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Unveiling Rare Earth dopant configurations and crystal field analysis in tetragonal $BaTiO_3$ via Machine Learning and Superposition Modeling

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S1. Optimized Atomic Coordinates of Nearest-Neighbor Ligands Surrounding the Central RE Ion Obtained Using CHGNet

This section presents the optimized atomic coordinates of oxygen ligands in the first coordination shell around the central RE ion, as obtained from CHGNet-optimized structures. The coordination number is 12 for RE substitution at the A-site (Ba) and 6 for substitution at the B-site (Ti). Cartesian coordinates of the central RE ion are provided for each model. Data are provided for both 2×2×2 and 3×3×3 supercells. The positions of the surrounding O ligands are reported in both Cartesian and spherical coordinate systems, defined relative to the RE ion as the origin. Additionally, the local site symmetry of each RE ion is specified beneath the corresponding table.

1. La-Model0a-2x2x2

Central atom: La at (4.0089, 4.0088, 4.3682)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.5788	48.4103	-0.0006	5.9376	4.0087	6.0799
O	2.5789	48.4127	90.0069	4.0087	5.9376	6.0799
O	2.5789	48.4133	-90.0066	4.0087	2.0799	6.0799
O	2.5791	48.4155	-179.9991	2.0798	4.0087	6.0799
O	2.7365	96.5124	45.0030	5.9313	5.9314	4.0578
O	2.7365	96.5126	-45.0034	5.9313	2.0861	4.0578
O	2.7368	96.5115	135.0038	2.0860	5.9314	4.0578
O	2.7369	96.5111	-135.0028	2.0860	2.0861	4.0578
O	3.0466	139.4993	0.0003	5.9875	4.0088	2.0516
O	3.0468	139.4950	90.0137	4.0084	5.9877	2.0515
O	3.0469	139.4940	-90.0149	4.0084	2.0298	2.0515
O	3.0471	139.4896	-179.9970	2.0296	4.0087	2.0515

◈ **Local site symmetry around La**: Low symmetry (C1 or Cs)

2. La-Model0b-2x2x2

Central atom: La at (2.0292, 2.0547, 2.2117)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3092	96.2424	-91.6504	1.9631	-0.2399	1.9606
O	2.3094	96.2232	1.4869	4.3242	2.1143	1.9613
O	2.3280	96.3356	91.6176	1.9639	4.3676	1.9548
O	2.3299	96.2504	178.5514	-0.2861	2.1133	1.9580
O	2.3498	0.6919	130.9837	2.0106	2.0761	4.5613
O	2.4932	179.1845	137.2585	2.0032	2.0788	-0.2813

◈ **Local site symmetry around La**: Octahedral (Oh)

3. Ce-Model0a-2x2x2

Central atom: Ce at (4.0077, 4.0076, 4.4815)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4921	50.2235	-90.0009	4.0076	2.0923	6.0759
O	2.4921	50.2243	0.0032	5.9230	4.0077	6.0759
O	2.4922	50.2251	179.9970	2.0923	4.0077	6.0759
O	2.4922	50.2260	90.0009	4.0076	5.9230	6.0759
O	2.7239	98.8974	-44.9988	5.9106	2.1047	4.0602
O	2.7240	98.8973	-135.0021	2.1046	2.1047	4.0602
O	2.7241	98.8967	45.0022	5.9106	5.9107	4.0602
O	2.7242	98.8965	134.9989	2.1046	5.9107	4.0602
O	3.1603	140.9522	-90.0017	4.0076	2.0167	2.0272
O	3.1604	140.9505	0.0073	5.9987	4.0078	2.0271
O	3.1604	140.9489	179.9924	2.0165	4.0078	2.0271
O	3.1605	140.9472	90.0028	4.0076	5.9988	2.0271

◈ **Local site symmetry around Ce**: Low symmetry (C1 or Cs)

4. Ce-Model0b-2x2x2

Central atom: Ce at (2.0755, 2.0528, 2.0782)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2048	91.5073	-88.6237	2.1284	-0.1506	2.0202
O	2.2068	91.4634	88.4672	2.1345	4.2581	2.0218
O	2.2072	91.2302	-178.1976	-0.1301	1.9834	2.0308
O	2.2117	2.1600	57.2644	2.1206	2.1229	4.2883
O	2.2307	91.3745	-1.6389	4.3046	1.9890	2.0246
O	2.2342	177.7181	53.4153	2.1285	2.1242	-0.1543

◈ **Local site symmetry around Ce**: Octahedral (Oh)

5. Ce-Model1-2x2x2 (1st Ce atom)

Central atom: Ce1 at (4.0382, 4.0384, 4.8966)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4224	52.2930	177.0185	2.1243	4.1381	6.3782
O	2.4226	52.2981	-87.0139	4.1381	2.1243	6.3781
O	2.4396	55.4603	88.2438	4.0998	6.0471	6.2798
O	2.4397	55.4642	1.7501	6.0471	4.0998	6.2797
O	2.5177	101.6390	-134.9979	2.2946	2.2947	4.3887
O	2.7370	105.8438	135.0626	2.1744	5.8982	4.1494
O	2.7375	105.8405	-45.0613	5.8984	2.1742	4.1494
O	2.8640	104.7558	44.9974	5.9967	5.9967	4.1671
O	3.5783	143.6131	86.6980	4.1605	6.1576	2.0160
O	3.5783	143.6091	3.2963	6.1577	4.1605	2.0161
O	3.6861	146.9229	174.0684	2.0372	4.2463	1.8079
O	3.6862	146.9189	-84.0620	4.2464	2.0372	1.8079

◈ **Local site symmetry around Ce1**: Low symmetry (C1 or Cs)

6. Ce-Model1-2x2x2 (2nd Ce atom)

Central atom: Ce2 at (2.0785, 2.0785, 2.1661)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1976	99.3830	91.0914	2.0372	4.2463	1.8079
O	2.1976	99.3805	-1.0920	4.2464	2.0372	1.8079
O	2.2196	89.5549	-179.6880	-0.1409	2.0664	2.1834
O	2.2196	89.5517	-90.3112	2.0665	-0.1410	2.1835
O	2.2434	7.8300	45.0100	2.2946	2.2947	4.3887
O	2.3758	176.3658	-134.9714	1.9721	1.9720	-0.2049

◈ **Local site symmetry around Ce2**: Octahedral (Oh)

7. Ce-Model2(i)-2x2x2

Central atom: Ce at (4.2580, 4.0484, 3.8456)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4681	135.5487	-0.0005	5.9864	4.0484	2.0838
O	2.5860	85.7075	48.6221	5.9627	5.9835	4.0392
O	2.5861	85.7076	-48.6225	5.9627	2.1134	4.0392
O	2.6086	131.7672	96.9146	4.0238	5.9800	2.1080
O	2.6087	131.7668	-96.9145	4.0238	2.1169	2.1080
O	2.7529	38.7778	-0.0005	5.9822	4.0484	5.9917
O	2.8216	128.8064	-179.9995	2.0592	4.0484	2.0773
O	2.9071	41.7817	98.7210	3.9643	5.9630	6.0134
O	2.9071	41.7821	-98.7208	3.9643	2.1338	6.0134
O	2.9537	85.1592	138.9796	2.0375	5.9801	4.0949
O	2.9538	85.1593	-138.9790	2.0374	2.1167	4.0949

◈ **Local site symmetry around Ce**: Low symmetry (C1 or Cs)

8. Ce-Model2(ii)-2x2x2

Central atom: Ce at (2.0703, 2.0751, 2.1526)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2197	92.5022	-178.3466	-0.1463	2.0111	2.0557
O	2.2211	92.4253	88.3984	2.1324	4.2934	2.0586
O	2.2329	92.4534	-1.4588	4.3004	2.0183	2.0571
O	2.2358	92.4062	-88.5898	2.1253	-0.1580	2.0588
O	2.2544	179.9211	-32.5394	2.0730	2.0734	-0.1017

◈ **Local site symmetry around Ce**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

9. Ce-Model2(iii)-2x2x2 (1st Ce atom)

Central atom: Ce1 at (4.3389, 4.3389, 4.5181)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3878	48.5749	96.3388	4.1412	6.1183	6.0980
O	2.3878	48.5751	-6.3388	6.1183	4.1412	6.0980
O	2.4908	98.9151	44.9999	6.0788	6.0788	4.1321
O	2.6309	55.9464	-174.0208	2.1710	4.1118	5.9914
O	2.6309	55.9464	-95.9789	4.1118	2.1710	5.9914
O	2.8653	98.4879	-51.1336	6.1171	2.1323	4.0952

O	2.8653	98.4879	141.1336	2.1323	6.1172	4.0952
O	2.9758	143.5222	98.6317	4.0733	6.0880	2.1253
O	2.9758	143.5221	-8.6318	6.0880	4.0733	2.1253

