	35	O	-1.33277E-01	3.79498E-01	-4.59690E-02
16	AL	1.03294E-01	-3.84575E-01	-1.12240E-01	36	O	-1.27777E-01	3.82382E-01	2.82896E-01
17	O	3.34945E-01	3.81762E-01	1.29152E-01	37	O	-1.35318E-01	3.76069E-01	-3.76531E-01
18	O	3.37611E-01	3.71106E-01	4.69016E-01	38	O	3.51711E-01	-1.35210E-01	-4.66125E-02
19	O	3.31789E-01	3.83420E-01	-2.03464E-01	39	O	3.48987E-01	-1.40814E-01	2.92159E-01
20	O	3.52549E-01	4.11288E-01	-4.67816E-02	40	O	3.49295E-01	-1.39342E-01	-3.70816E-01

5.7 η-ZS-Al_2O_3

Primitive cell (1×1×3-supercell) with the space group $Fd\bar{3}m$ (no. 227) and the lattice constants:

a = 5.748 Å, b = 5.748 Å, c = 17.244 Å, $\alpha = 60.0°$, $\beta = 60.0°$, $\gamma = 60.0°$

atoms in the asymmetric unit: 40

		x/a	y/b	z/c			x/a	y/b	z/c
1	AL	-3.78968E-01	4.66520E-01	2.52108E-01	21	O	3.88626E-01	2.63493E-01	3.09740E-01
2	AL	-3.87480E-01	-4.25598E-01	-4.49039E-01	22	O	3.68178E-01	3.57960E-01	-3.73851E-01
3	AL	-3.99524E-01	-3.64529E-01	-1.21484E-01	23	O	-2.13068E-01	4.82007E-01	1.30353E-01
4	AL	-3.92363E-01	-3.55916E-01	-2.95439E-01	24	O	-1.24345E-01	3.26690E-01	4.72472E-01
5	AL	1.25293E-01	4.69087E-01	2.52284E-01	25	O	-1.61415E-01	3.94409E-01	-2.10305E-01
6	AL	1.33020E-01	-4.25437E-01	-4.49055E-01	26	O	3.45975E-01	-1.85117E-02	1.00353E-01
7	AL	1.00891E-01	-3.64851E-01	-1.21593E-01	27	O	3.74067E-01	-2.09702E-01	4.78242E-01
8	AL	-3.93468E-01	1.42842E-01	-1.27736E-01	28	O	3.73839E-01	-1.36761E-01	-2.12695E-01
9	AL	2.21630E-01	-1.34225E-01	5.93350E-02	29	O	-7.40006E-02	-2.35505E-01	2.86133E-01
10	AL	4.30663E-03	-3.20422E-02	-3.34470E-01	30	O	-1.18449E-01	-1.78400E-01	-3.73641E-01
11	AL	-2.90778E-01	-1.36170E-01	5.92526E-02	31	O	-1.34525E-01	-9.37017E-02	-6.17825E-02
12	AL	6.30059E-02	-1.42040E-01	3.29918E-01	32	O	-1.54395E-01	-3.02213E-02	1.03901E-01
13	AL	-3.06614E-01	3.41357E-01	8.06229E-02	33	O	-1.13748E-01	-1.89793E-01	4.63661E-01
14	AL	-2.87504E-01	1.79449E-01	4.55876E-01	34	O	-1.41867E-01	-1.28925E-01	-2.04954E-01
15	AL	2.30812E-01	2.50111E-01	-2.46391E-01	35	O	-1.64162E-01	4.39448E-01	-4.64538E-02
16	AL	2.51126E-01	1.60953E-01	4.36238E-01	36	O	-1.10574E-01	2.51326E-01	3.13863E-01
17	O	3.10464E-01	4.83787E-01	1.30567E-01	37	O	-1.36699E-01	3.70825E-01	-3.74853E-01
18	O	3.52363E-01	3.26336E-01	4.72570E-01	38	O	3.85923E-01	-9.34166E-02	-6.16160E-02
19	O	3.70224E-01	3.94518E-01	-2.10281E-01	39	O	4.24975E-01	-2.38129E-01	2.86035E-01
20	O	3.80396E-01	4.16029E-01	-6.82319E-02	40	O	3.91010E-01	-1.78388E-01	-3.73674E-01