◈ **Local site symmetry around Ce1**: Low symmetry (C1 or Cs)

10. Ce-Model2(iii)-2x2x2 (2nd Ce atom)

Central atom: Ce2 at (2.0635, 2.0635, 2.1807)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2024	95.2198	-3.5252	4.2527	1.9287	1.9803
O	2.2024	95.2198	93.5253	1.9287	4.2527	1.9803
O	2.2400	93.1760	-178.2304	-0.1719	1.9945	2.0566
O	2.2400	93.1761	-91.7694	1.9945	-0.1719	2.0566
O	2.2914	179.7249	44.9852	2.0713	2.0713	-0.1108

◈ **Local site symmetry around Ce2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

11. Ce-Model2(iv)a-2x2x2

Central atom: Ce at (3.8363, 3.8363, 4.0974)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4708	90.3964	-135.0001	2.0892	2.0892	4.0803
O	2.6116	42.2230	-83.6913	4.0291	2.0919	6.0314
O	2.6116	42.2231	173.6912	2.0919	4.0291	6.0314
O	2.6413	138.3175	173.6174	2.0907	4.0315	2.1248
O	2.6413	138.3176	-83.6174	4.0315	2.0907	2.1248
O	2.7386	90.4161	-39.0353	5.9635	2.1115	4.0775
O	2.7386	90.4161	129.0353	2.1115	5.9635	4.0775
O	3.0001	46.9323	6.1998	6.0152	4.0730	6.1461
O	3.0001	46.9323	83.8003	4.0730	6.0152	6.1461
O	3.0368	133.5925	6.2616	6.0226	4.0762	2.0035
O	3.0368	133.5925	83.7385	4.0762	6.0226	2.0035
O	3.0465	90.3929	45.0001	5.9904	5.9904	4.0765

◈ **Local site symmetry around Ce**: Low symmetry (C1 or Cs)

12. Ce-Model2(iv)b-2x2x2

Central atom: Ce at (2.0589, 2.0395, 2.1123)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2149	92.2766	-178.5329	-0.1536	1.9829	2.0243
O	2.2187	92.2435	88.1534	2.1303	4.2554	2.0255
O	2.2239	92.3399	-1.1645	4.2805	1.9944	2.0215
O	2.2325	92.1739	-88.3102	2.1247	-0.1904	2.0276
O	2.2544	1.3945	-159.6848	2.0074	2.0205	4.3660
O	2.2786	178.7491	-152.5882	2.0147	2.0166	-0.1657

◈ **Local site symmetry around Ce**: Octahedral (Oh)

13. Model3a-Ce-Ti-2x2x2

Central atom: Ce at (2.0639, 2.0639, 2.1322)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1747	94.4133	93.5618	1.9292	4.2280	1.9648
O	2.1747	94.4134	-3.5617	4.2280	1.9292	1.9648
O	2.1883	4.5401	-135.0007	1.9414	1.9414	4.3136
O	2.2343	92.6061	-178.1185	-0.1669	1.9906	2.0306
O	2.2343	92.6060	-91.8815	1.9906	-0.1669	2.0306
O	2.2761	178.0899	-135.0006	2.0102	2.0102	-0.1426

14. Ce-Model3b-2x2x2

Central atom: Ce at (4.6273, 3.5864, 3.8114)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1226	82.5911	-45.0025	6.1157	2.0979	4.0851
O	2.1422	136.7464	26.9627	5.9357	4.2520	2.2511
O	2.1422	136.7469	-116.9638	3.9618	2.2781	2.2511
O	2.4859	37.8276	22.6806	6.0340	4.1743	5.7748
O	2.4859	37.8282	-112.6847	4.0394	2.1797	5.7749
O	3.0001	85.7503	62.0351	6.0303	6.2289	4.0337
O	3.0001	85.7500	-152.0365	1.9848	2.1835	4.0337
O	3.2676	123.7715	104.4955	3.9475	6.2162	1.9949
O	3.2677	123.7713	165.5050	1.9975	4.2663	1.9949

◈ **Local site symmetry around Ce**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

15. Pr-Model0a-2x2x2

Central atom: Pr at (4.0053, 4.0053, 4.4438)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.5365	49.2794	-0.0013	5.9277	4.0052	6.0985
O	2.5365	49.2793	90.0020	4.0052	5.9277	6.0985
O	2.5366	49.2805	-179.9981	2.0828	4.0052	6.0985
O	2.5366	49.2806	-90.0009	4.0052	2.0828	6.0985
O	2.7062	98.0821	45.0005	5.8998	5.8998	4.0633
O	2.7063	98.0813	-45.0014	5.8999	2.1106	4.0633
O	2.7063	98.0812	135.0023	2.1106	5.8998	4.0633
O	2.7063	98.0812	-134.9996	2.1106	2.1106	4.0633
O	3.1238	140.5526	-0.0041	5.9900	4.0051	2.0315
O	3.1238	140.5524	90.0076	4.0050	5.9900	2.0315
O	3.1239	140.5496	-90.0017	4.0052	2.0203	2.0315
O	3.1239	140.5494	-179.9960	2.0203	4.0051	2.0315

◈ **Local site symmetry around Pr**: Low symmetry (C1 or Cs)

16. Pr-Model0b-2x2x2

Central atom: Pr at (2.0625, 2.0749, 2.1057)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3085	92.4126	93.1664	1.9351	4.3778	2.0086
O	2.3099	92.8655	-2.6242	4.3671	1.9692	1.9903
O	2.3100	92.5853	-177.8177	-0.2435	1.9870	2.0015

O	2.3101	3.8802	-26.3605	2.2026	2.0054	4.4106
O	2.3418	91.9995	-92.7946	1.9484	-0.2627	2.0240
O	2.3515	176.4947	-45.5814	2.1632	1.9722	-0.2413

◈ **Local site symmetry around Pr**: Octahedral (Oh)

17. Pr-Model1-2x2x2 (1st Pr atom)

Central atom: Pr at (2.1068, 2.1067, 2.3445)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3080	4.9026	45.0098	2.2462	2.2462	4.6441
O	2.3107	105.6353	-2.4634	4.3299	2.0111	1.7218
O	2.3107	105.6354	92.4617	2.0112	4.3299	1.7218
O	2.3295	92.3730	-91.3734	2.0510	-0.2201	2.2481
O	2.3295	92.3731	-178.6291	-0.2201	2.0511	2.2481
O	2.6836	173.9519	-135.0047	1.9068	1.9068	-0.3241
O	4.1434	60.9126	1.4558	5.7264	2.1987	4.3588
O	4.1434	60.9133	88.5446	2.1987	5.7264	4.3588
O	4.4531	92.9379	26.8917	6.0731	4.1183	2.1163
O	4.4532	92.9373	63.1093	4.1183	6.0732	2.1163
O	4.4772	87.9202	118.1385	-0.0033	6.0522	2.5070
O	4.4772	87.9201	-28.1378	6.0523	-0.0033	2.5070

◈ Local site symmetry around Pr (index 7): Low symmetry (C1 or Cs)

18. Pr-Model1-2x2x2 (2nd Pr atom)

Central atom: Pr at (2.1068, 2.1067, 2.3445)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3080	4.9026	45.0098	2.2462	2.2462	4.6441
O	2.3107	105.6353	-2.4634	4.3299	2.0111	1.7218
O	2.3107	105.6354	92.4617	2.0112	4.3299	1.7218
O	2.3295	92.3730	-91.3734	2.0510	-0.2201	2.2481
O	2.3295	92.3731	-178.6291	-0.2201	2.0511	2.2481
O	2.6836	173.9519	-135.0047	1.9068	1.9068	-0.3241

◈ Local site symmetry around Pr (index 8): Octahedral (Oh)

19. Pr-Model2(i)-2x2x2

Central atom: Pr at (4.1656, 4.0432, 3.8606)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.5268	134.1815	-0.0002	5.9776	4.0432	2.0996
O	2.6088	131.9196	94.0000	4.0302	5.9796	2.1177
O	2.6088	131.9194	-93.9999	4.0302	2.1067	2.1177
O	2.6507	85.6382	47.1651	5.9625	5.9813	4.0622
O	2.6507	85.6382	-47.1653	5.9625	2.1050	4.0622
O	2.7513	130.3542	-179.9998	2.0689	4.0432	2.0791
O	2.8352	84.8634	137.9980	2.0671	5.9327	4.1144
O	2.8352	84.8635	-137.9977	2.0671	2.1536	4.1144
O	2.8508	40.2467	-0.0003	6.0074	4.0432	6.0365
O	2.8885	41.3288	95.8132	3.9724	5.9408	6.0296
O	2.8885	41.3291	-95.8130	3.9724	2.1455	6.0296

◈ **Local site symmetry around Pr**: Low symmetry (C1 or Cs)

20. Pr-Model2(ii)-2x2x2

Central atom: Pr at (2.1142, 2.0843, 2.2024)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2833	94.9141	-92.7794	2.0039	-0.1880	2.0068
O	2.2911	179.7608	-89.8261	2.1142	2.0747	-0.0887
O	2.2957	94.7565	92.7013	2.0064	4.3695	2.0121
O	2.2989	93.4912	1.5292	4.4080	2.1455	2.0624
O	2.3303	93.8212	178.6858	-0.2103	2.1376	2.0471

◈ **Local site symmetry around Pr**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

21. Pr-Model2(iii)-2x2x2 (1st Pr atom)

Central atom: Pr1 at (4.3180, 4.3180, 4.4379)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4359	47.2850	96.6544	4.1106	6.0956	6.0903
O	2.4359	47.2850	-6.6543	6.0956	4.1106	6.0903
O	2.5801	96.1756	45.0000	6.1318	6.1318	4.1604
O	2.6662	55.5414	-97.5018	4.0309	2.1384	5.9465
O	2.6662	55.5414	-172.4982	2.1384	4.0309	5.9465
O	2.8800	96.4211	140.4727	2.1105	6.1394	4.1159
O	2.8800	96.4210	-50.4727	6.1394	2.1105	4.1159
O	2.9330	140.8060	92.7714	4.2283	6.1693	2.1648
O	2.9330	140.8060	-2.7715	6.1693	4.2283	2.1648
O	3.2884	138.2300	-89.6141	4.3327	2.1274	1.9853
O	3.2884	138.2299	179.6141	2.1274	4.3327	1.9853
O	5.0488	69.9660	-67.0057	6.1709	-0.0484	6.1675

◈ **Local site symmetry around Pr1**: Low symmetry (C1 or Cs)

22. Pr-Model2(iii)-2x2x2 (2nd Pr atom)

Central atom: Pr2 at (2.0766, 2.0766, 2.2223)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2691	95.9942	88.7094	2.1274	4.3327	1.9853
O	2.2691	95.9942	1.2908	4.3327	2.1274	1.9853
O	2.2851	95.5732	178.2829	-0.1966	2.1448	2.0004
O	2.2851	95.5731	-88.2828	2.1448	-0.1966	2.0004
O	2.3527	179.7650	44.9592	2.0834	2.0834	-0.1304

◈ **Local site symmetry around Pr2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

23. Pr-Model2(iv)a-2x2x2

Central atom: Pr at (3.8642, 3.8642, 4.1079)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.5189	90.6933	-134.9999	2.0832	2.0832	4.0774
O	2.6132	42.7324	174.6733	2.0986	4.0288	6.0274
O	2.6132	42.7324	-84.6731	4.0288	2.0986	6.0274

O	2.6575	138.0569	174.6085	2.0958	4.0311	2.1312
O	2.6575	138.0568	-84.6084	4.0311	2.0958	2.1312
O	2.7443	90.5683	129.7233	2.1104	5.9749	4.0807
O	2.7443	90.5683	-39.7233	5.9749	2.1104	4.0807
O	2.9519	46.8449	84.3676	4.0755	6.0072	6.1270
O	2.9519	46.8450	5.6323	6.0073	4.0755	6.1270
O	3.0037	133.9278	84.3130	4.0786	6.0169	2.0241
O	3.0037	133.9278	5.6869	6.0169	4.0786	2.0241
O	3.0103	90.5747	45.0000	5.9927	5.9927	4.0777

◈ **Local site symmetry around Pr**: Low symmetry (C1 or Cs)

24. Pr-Model2(iv)b-2x2x2

Central atom: Pr at (2.0931, 2.0521, 2.1210)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3090	92.7341	88.0289	2.1724	4.3571	2.0108
O	2.3093	92.7275	-178.0621	-0.2122	1.9741	2.0111
O	2.3299	1.2349	-44.6973	2.1288	2.0168	4.4503
O	2.3357	92.2938	-88.0190	2.1738	-0.2804	2.0275
O	2.3360	92.2443	-1.9738	4.4259	1.9717	2.0295
O	2.3668	178.3339	-43.7281	2.1428	2.0045	-0.2449

◈ **Local site symmetry around Pr**: Octahedral (Oh)

25. Model3a-Pr-Ti-2x2x2

Central atom: Pr at (2.0967, 2.0968, 2.3098)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3237	5.5691	-134.9889	1.9373	1.9373	4.6225
O	2.3275	96.3179	98.3148	1.7622	4.3859	2.0537
O	2.3276	96.3226	-8.3115	4.3858	1.7624	2.0535
O	2.3556	97.0797	-176.6307	-0.2369	1.9594	2.0195
O	2.3558	97.0774	-93.3672	1.9594	-0.2370	2.0196
O	2.5448	178.6275	-134.9799	2.0536	2.0537	-0.2343

◈ **Local site symmetry around Pr**: Octahedral (Oh)

26. Pr-Model3b-2x2x2

Central atom: Pr at (4.2262, 3.8468, 4.1924)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4404	89.0668	-45.0001	5.9516	2.1214	4.2321
O	2.5530	43.7388	6.9521	5.9782	4.0605	6.0369
O	2.5530	43.7388	-96.9522	4.0125	2.0948	6.0369
O	2.5683	140.8441	8.3504	5.8307	4.0824	2.2009
O	2.5683	140.8439	-98.3504	3.9906	2.2423	2.2008
O	2.7284	92.3146	51.0966	5.9382	5.9683	4.0822
O	2.7284	92.3146	-141.0963	2.1047	2.1348	4.0822
O	2.9174	49.4745	96.7288	3.9663	6.0491	6.0881
O	2.9174	49.4745	173.2717	2.0239	4.1067	6.0881
O	3.0988	134.4555	96.7428	3.9665	6.0434	2.0221
O	3.0988	134.4553	173.2574	2.0296	4.1065	2.0221
O	3.1681	93.2628	135.0002	1.9896	6.0834	4.0121

◈ **Local site symmetry around Pr**: Low symmetry (C1 or Cs)

27. Nd-Model0a-2x2x2

Central atom: Nd at (4.0013, 4.0011, 4.5357)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4901	50.3558	-89.9948	4.0014	2.0837	6.1244
O	2.4902	50.3581	179.9890	2.0837	4.0015	6.1244
O	2.4904	50.3626	0.0102	5.9191	4.0014	6.1244
O	2.4906	50.3648	89.9946	4.0014	5.9191	6.1244
O	2.6913	99.8918	-135.0034	2.1264	2.1265	4.0733
O	2.6916	99.8896	-44.9910	5.8765	2.1264	4.0734
O	2.6919	99.8880	134.9904	2.1263	5.8766	4.0734
O	2.6922	99.8871	45.0028	5.8766	5.8766	4.0734
O	3.2128	141.6769	-89.9831	4.0018	2.0088	2.0151
O	3.2131	141.6716	179.9656	2.0086	4.0023	2.0151
O	3.2136	141.6605	0.0278	5.9947	4.0021	2.0151
O	3.2139	141.6551	89.9851	4.0018	5.9950	2.0151

◈ **Local site symmetry around Nd**: Low symmetry (C1 or Cs)

28. Nd-Model0b-2x2x2

Central atom: Nd at (2.0991, 2.0845, 2.0802)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2876	92.0182	-93.5151	1.9589	-0.1974	1.9996
O	2.2911	3.9026	26.5918	2.2385	2.1543	4.3659
O	2.3053	91.9974	2.1556	4.4014	2.1712	1.9998
O	2.3093	91.9646	177.9328	-0.2074	2.1678	2.0010
O	2.3217	176.7264	37.9618	2.2036	2.1661	-0.2378
O	2.3219	92.0344	93.1419	1.9719	4.4015	1.9977

◈ **Local site symmetry around Nd**: Octahedral (Oh)

29. Nd-Model1-2x2x2 (1st Nd atom)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4448	51.0581	-86.7645	4.0622	2.0564	6.7452
O	2.4448	51.0581	176.7644	2.0564	4.0622	6.7452
O	2.4730	54.4055	1.3927	5.9652	4.0037	6.6480
O	2.4730	54.4057	88.6076	4.0037	5.9652	6.6480
O	2.4732	103.3648	-134.9999	2.2534	2.2534	4.6369
O	2.6065	108.9980	135.0338	2.2112	5.6965	4.3601
O	2.6065	108.9978	-45.0338	5.6965	2.2112	4.3601
O	2.6487	107.3875	45.0001	5.7422	5.7422	4.4171
O	3.7527	145.8975	3.9417	6.0539	4.0995	2.1013
O	3.7527	145.8976	86.0581	4.0995	6.0539	2.1013
O	3.9994	150.3003	-80.0100	4.2986	2.0034	1.7346
O	3.9994	150.3003	170.0099	2.0034	4.2986	1.7346