5.8 δ-FE-Al_2O_3

Primitive cell with the space group $P4_12_12$ (no. 92) and the lattice constants:

a = 7.945 Å, b = 7.945 Å, c = 23.790 Å, $\alpha = 90.0°$, $\beta = 90.0°$, $\gamma = 90.0°$

atoms in the asymmetric unit: 21

		x/a	y/b	z/c
1	AL	-2.54029E-01	-1.52454E-02	4.08235E-02
2	AL	-2.52942E-01	-2.31714E-03	3.73415E-01
3	AL	-2.56100E-01	4.17531E-03	-2.93181E-01
4	AL	-3.92174E-01	-3.92174E-01	0.00000E+00
5	AL	-3.73490E-01	-3.85694E-01	3.36495E-01
6	AL	3.67051E-01	-1.40258E-01	-3.71838E-03
7	AL	3.73365E-01	-1.15938E-01	3.31960E-01
8	AL	3.57885E-01	-1.19572E-01	-3.37387E-01
9	AL	1.20696E-01	1.20696E-01	0.00000E+00
10	O	-3.93520E-01	-1.38698E-01	-4.27950E-03
11	O	-3.82900E-01	-1.41298E-01	3.28675E-01
12	O	-3.84747E-01	-1.32389E-01	-3.37269E-01
13	O	1.14955E-01	3.61071E-01	-2.90667E-03
14	O	1.16955E-01	3.90356E-01	3.29694E-01
15	O	1.15021E-01	3.94222E-01	-3.35042E-01
16	O	1.29038E-01	-1.19640E-01	1.73255E-03
17	O	1.42367E-01	-1.41751E-01	3.36638E-01
18	O	1.28830E-01	-1.33198E-01	-3.29402E-01
19	O	3.75191E-01	-3.71130E-01	3.59134E-03
20	O	3.88216E-01	-3.70604E-01	3.30717E-01
21	O	3.86833E-01	-3.56057E-01	-3.28362E-01

5.9 δ-RH-Al_2O_3

Primitive cell with the space group $P\bar{4}m2$ (no. 115) and the lattice constants:

a = 5.633 Å, b = 5.633 Å, c = 23.560 Å, $\alpha = 90.0°$, $\beta = 90.0°$, $\gamma = 90.0°$

atoms in the asymmetric unit: 41

		x/a	y/b	z/c			x/a	y/b	z/c
1	AL	-4.21935E-01	4.21935E-01	0.00000E+00	22	O	-1.80944E-01	4.19251E-01	4.60146E-01
2	AL	7.80648E-02	-7.80648E-02	-5.00000E-01	23	O	3.55285E-01	4.19585E-01	4.62416E-01
3	AL	-4.38531E-01	4.26244E-01	3.34002E-01	24	O	-1.69150E-01	4.42502E-01	-3.77177E-01
4	AL	-4.24571E-01	-7.54124E-02	2.50000E-01	25	O	3.20718E-01	4.41378E-01	-3.77713E-01
5	AL	-4.20272E-01	-9.20180E-02	-4.15996E-01	26	O	-1.95410E-01	4.27143E-01	-2.06802E-01
6	AL	-4.07982E-01	-7.97349E-02	-8.40014E-02	27	O	3.46389E-01	4.28911E-01	-2.13017E-01
7	AL	7.37588E-02	-6.14610E-02	1.65998E-01	28	O	-1.51113E-01	4.19363E-01	-4.31962E-02
8	AL	-1.81575E-01	4.42379E-01	2.04300E-01	29	O	3.07089E-01	4.17618E-01	-3.69832E-02
9	AL	3.25359E-01	4.39901E-01	2.05292E-01	30	O	-1.79277E-01	-5.86030E-02	1.22287E-01
10	AL	-1.64940E-01	4.04155E-01	-4.54299E-01	31	O	3.30868E-01	-5.74789E-02	1.22826E-01
11	AL	3.28119E-01	4.06607E-01	-4.55295E-01	32	O	-1.53593E-01	-7.10778E-02	2.86982E-01
12	AL	-1.73297E-01	4.23242E-01	-1.24997E-01	33	O	3.04605E-01	-7.28400E-02	2.93194E-01
13	AL	-1.71885E-01	-9.34138E-02	4.47067E-02	34	O	-1.92908E-01	-8.23923E-02	4.63016E-01
14	AL	3.35054E-01	-9.58364E-02	4.57068E-02	35	O	3.48884E-01	-8.06332E-02	4.56802E-01
15	AL	3.26755E-01	-7.67502E-02	3.74998E-01	36	O	-1.67240E-01	-9.48683E-02	-3.72284E-01
16	AL	-1.74652E-01	-6.01035E-02	-2.94703E-01	37	O	3.22619E-01	-9.59771E-02	-3.72823E-01
17	AL	3.18416E-01	-5.76372E-02	-2.95702E-01	38	O	-2.01823E-01	-7.30707E-02	-2.12415E-01
18	O	-1.77366E-01	4.04042E-01	1.27176E-01	39	O	3.34416E-01	-7.27387E-02	-2.10145E-01
19	O	3.32776E-01	4.05158E-01	1.27711E-01	40	O	-1.44706E-01	-8.04129E-02	-3.75845E-02
20	O	-1.65573E-01	4.27272E-01	2.89855E-01	41	O	3.19053E-01	-8.07446E-02	-3.98565E-02
21	O	2.98193E-01	4.26943E-01	2.87582E-01					

5.10 ι-Al_2O_3

Primitive cell (1×1×3-supercell) with the space group *Pbam* (no. 55) and the lattice constants:

a = 7.613 Å, b = 7.218 Å, c = 9.135 Å, $\alpha = 90.0°$, $\beta = 90.0°$, $\gamma = 90.0°$

atoms in the asymmetric unit: 30

		x/a	y/b	z/c			x/a	y/b	z/c
1	AL	3.76643E-01	4.80128E-01	0.00000E+00	16	O	-2.81746E-02	1.08684E-01	5.00000E-01
2	AL	3.78932E-01	4.85577E-01	3.34635E-01	17	O	2.00109E-01	-4.84143E-01	-1.59385E-01
3	AL	-1.29122E-01	-7.67545E-03	0.00000E+00	18	O	2.36760E-01	-4.51687E-01	5.00000E-01
4	AL	-1.22931E-01	-1.42803E-02	3.33098E-01	19	O	-4.82024E-01	4.24629E-01	-1.71446E-01
5	AL	-4.15920E-01	-2.84952E-01	5.00000E-01	20	O	-4.46120E-01	4.54566E-01	5.00000E-01
6	AL	1.36837E-02	-3.20419E-01	-1.64664E-01	21	O	-1.69602E-01	-4.80746E-01	-1.70075E-01
7	AL	2.53500E-02	-3.16296E-01	5.00000E-01	22	O	-7.41177E-02	4.54237E-01	5.00000E-01
8	AL	-2.71253E-01	2.91776E-01	-1.69200E-01	23	O	-4.93694E-01	-3.01926E-01	0.00000E+00
9	AL	-2.58495E-01	2.95057E-01	5.00000E-01	24	O	4.89691E-01	-2.81960E-01	3.23926E-01
10	AL	-3.71148E-01	-3.25518E-01	-1.66652E-01	25	O	2.81609E-01	2.32769E-01	0.00000E+00
11	AL	1.70027E-01	2.56534E-01	-1.67686E-01	26	O	2.62454E-01	2.57715E-01	3.43237E-01
12	AL	1.24531E-01	2.97204E-01	5.00000E-01	27	O	4.78601E-02	-1.91615E-01	0.00000E+00
13	O	-2.17988E-01	-1.36339E-01	-1.66777E-01	28	O	5.21940E-02	-1.97458E-01	3.29970E-01
14	O	-2.12657E-01	-1.72169E-01	5.00000E-01	29	O	-2.98767E-01	1.76488E-01	0.00000E+00
15	O	-3.27267E-02	1.44188E-01	-1.66600E-01	30	O	-2.96520E-01	1.68716E-01	3.36807E-01

5.11 Rh_2O_3-$\mathbf{Al_2O_3}$

Primitive cell (at 113 GPa) with the space group *Pbcn* (no. 60) and the lattice constants:

a = 6.418 Å, b = 4.412 Å, c = 4.576 Å, $\alpha = 90.0°$, $\beta = 90.0°$, $\gamma = 90.0°$

atoms in the asymmetric unit: 3

		x/a	y/b	z/c
1	AL	1.12507E-01	-2.47216E-01	3.93485E-02
2	O	-1.54859E-01	-3.92840E-01	1.02613E-01
3	O	-4.91782E-20	5.74690E-02	2.50000E-01

5.12 $CaIrO_3$-$\mathbf{Al_2O_3}$

Conventional cell with the space group *Cmcm* (no. 63) and the lattice constants:

a = 2.441 Å, b = 8.017 Å, c = 6.078 Å, $\alpha = 90.0°$, $\beta = 90.0°$, $\gamma = 90.0°$

atoms in the asymmetric unit: 4

		x/a	y/b	z/c
1	AL	0.00000E+00	-2.50884E-01	2.49999E-01
2	AL	0.00000E+00	0.00000E+00	0.00000E+00
3	O	0.00000E+00	9.18068E-02	2.49999E-01
4	O	5.00000E-01	-1.44137E-01	4.29453E-01