◈ Local site symmetry around Nd (index 7): Low symmetry (C1 or Cs)

30. Nd-Model1-2x2x2 (2nd Nd atom)

Central atom: Nd2 at (2.1039, 2.1039, 2.3703)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2765	5.3285	44.9988	2.2534	2.2534	4.6369
O	2.2871	106.1377	-2.6226	4.2986	2.0034	1.7346
O	2.2871	106.1380	92.6226	2.0034	4.2986	1.7346
O	2.3146	92.3198	-178.5453	-0.2080	2.0452	2.2766
O	2.3146	92.3199	-91.4545	2.0452	-0.2080	2.2766
O	2.7082	173.7990	-135.0002	1.8971	1.8971	-0.3221

◈ **Local site symmetry around Nd2**: Octahedral (Oh)

31. Nd-Model2(i)-2x2x2

Central atom: Nd at (4.1837, 4.0435, 3.8075)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4822	133.7606	-0.0001	5.9764	4.0435	2.0907
O	2.5669	131.1476	94.5661	4.0298	5.9703	2.1185
O	2.5669	131.1474	-94.5660	4.0298	2.1167	2.1185
O	2.6274	84.5985	47.4211	5.9536	5.9696	4.0549
O	2.6275	84.5986	-47.4212	5.9536	2.1174	4.0549
O	2.7205	129.1960	-179.9998	2.0754	4.0435	2.0883
O	2.8598	83.9069	138.1363	2.0659	5.9413	4.1111
O	2.8598	83.9069	-138.1361	2.0659	2.1458	4.1111
O	2.8733	39.2506	-0.0002	6.0017	4.0435	6.0326
O	2.9431	40.9005	96.3287	3.9713	5.9588	6.0321
O	2.9431	40.9007	-96.3287	3.9713	2.1282	6.0321

◈ **Local site symmetry around Nd**: Low symmetry (C1 or Cs)

32. Nd-Model2(ii)-2x2x2

Central atom: Nd at (2.0807, 2.0846, 2.1744)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2663	179.5682	77.7001	2.0843	2.1013	-0.0918
O	2.2784	93.4967	-177.6058	-0.1915	1.9896	2.0355
O	2.2823	93.5398	87.5138	2.1795	4.3604	2.0335
O	2.2909	94.2263	-88.0311	2.1592	-0.1988	2.0056
O	2.3035	93.5028	-2.1399	4.3783	1.9987	2.0337

◈ **Local site symmetry around Nd**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

33. Nd-Model2(iii)-2x2x2 (1st Nd atom)

Central atom: Nd1 at (4.3779, 4.3780, 4.4659)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4084	47.6448	97.4087	4.1485	6.1429	6.0885
O	2.4084	47.6459	-7.4101	6.1429	4.1485	6.0885
O	2.4654	97.3923	44.9993	6.1068	6.1068	4.1487
O	2.6589	55.0640	-174.2172	2.2093	4.1584	5.9886
O	2.6590	55.0653	-95.7815	4.1584	2.2093	5.9885
O	2.8615	142.8665	99.3905	4.0961	6.0823	2.1846
O	2.8616	142.8654	-9.3917	6.0823	4.0961	2.1846
O	2.8981	96.7894	141.5661	2.1237	6.1668	4.1233
O	2.8982	96.7893	-51.5660	6.1669	2.1237	4.1233

◈ **Local site symmetry around Nd1**: Low symmetry (C1 or Cs)

34. Nd-Model2(iii)-2x2x2 (2nd Nd atom)

Central atom: Nd2 at (2.0638, 2.0638, 2.1941)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2585	95.1706	93.3318	1.9331	4.3093	1.9906
O	2.2585	95.1704	-3.3316	4.3093	1.9331	1.9906
O	2.2937	94.4019	-91.7828	1.9927	-0.2221	2.0181
O	2.2937	94.4024	-178.2175	-0.2221	1.9927	2.0181
O	2.3073	179.1548	44.9918	2.0879	2.0879	-0.1129

◈ **Local site symmetry around Nd2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

35. Nd-Model2(iv)a-2x2x2

Central atom: Nd at (3.8230, 3.8230, 4.0938)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4623	90.3383	-134.9999	2.0819	2.0819	4.0793
O	2.5874	42.0323	173.2858	2.1025	4.0255	6.0156
O	2.5874	42.0325	-83.2855	4.0255	2.1025	6.0156
O	2.6050	138.3955	173.2025	2.1054	4.0277	2.1459
O	2.6050	138.3953	-83.2022	4.0277	2.1054	2.1459
O	2.7394	90.3164	128.3790	2.1222	5.9704	4.0787
O	2.7394	90.3164	-38.3790	5.9704	2.1222	4.0787
O	3.0097	47.1846	83.3422	4.0789	6.0159	6.1394
O	3.0097	47.1847	6.6576	6.0159	4.0789	6.1393
O	3.0423	133.2299	83.2477	4.0836	6.0242	2.0101
O	3.0423	133.2298	6.7520	6.0242	4.0836	2.0101
O	3.0723	90.3321	44.9999	5.9954	5.9954	4.0760

◈ **Local site symmetry around Nd**: Low symmetry (C1 or Cs)

36. Nd-Model2(iv)b-2x2x2

Central atom: Nd at (2.0696, 2.0522, 2.1234)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2924	92.5546	-178.0807	-0.2192	1.9755	2.0212
O	2.2980	92.7165	86.9527	2.1916	4.3443	2.0145
O	2.3071	92.4064	-1.7254	4.3737	1.9828	2.0265
O	2.3189	2.2320	-157.9099	1.9859	2.0182	4.4406
O	2.3216	92.2838	-87.3779	2.1757	-0.2652	2.0309
O	2.3601	178.1500	-142.2368	2.0094	2.0055	-0.2354

◈ **Local site symmetry around Nd**: Octahedral (Oh)

37. Model3a-Nd-Ti-2x2x2

Central atom: Nd at (2.0785, 2.0784, 2.3017)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)

O	2.3007	95.8756	-7.0766	4.3496	1.7965	2.0662
O	2.3007	95.8757	97.0772	1.7965	4.3496	2.0662
O	2.3110	4.6648	-135.0017	1.9456	1.9455	4.6051
O	2.3273	97.1166	-93.1123	1.9531	-0.2275	2.0134
O	2.3273	97.1161	-176.8886	-0.2275	1.9531	2.0134
O	2.5306	179.0261	-135.0109	2.0480	2.0480	-0.2285

◈ **Local site symmetry around Nd**: Octahedral (Oh)

38. Nd-Model3b-2x2x2

Central atom: Nd at (4.2562, 3.8144, 4.1743)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3985	88.8132	-45.0003	5.9518	2.1188	4.2240
O	2.5289	140.9947	9.5833	5.8256	4.0794	2.2091
O	2.5289	140.9946	-99.5835	3.9912	2.2450	2.2091
O	2.5308	43.1948	8.0081	5.9716	4.0558	6.0193
O	2.5308	43.1949	-98.0084	4.0148	2.0990	6.0193
O	2.7263	91.9800	52.0602	5.9314	5.9633	4.0801
O	2.7263	91.9800	-142.0602	2.1074	2.1392	4.0801
O	2.9554	49.7774	97.4896	3.9620	6.0517	6.0828
O	2.9554	49.7775	172.5108	2.0189	4.1086	6.0828
O	3.1158	133.8001	97.5083	3.9623	6.0440	2.0177
O	3.1158	133.8002	172.4922	2.0266	4.1083	2.0177
O	3.2230	92.9090	135.0001	1.9801	6.0905	4.0107

◈ **Local site symmetry around Nd**: Low symmetry (C1 or Cs)

39. Pm-Model0a-2x2x2

Central atom: Pm at (3.9909, 3.9909, 4.6919)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4444	51.5664	90.0000	3.9909	5.9057	6.2114
O	2.4444	51.5665	-179.9999	2.0762	3.9909	6.2114
O	2.4444	51.5666	-0.0001	5.9057	3.9909	6.2114
O	2.4444	51.5666	-90.0000	3.9909	2.0762	6.2114
O	2.6576	102.8244	135.0000	2.1586	5.8233	4.1020
O	2.6576	102.8243	44.9999	5.8233	5.8233	4.1020
O	2.6576	102.8243	-134.9999	2.1586	2.1586	4.1020
O	2.6576	102.8242	-45.0000	5.8233	2.1586	4.1020
O	3.3596	143.3995	-179.9995	1.9878	3.9909	1.9948
O	3.3596	143.3994	89.9995	3.9910	5.9940	1.9948
O	3.3596	143.3991	-0.0005	5.9941	3.9909	1.9948
O	3.3596	143.3991	-89.9995	3.9910	1.9878	1.9948

◈ **Local site symmetry around Pm**: Low symmetry (C1 or Cs)

40. Pm-Model0b-2x2x2

Central atom: Pm at (2.0645, 2.0793, 2.0778)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2788	91.8952	1.9043	4.3408	2.1550	2.0025

O	2.2790	2.8218	135.2350	1.9848	2.1583	4.3541
O	2.2799	91.8556	-91.9013	1.9889	-0.1981	2.0040
O	2.3072	177.1043	135.6494	1.9811	2.1608	-0.2264
O	2.3079	92.0642	178.0932	-0.2406	2.1560	1.9947
O	2.3086	92.0374	91.8989	1.9880	4.3851	1.9958

◈ **Local site symmetry around Pm**: Octahedral (Oh)

41. Pm-Model1-2x2x2 (1st Pm atom)

Central atom: Pm1 at (3.9459, 3.9459, 5.2075)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4268	51.1421	-86.5938	4.0582	2.0595	6.7301
O	2.4268	51.1417	176.5940	2.0595	4.0582	6.7301
O	2.4419	103.8835	-135.0000	2.2697	2.2697	4.6216
O	2.4606	54.9019	88.3720	4.0031	5.9583	6.6223
O	2.4606	54.9019	1.6279	5.9583	4.0031	6.6223
O	2.5874	109.3243	134.7759	2.2262	5.6791	4.3513
O	2.5874	109.3247	-44.7760	5.6791	2.2262	4.3513
O	2.6536	107.8846	45.0000	5.7316	5.7316	4.3926
O	3.7694	146.0317	3.8321	6.0473	4.0867	2.0813
O	3.7694	146.0308	86.1690	4.0867	6.0474	2.0814
O	3.9875	150.3240	170.2554	2.0002	4.2801	1.7430
O	3.9875	150.3245	-80.2558	4.2801	2.0002	1.7430

◈ **Local site symmetry around Pm1**: Low symmetry (C1 or Cs)

42. Pm-Model1-2x2x2 (2nd Pm atom)

Central atom: Pm2 at (2.0949, 2.0949, 2.3422)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2678	105.3218	-2.4802	4.2801	2.0002	1.7430
O	2.2678	105.3213	92.4805	2.0002	4.2801	1.7430
O	2.2927	6.1907	44.9981	2.2697	2.2697	4.6216
O	2.2981	91.2999	-178.5803	-0.2020	2.0380	2.2901
O	2.2981	91.2993	-91.4206	2.0379	-0.2020	2.2901
O	2.6632	173.9556	-134.9994	1.8966	1.8966	-0.3062

◈ **Local site symmetry around Pm2**: Octahedral (Oh)

43. Pm-Model2(i)-2x2x2

Central atom: Pm at (4.2676, 4.0477, 3.7637)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4177	134.5907	0.0001	5.9894	4.0477	2.0664
O	2.5336	130.5101	97.1415	4.0282	5.9590	2.1180
O	2.5336	130.5102	-97.1414	4.0282	2.1364	2.1180
O	2.5460	83.8406	-48.7832	5.9356	2.1436	4.0369
O	2.5460	83.8407	48.7834	5.9356	5.9518	4.0369
O	2.7468	127.1511	179.9999	2.0784	4.0477	2.1049
O	2.8123	37.1659	0.0003	5.9666	4.0477	6.0048
O	2.9768	83.3577	-138.9541	2.0377	2.1061	4.1081
O	2.9768	83.3576	138.9540	2.0377	5.9893	4.1081
O	3.0138	40.9439	-99.0387	3.9574	2.0972	6.0402
O	3.0138	40.9440	99.0387	3.9574	5.9982	6.0402

◈ **Local site symmetry around Pm**: Low symmetry (C1 or Cs)

44. Pm-Model2(ii)-2x2x2

Central atom: Pm at (2.0893, 2.0808, 2.1487)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2469	179.4139	-100.1755	2.0852	2.0582	-0.0981
O	2.2645	92.4210	-92.1176	2.0057	-0.1801	2.0530
O	2.2650	93.2371	91.8027	2.0182	4.3411	2.0208
O	2.2653	92.3338	1.9593	4.3514	2.1582	2.0564
O	2.2815	92.3895	178.2593	-0.1892	2.1501	2.0535

◈ **Local site symmetry around Pm**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

45. Pm-Model2(iii)-2x2x2 (1st Pm atom)

Central atom: Pm1 at (4.4112, 4.4111, 4.4427)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3747	47.0332	-8.8237	6.1283	4.1445	6.0613
O	2.3748	47.0348	98.8263	4.1445	6.1283	6.0613
O	2.4190	96.8481	45.0013	6.1094	6.1094	4.1543
O	2.7049	55.1650	-96.7584	4.1499	2.2063	5.9878
O	2.7050	55.1663	-173.2439	2.2063	4.1499	5.9878
O	2.7742	142.9808	-11.0697	6.0504	4.0904	2.2277
O	2.7743	142.9791	101.0720	4.0904	6.0504	2.2277
O	2.9171	96.3144	-53.0499	6.1540	2.0940	4.1219
O	2.9173	96.3141	143.0496	2.0940	6.1541	4.1219

◈ **Local site symmetry around Pm1**: Low symmetry (C1 or Cs)

46. Pm-Model2(iii)-2x2x2 (2nd Pm atom)

Central atom: Pm2 at (2.0602, 2.0602, 2.1607)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2462	94.9410	-3.4532	4.2939	1.9254	1.9672
O	2.2462	94.9410	93.4534	1.9254	4.2939	1.9672
O	2.2813	93.3396	-178.4718	-0.2164	1.9994	2.0278
O	2.2813	93.3400	-91.5279	1.9995	-0.2164	2.0278
O	2.2824	179.4496	45.0012	2.0757	2.0757	-0.1216

◈ **Local site symmetry around Pm2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

47. Pm-Model2(iv)a-2x2x2

Central atom: Pm at (3.7497, 3.7497, 4.0821)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3830	89.9988	-135.0003	2.0646	2.0646	4.0821
O	2.5332	40.8636	-80.3930	4.0263	2.1156	5.9978

O	2.5332	40.8640	170.3925	2.1156	4.0263	5.9978
O	2.5361	139.2285	-80.3226	4.0281	2.1171	2.1614
O	2.5361	139.2281	170.3221	2.1171	4.0281	2.1615
O	2.7277	90.0327	-35.8292	5.9612	2.1530	4.0805
O	2.7277	90.0326	125.8291	2.1530	5.9613	4.0805
O	3.1248	48.0462	8.6085	6.0474	4.0975	6.1711
O	3.1248	48.0464	81.3919	4.0975	6.0474	6.1711
O	3.1315	131.9908	8.6220	6.0509	4.0986	1.9870
O	3.1315	131.9907	81.3784	4.0986	6.0509	1.9870
O	3.2300	90.0579	45.0002	6.0336	6.0336	4.0788

◈ **Local site symmetry around Pm**: Low symmetry (C1 or Cs)

48. Pm-Model2(iv)b-2x2x2

Central atom: Pm at (2.0695, 2.0603, 2.1124)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2832	92.1470	87.6033	2.1649	4.3399	2.0269
O	2.2840	92.1113	-177.6396	-0.2110	1.9663	2.0283
O	2.2914	92.3078	-87.7491	2.1594	-0.2275	2.0202
O	2.2929	92.2872	-2.1908	4.3589	1.9727	2.0209
O	2.3075	2.7022	135.0502	1.9925	2.1372	4.4174
O	2.3434	177.9786	135.3829	2.0107	2.1184	-0.2295

◈ **Local site symmetry around Pm**: Octahedral (Oh)

49. Model3a-Pm-Ti-2x2x2

Central atom: Pm at (2.0710, 2.0712, 2.2911)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2821	96.3990	-6.3668	4.3249	1.8197	2.0367
O	2.2821	96.3927	96.3619	1.8197	4.3252	2.0370
O	2.3110	4.6221	-134.9769	1.9394	1.9395	4.5945
O	2.3115	96.6681	-177.0574	-0.2218	1.9533	2.0227
O	2.3116	96.6623	-92.9495	1.9529	-0.2217	2.0229
O	2.5197	179.0445	-134.8792	2.0414	2.0414	-0.2283

◈ **Local site symmetry around Pm**: Octahedral (Oh)

50. Pm-Model3b-2x2x2

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3409	87.7503	-44.9896	6.0217	2.1630	4.1154
O	2.3826	138.0171	14.7826	5.9084	4.2233	2.2525
O	2.3826	138.0383	-104.7531	3.9617	2.2761	2.2518
O	2.5365	42.0938	-100.9718	4.0438	2.1474	5.9058
O	2.5369	42.1095	10.9964	6.0373	4.1411	5.9056
O	2.7853	89.8657	-144.0591	2.1124	2.1818	4.0301
O	2.7870	89.8661	54.0571	6.0033	6.0730	4.0301
O	3.0904	50.4340	170.5683	2.0172	4.2071	5.9920
O	3.0913	50.4451	99.4067	3.9778	6.1681	5.9922
O	3.1141	130.2997	170.1961	2.0271	4.2211	2.0094
O	3.1146	130.2909	99.7808	3.9638	6.1579	2.0094