5.13 Boehmite

Conventional cell with the space group $Cmcm$ (no. 63) and the lattice constants:

a = 2.872 Å, b = 12.125 Å, c = 3.742 Å, $\alpha = 90.0°$, $\beta = 90.0°$, $\gamma = 90.0°$

atoms in the asymmetric unit: 4

		x/a	y/b	z/c
1	AL	5.00000E-01	1.81775E-01	2.30401E-01
2	O	5.00000E-01	-2.09364E-01	2.31622E-01
3	O	5.10696E-18	7.91124E-02	2.31858E-01
4	H	1.27674E-18	3.09680E-02	4.48117E-01

5.14 Gibbsite

Primitive cell with the space group $P2_1/c$ (no. 14) and the lattice constants:

a = 9.681 Å, b = 5.064 Å, c = 12.877 Å, $\alpha = 90.0°$, $\beta = 137.8°$, $\gamma = 90.0°$

atoms in the asymmetric unit: 14

		x/a	y/b	z/c
1	AL	-1.69955E-01	-4.64650E-01	-1.68168E-01
2	AL	-3.36255E-01	2.96652E-02	-3.35039E-01
3	O	-2.96479E-01	2.21536E-01	-1.84670E-01
4	O	2.21184E-01	-3.51868E-01	3.25701E-01
5	O	3.87189E-01	1.37295E-01	4.92651E-01
6	O	-9.31922E-02	-3.66272E-01	1.43580E-02
7	O	-4.13560E-01	-2.79419E-01	-3.07375E-01
8	O	6.50713E-02	1.39217E-01	1.68732E-01
9	H	-2.01507E-01	1.37082E-01	-8.33770E-02
10	H	3.19291E-01	-4.48969E-01	4.24248E-01
11	H	2.91649E-01	1.08495E-01	4.97874E-01
12	H	-6.59950E-02	-1.81141E-01	4.71472E-02
13	H	4.97810E-01	-2.66510E-01	-2.94685E-01
14	H	-1.98756E-02	1.60401E-01	1.85011E-01

5.15 Bayerite

Primitive cell with the space group $P2_1/c$ (no. 14) and the lattice constants:

a = 9.348 Å, b = 8.699 Å, c = 10.610 Å, $\alpha = 90.0°$, $\beta = 151.489731°$, $\gamma = 90.0°$

atoms in the asymmetric unit: 14

		x/a	y/b	z/c
1	AL	4.68519E-01	1.65697E-01	4.72145E-01
2	AL	-3.86664E-02	3.33209E-01	-3.40916E-02
3	O	2.58994E-01	-4.89766E-01	-1.27913E-01
4	O	-2.50035E-01	3.27419E-01	-3.56779E-01
5	O	-3.40496E-01	3.05297E-01	2.76828E-01
6	O	2.39135E-01	4.87014E-01	1.27389E-01
7	O	-2.52119E-01	-3.22691E-01	3.51901E-01
8	O	-1.55001E-01	-3.05489E-01	-2.74229E-01
9	H	2.54884E-01	-4.92506E-01	-3.79614E-02
10	H	-1.16170E-01	2.98558E-01	-3.23735E-01
11	H	-4.79661E-01	2.68912E-01	2.34750E-01
12	H	4.39567E-01	4.61367E-01	3.14613E-01
13	H	-1.58935E-01	-4.20299E-01	4.48909E-01
14	H	-1.92591E-01	-3.97961E-01	-3.52437E-01

5.16 Tohdite

Primitive cell with the space group $P6_3mc$ (no. 186) and the lattice constants:

a = 5.612 Å, b = 5.612 Å, c = 8.777 Å, $\alpha = 90.0°$, $\beta = 90.0°$, $\gamma = 120.0°$

atoms in the asymmetric unit: 8

		x/a	y/b	z/c
1	AL	1.65800E-01	3.31601E-01	3.74973E-01
2	AL	-3.33333E-01	3.33333E-01	1.67726E-01
3	AL	3.33333E-01	-3.33333E-01	5.50480E-02
4	O	0.00000E+00	0.00000E+00	-5.16662E-03
5	O	-4.84874E-01	3.02508E-02	9.63217E-03
6	O	-1.65593E-01	-3.31187E-01	2.71697E-01
7	O	3.33333E-01	-3.33333E-01	2.63499E-01
8	H	0.00000E+00	0.00000E+00	1.08283E-01