◈ **Local site symmetry around Pm**: Low symmetry (C1 or Cs)

51. Sm-Model0a-2x2x2

Central atom: Sm at (3.9943, 3.9934, 4.6669)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4232	51.7474	0.0002	5.8973	3.9934	6.1672
O	2.4239	51.7599	-90.0303	3.9933	2.0896	6.1672
O	2.4239	51.7601	90.0298	3.9934	5.8971	6.1672
O	2.4245	51.7729	179.9996	2.0897	3.9934	6.1672
O	2.6810	102.1976	-45.0200	5.8467	2.1397	4.1005
O	2.6810	102.1969	45.0195	5.8467	5.8470	4.1005
O	2.6830	102.1863	135.0194	2.1393	5.8471	4.1006
O	2.6830	102.1860	-135.0203	2.1393	2.1396	4.1006
O	3.3229	143.0895	0.0015	5.9900	3.9934	2.0100
O	3.3249	143.0457	-90.1259	3.9899	1.9945	2.0099
O	3.3249	143.0452	90.1172	3.9903	5.9923	2.0099
O	3.3269	143.0016	-179.9996	1.9922	3.9933	2.0099

◈ **Local site symmetry around Sm**: Low symmetry (C1 or Cs)

52. Sm-Model0b-2x2x2

Central atom: Sm at (2.0787, 2.0645, 2.0780)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2639	91.8476	-178.0485	-0.1828	1.9875	2.0050
O	2.2661	2.2647	-46.1216	2.1407	2.0000	4.3424
O	2.2666	91.7877	88.2632	2.1473	4.3290	2.0073
O	2.2948	91.8163	-1.9830	4.3709	1.9852	2.0053
O	2.2968	177.2208	-45.6717	2.1565	1.9849	-0.2161
O	2.2994	91.7833	-88.1936	2.1511	-0.2326	2.0065

◈ **Local site symmetry around Sm**: Octahedral (Oh)

53. Sm-Model1-2x2x2 (1st Sm atom)

Central atom: Sm1 at (3.9306, 3.9306, 5.2566)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4128	51.2216	176.9538	2.0523	4.0305	6.7677
O	2.4128	51.2216	-86.9537	4.0305	2.0523	6.7677
O	2.4351	105.2134	-135.0000	2.2690	2.2690	4.6176
O	2.4429	54.9096	88.5068	3.9826	5.9288	6.6609
O	2.4429	54.9097	1.4930	5.9288	3.9826	6.6609
O	2.5729	110.2793	-44.6478	5.6476	2.2345	4.3648
O	2.5730	110.2792	134.6480	2.2345	5.6476	4.3648
O	2.6308	108.6764	45.0000	5.6928	5.6928	4.4141
O	3.8068	146.5477	3.7542	6.0245	4.0680	2.0804
O	3.8068	146.5473	86.2458	4.0680	6.0246	2.0804
O	4.0115	150.6749	170.5957	1.9923	4.2516	1.7591
O	4.0115	150.6747	-80.5961	4.2516	1.9923	1.7591

◈ **Local site symmetry around Sm1**: Low symmetry (C1 or Cs)

54. Sm-Model1-2x2x2 (2nd Sm atom)

Central atom: Sm2 at (2.0935, 2.0935, 2.3923)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2391	6.3659	45.0015	2.2690	2.2690	4.6176
O	2.2513	106.3347	-2.6853	4.2516	1.9923	1.7591
O	2.2514	106.3346	92.6851	1.9923	4.2516	1.7591
O	2.2858	91.8287	-91.5624	2.0312	-0.1903	2.3194
O	2.2858	91.8288	-178.4386	-0.1903	2.0312	2.3194
O	2.7213	173.7245	-135.0020	1.8831	1.8831	-0.3127

◈ **Local site symmetry around Sm2**: Octahedral (Oh)

55. Sm-Model2(i)-2x2x2

Central atom: Sm at (4.2312, 4.0427, 3.7642)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4259	133.9386	-0.0002	5.9781	4.0426	2.0809
O	2.5244	130.5360	96.0743	4.0282	5.9504	2.1235
O	2.5244	130.5356	-96.0743	4.0282	2.1349	2.1235
O	2.5711	83.7664	48.1267	5.9372	5.9458	4.0433
O	2.5711	83.7665	-48.1268	5.9372	2.1395	4.0433
O	2.7258	127.7477	-179.9997	2.0759	4.0426	2.0955
O	2.8613	37.8664	-0.0004	5.9876	4.0426	6.0230
O	2.9193	83.2644	138.6914	2.0535	5.9564	4.1066
O	2.9193	83.2645	-138.6911	2.0535	2.1288	4.1066
O	2.9835	40.6006	97.9328	3.9633	5.9657	6.0294
O	2.9835	40.6009	-97.9327	3.9633	2.1196	6.0294

◈ **Local site symmetry around Sm**: Low symmetry (C1 or Cs)

56. Sm-Model2(ii)-2x2x2

Central atom: Sm at (2.0762, 2.0876, 2.1356)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2297	179.4916	-173.0888	2.0566	2.0852	-0.0941
O	2.2505	91.8584	88.1235	2.1498	4.3356	2.0626
O	2.2526	91.8638	-178.0424	-0.1739	2.0107	2.0623
O	2.2558	92.7168	-1.7229	4.3285	2.0198	2.0286
O	2.2696	91.9840	-88.2733	2.1445	-0.1797	2.0570

◈ **Local site symmetry around Sm**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

57. Sm-Model2(iii)-2x2x2 (1st Sm atom)

Central atom: Sm1 at (4.2551, 4.2551, 4.8111)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3448	51.6480	-4.0223	6.0894	4.1262	6.2660
O	2.3448	51.6482	94.0226	4.1262	6.0894	6.2660
O	2.4923	57.9062	-95.9252	4.0372	2.1550	6.1352
O	2.4923	57.9061	-174.0749	2.1550	4.0372	6.1353
O	2.5182	104.1697	45.0001	5.9816	5.9816	4.1946
O	2.7531	103.1325	-48.8626	6.0190	2.2359	4.1855
O	2.7531	103.1325	138.8628	2.2359	6.0190	4.1855

◈ **Local site symmetry around Sm1**: Low symmetry (C1 or Cs)

58. Sm-Model2(iii)-2x2x2 (2nd Sm atom)

Central atom: Sm2 at (2.0588, 2.0588, 2.1674)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2242	95.0690	-3.4928	4.2701	1.9238	1.9709
O	2.2242	95.0687	93.4928	1.9238	4.2701	1.9709
O	2.2687	91.1256	-92.0608	1.9772	-0.2081	2.1229
O	2.2688	91.1259	-177.9397	-0.2081	1.9772	2.1228
O	2.2856	178.9784	-135.0050	2.0299	2.0299	-0.1179

◈ **Local site symmetry around Sm2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

59. Sm-Model2(iv)a-2x2x2

Central atom: Sm at (3.7612, 3.7613, 4.1007)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3788	90.5200	-134.9996	2.0793	2.0793	4.0792
O	2.5291	41.3945	171.0612	2.1092	4.0211	5.9980
O	2.5291	41.3949	-81.0604	4.0211	2.1092	5.9980
O	2.5594	139.3406	170.8471	2.1148	4.0265	2.1592
O	2.5595	139.3400	-80.8462	4.0265	2.1148	2.1592
O	2.7392	90.4627	126.4338	2.1345	5.9650	4.0786
O	2.7393	90.4627	-36.4339	5.9650	2.1345	4.0786
O	3.0650	48.2025	81.8438	4.0854	6.0231	6.1436
O	3.0650	48.2028	8.1555	6.0231	4.0854	6.1436
O	3.1199	132.4720	81.7773	4.0904	6.0389	1.9941
O	3.1199	132.4717	8.2219	6.0389	4.0904	1.9941
O	3.1958	90.4888	44.9997	6.0209	6.0209	4.0735

◈ **Local site symmetry around Sm**: Low symmetry (C1 or Cs)

60. Sm-Model2(iv)b-2x2x2

Central atom: Sm at (2.0831, 2.0676, 2.1045)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2704	92.0232	-88.5520	2.1405	-0.2007	2.0244
O	2.2711	92.1957	177.6254	-0.1844	2.1616	2.0175
O	2.2810	92.1099	88.6442	2.1371	4.3463	2.0205
O	2.2892	91.8939	2.1177	4.3696	2.1521	2.0289
O	2.2956	1.8972	-68.3289	2.1112	1.9969	4.3988
O	2.3273	178.3417	-52.2366	2.1244	2.0143	-0.2218

◈ **Local site symmetry around Sm**: Octahedral (Oh)

61. Model3a-Sm-Ti-2x2x2

Central atom: Sm at (2.0798, 2.0798, 2.2343)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2338	96.6374	94.3029	1.9133	4.2923	1.9761
O	2.2338	96.6368	-4.3033	4.2924	1.9133	1.9761

O	2.2576	5.2823	-134.9972	1.9328	1.9328	4.4823
O	2.2903	95.2607	-92.6378	1.9748	-0.1985	2.0243
O	2.2904	95.2606	-177.3633	-0.1985	1.9748	2.0243
O	2.4369	177.8224	-135.0085	2.0143	2.0143	-0.2008

◈ **Local site symmetry around Sm**: Octahedral (Oh)

62. Sm-Model3b-2x2x2

Central atom: Sm at (4.3827, 3.8162, 4.1363)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3274	89.5749	-44.9970	6.0285	2.1706	4.1535
O	2.3640	138.4339	-107.0910	3.9218	2.3170	2.3676
O	2.3641	138.4266	17.0984	5.8821	4.2774	2.3677
O	2.4786	43.7991	-100.9941	4.0556	2.1322	5.9253
O	2.4787	43.8030	10.9990	6.0670	4.1436	5.9252
O	2.8203	92.2719	-143.5193	2.1168	2.1407	4.0245
O	2.8206	92.2718	53.5197	6.0584	6.0824	4.0245
O	2.9472	52.5770	170.9159	2.0715	4.1857	5.9273
O	2.9474	52.5792	99.0775	4.0134	6.1277	5.9273
O	3.2355	131.6977	170.0557	2.0032	4.2334	1.9841
O	3.2358	131.6956	99.9365	3.9658	6.1961	1.9839

◈ **Local site symmetry around Sm**: Low symmetry (C1 or Cs)

63. Eu-Model0a-2x2x2

Central atom: Eu at (3.9965, 3.9972, 4.4043)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.6209	47.9746	89.9865	3.9970	5.9442	6.1589
O	2.6211	47.9781	-179.9775	2.0494	3.9965	6.1589
O	2.6217	47.9887	-0.0266	5.9445	3.9963	6.1589
O	2.6219	47.9922	-89.9865	3.9970	2.0491	6.1589
O	2.7415	96.8443	135.0003	2.0718	5.9219	4.0776
O	2.7421	96.8424	44.9851	5.9222	5.9219	4.0776
O	2.7422	96.8427	-134.9857	2.0718	2.0716	4.0776
O	2.7429	96.8399	-45.0008	5.9222	2.0715	4.0776
O	3.0809	139.8829	-179.9733	2.0114	3.9963	2.0483
O	3.0810	139.8808	89.9654	3.9977	5.9826	2.0483
O	3.0820	139.8603	-89.9617	3.9979	2.0104	2.0482
O	3.0821	139.8580	-0.0321	5.9835	3.9961	2.0482

◈ **Local site symmetry around Eu**: Low symmetry (C1 or Cs)

64. Eu-Model0b-2x2x2

Central atom: Eu at (2.0746, 2.0608, 2.0880)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2340	92.3651	-92.4652	1.9786	-0.1693	1.9958
O	2.2427	2.9717	136.1180	1.9908	2.1414	4.3277
O	2.2428	92.1283	2.1666	4.3143	2.1455	2.0047
O	2.2673	92.1278	92.0753	1.9926	4.3250	2.0039
O	2.2808	177.3923	137.5379	1.9981	2.1308	-0.1904
O	2.2821	91.8498	178.3300	-0.2053	2.1272	2.0144

◈ Local site symmetry around Eu (index 8): Octahedral (Oh)

65. Eu-Model1-2x2x2 (1st Eu atom)

Central atom: Eu1 at (3.9900, 3.9900, 4.8172)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4205	99.0395	-135.0008	2.2997	2.2997	4.4369
O	2.4524	50.3761	-84.5085	4.1708	2.1096	6.3812
O	2.4525	50.3768	174.5075	2.1097	4.1708	6.3813
O	2.5415	55.1607	3.6859	6.0716	4.1241	6.2691
O	2.5415	55.1608	86.3155	4.1241	6.0716	6.2691
O	2.7681	103.6527	-43.7897	5.9318	2.1285	4.1639
O	2.7682	103.6521	133.7898	2.1285	5.9318	4.1639
O	2.9700	102.8902	45.0005	6.0372	6.0372	4.1547
O	3.5182	142.1185	4.6182	6.1433	4.1639	2.0404
O	3.5182	142.1181	85.3822	4.1639	6.1433	2.0404
O	3.5737	146.9133	-81.3844	4.2823	2.0611	1.8231
O	3.5737	146.9124	171.3839	2.0611	4.2822	1.8231

◈ **Local site symmetry around Eu1**: Low symmetry (C1 or Cs)

66. Eu-Model1-2x2x2 (2nd Eu atom)

Central atom: Eu2 at (2.0788, 2.0788, 2.1833)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2328	99.2845	90.4605	2.0611	4.2822	1.8231
O	2.2328	99.2849	-0.4603	4.2823	2.0611	1.8231
O	2.2499	90.8051	-89.8203	2.0859	-0.1709	2.1517
O	2.2500	90.8043	179.8204	-0.1709	2.0858	2.1517
O	2.2752	7.8924	45.0007	2.2997	2.2997	4.4369
O	2.4356	177.0072	-135.0057	1.9889	1.9889	-0.2490

◈ **Local site symmetry around Eu2**: Octahedral (Oh)

67. Eu-Model2(i)-2x2x2

Central atom: Eu at (4.1342, 4.0395, 4.0176)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.7156	136.3486	-0.0001	6.0087	4.0395	2.0527
O	2.7195	89.8443	46.6863	5.9997	6.0182	4.0250
O	2.7195	89.8443	-46.6863	5.9997	2.0607	4.0250
O	2.7767	43.1418	-0.0001	6.0329	4.0395	6.0437
O	2.7826	43.2863	94.4431	3.9864	5.9416	6.0432
O	2.7826	43.2864	-94.4431	3.9864	2.1373	6.0432
O	2.7944	134.5563	93.3106	4.0192	6.0274	2.0570
O	2.7945	134.5562	-93.3106	4.0192	2.0516	2.0570
O	2.8316	88.7415	137.4621	2.0483	5.9534	4.0798
O	2.8316	88.7414	-137.4620	2.0483	2.1255	4.0798
O	2.8839	133.2439	-179.9998	2.0334	4.0395	2.0418

◈ **Local site symmetry around Eu**: Low symmetry (C1 or Cs)

68. Eu-Model2(ii)-2x2x2

Central atom: Eu at (2.0863, 2.0649, 2.2087)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2645	94.6551	2.7767	4.3407	2.1742	2.0249
O	2.2666	94.4802	-92.6430	1.9821	-0.1924	2.0316
O	2.2973	94.6321	177.6688	-0.2016	2.1580	2.0231
O	2.3007	94.5709	92.1263	2.0012	4.3567	2.0253
O	2.3094	179.8978	-67.7006	2.0879	2.0611	-0.1008

◈ **Local site symmetry around Eu**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

69. Eu-Model2(iii)-2x2x2 (1st Eu atom)

Central atom: Eu1 at (4.4080, 4.4080, 4.2772)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4840	93.5553	45.0000	6.1611	6.1611	4.1232
O	2.5341	44.9501	-9.0397	6.1761	4.1267	6.0706
O	2.5341	44.9502	99.0398	4.1267	6.1761	6.0706
O	2.7290	140.4188	100.3844	4.0946	6.1184	2.1739
O	2.7290	140.4187	-10.3846	6.1184	4.0946	2.1739
O	2.8195	52.5206	-174.1706	2.1821	4.1808	5.9928
O	2.8195	52.5206	-95.8294	4.1807	2.1821	5.9928
O	2.9679	93.0709	-52.1634	6.2260	2.0674	4.1182
O	2.9679	93.0709	142.1634	2.0674	6.2260	4.1182
O	3.3359	132.5388	-91.8047	4.3306	1.9513	2.0218
O	3.3359	132.5385	-178.1952	1.9513	4.3306	2.0218

◈ **Local site symmetry around Eu1**: Low symmetry (C1 or Cs)

70. Eu-Model2(iii)-2x2x2 (2nd Eu atom)

Central atom: Eu2 at (2.0869, 2.0869, 2.2399)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2583	95.5399	93.4600	1.9513	4.3306	2.0218
O	2.2583	95.5403	-3.4595	4.3306	1.9513	2.0218
O	2.3075	95.6796	-177.7547	-0.2075	1.9970	2.0115
O	2.3075	95.6799	-92.2452	1.9970	-0.2075	2.0115
O	2.3464	179.8677	45.0043	2.0907	2.0907	-0.1065

◈ **Local site symmetry around Eu2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

71. Eu-Model2(iv)a-2x2x2

Central atom: Eu at (3.9296, 3.9296, 4.2634)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.6614	94.1996	-135.0000	2.0527	2.0527	4.0685
O	2.6664	45.2854	-87.5115	4.0119	2.0366	6.1394
O	2.6664	45.2855	177.5115	2.0366	4.0119	6.1394
O	2.7851	94.2198	-42.5651	5.9753	2.0508	4.0585
O	2.7851	94.2198	132.5652	2.0508	5.9753	4.0585
O	2.8363	46.6483	2.9760	5.9892	4.0367	6.2104
O	2.8363	46.6483	87.0240	4.0367	5.9892	6.2104
O	2.8841	92.6237	45.0000	5.9668	5.9668	4.1314

O	2.9162	139.2021	177.5676	2.0259	4.0105	2.0558
O	2.9162	139.2021	-87.5677	4.0105	2.0259	2.0558
O	3.0586	137.1136	86.9811	4.0392	6.0083	2.0224
O	3.0586	137.1137	3.0189	6.0083	4.0392	2.0223

◈ **Local site symmetry around Eu**: Low symmetry (C1 or Cs)

72. Eu-Model2(iv)b-2x2x2

Central atom: Eu at (2.0696, 2.0482, 2.1174)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2740	92.6430	87.2903	2.1769	4.3173	2.0125
O	2.2797	92.1496	-178.0735	-0.2072	1.9717	2.0319
O	2.2900	92.3417	-1.6017	4.3568	1.9843	2.0238
O	2.3018	92.3724	-87.6297	2.1647	-0.2496	2.0221
O	2.3043	2.2969	-157.8117	1.9840	2.0134	4.4198
O	2.3538	178.1907	-145.4814	2.0083	2.0061	-0.2352

◈ **Local site symmetry around Eu**: Octahedral (Oh)

73. Model3a-Eu-Ti-2x2x2

Central atom: Eu at (2.0570, 2.0570, 2.1861)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1981	96.0926	-4.2887	4.2366	1.8936	1.9528
O	2.1981	96.0929	94.2874	1.8936	4.2366	1.9528
O	2.2513	93.7253	-177.8149	-0.1879	1.9714	2.0398
O	2.2514	93.7237	-92.1852	1.9714	-0.1879	2.0399
O	2.2726	4.9123	-135.0113	1.9194	1.9195	4.4504
O	2.3737	177.9503	-134.9987	1.9970	1.9970	-0.1861

◈ **Local site symmetry around Eu**: Octahedral (Oh)

74. Eu-Model3b-2x2x2

Central atom: Eu at (4.4189, 3.7755, 4.0079)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3014	86.8817	-45.0024	6.0438	2.1505	4.1331
O	2.3405	137.5700	16.9416	5.9295	4.2356	2.2804
O	2.3405	137.5661	-106.9492	3.9586	2.2649	2.2805
O	2.5561	41.4564	12.3649	6.0719	4.1379	5.9236
O	2.5561	41.4592	-102.3702	4.0564	2.1224	5.9236
O	2.8214	89.6635	54.5904	6.0537	6.0750	4.0245
O	2.8217	89.6632	-144.5910	2.1192	2.1406	4.0245
O	3.1291	50.8693	99.9046	4.0014	6.1666	5.9827
O	3.1294	50.8721	170.1017	2.0275	4.1928	5.9827
O	3.1601	129.5096	100.5322	3.9733	6.1725	1.9974
O	3.1603	129.5066	169.4725	2.0216	4.2210	1.9974

◈ **Local site symmetry around Eu**: Low symmetry (C1 or Cs)

75. Gd-Model0a-2x2x2

Central atom: Gd at (3.9865, 3.9868, 4.7634)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3907	52.6725	90.0039	3.9864	5.8878	6.2130
O	2.3909	52.6755	-0.0115	5.8878	3.9864	6.2130
O	2.3911	52.6793	-179.9894	2.0850	3.9864	6.2130
O	2.3912	52.6824	-90.0045	3.9864	2.0851	6.2130
O	2.6806	103.8586	44.9955	5.8270	5.8269	4.1213
O	2.6809	103.8589	135.0086	2.1458	5.8270	4.1212
O	2.6813	103.8568	-45.0096	5.8270	2.1457	4.1212
O	2.6816	103.8538	-134.9965	2.1457	2.1457	4.1213
O	3.4099	144.1100	90.0072	3.9863	5.9857	2.0009
O	3.4103	144.0995	-0.0396	5.9863	3.9854	2.0009
O	3.4108	144.0861	-179.9490	1.9859	3.9850	2.0009
O	3.4113	144.0756	-90.0280	3.9856	1.9853	2.0010

◈ **Local site symmetry around Gd**: Low symmetry (C1 or Cs)

76. Gd-Model0b-2x2x2

Central atom: Gd at (2.0579, 2.0759, 2.0886)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2261	92.1359	-177.9549	-0.1652	1.9966	2.0056
O	2.2303	91.9459	88.1461	2.1300	4.3038	2.0129
O	2.2304	2.5067	-49.4977	2.1213	2.0018	4.3169
O	2.2738	92.1139	-2.1123	4.3286	1.9922	2.0047
O	2.2845	177.0920	-49.5160	2.1332	1.9878	-0.1929
O	2.2853	91.9963	-88.0852	2.1342	-0.2067	2.0090

◈ **Local site symmetry around Gd**: Octahedral (Oh)

77. Gd-Model1-2x2x2 (1st Gd atom)

Central atom: Gd1 at (3.9591, 3.9591, 5.0401)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3551	51.7885	-85.3996	4.1076	2.1146	6.4969
O	2.3551	51.7883	175.3996	2.1146	4.1076	6.4969
O	2.3962	103.3782	-135.0001	2.3107	2.3107	4.4857
O	2.4283	56.7407	87.0858	4.0624	5.9871	6.3719
O	2.4283	56.7405	2.9142	5.9871	4.0624	6.3719
O	2.6566	107.8884	134.1810	2.1972	5.7722	4.2241
O	2.6566	107.8885	-44.1809	5.7722	2.1972	4.2241
O	2.8565	106.4076	44.9999	5.8968	5.8968	4.2333
O	3.6833	144.5438	85.8969	4.1120	6.0903	2.0398
O	3.6834	144.5438	4.1033	6.0903	4.1120	2.0398
O	3.7920	148.9037	-81.5544	4.2468	2.0219	1.7930
O	3.7920	148.9035	171.5542	2.0219	4.2468	1.7930

◈ **Local site symmetry around Gd1**: Low symmetry (C1 or Cs)

78. Gd-Model1-2x2x2 (2nd Gd atom)

Central atom: Gd2 at (2.0765, 2.0765, 2.2467)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)

O	2.2179	101.8031	91.4416	2.0219	4.2468	1.7930
O	2.2179	101.8030	-1.4415	4.2468	2.0219	1.7930
O	2.2490	90.3112	-179.2295	-0.1723	2.0463	2.2345
O	2.2490	90.3110	-90.7702	2.0463	-0.1723	2.2345
O	2.2634	8.4156	44.9997	2.3107	2.3107	4.4857
O	2.5157	175.3300	-134.9983	1.9317	1.9317	-0.2606

◈ **Local site symmetry around Gd2**: Octahedral (Oh)

79. Gd-Model2(i)-2x2x2

Central atom: Gd at (4.3268, 4.0442, 3.7205)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3237	134.7228	-0.0001	5.9778	4.0441	2.0854
O	2.4878	129.7240	99.0920	4.0245	5.9336	2.1305
O	2.4878	129.7239	-99.0919	4.0245	2.1547	2.1305
O	2.5040	82.7473	49.7836	5.9307	5.9410	4.0366
O	2.5041	82.7473	-49.7838	5.9307	2.1473	4.0366
O	2.8000	125.6285	-179.9999	2.0509	4.0441	2.0894
O	2.8117	35.6385	-0.0002	5.9651	4.0441	6.0056
O	3.0402	82.7396	139.7332	2.0256	5.9934	4.1047
O	3.0402	82.7396	-139.7331	2.0256	2.0949	4.1047
O	3.0576	40.6337	100.7320	3.9561	6.0005	6.0408
O	3.0576	40.6338	-100.7319	3.9561	2.0878	6.0408

◈ **Local site symmetry around Gd**: Low symmetry (C1 or Cs)

80. Gd-Model2(ii)-2x2x2

Central atom: Gd at (2.0727, 2.0797, 2.1164)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2095	179.4696	-173.8004	2.0523	2.0775	-0.0930
O	2.2289	91.4035	88.1166	2.1459	4.3067	2.0618
O	2.2317	91.2623	-178.0703	-0.1572	2.0046	2.0672
O	2.2370	91.8427	-1.5552	4.3077	2.0190	2.0444
O	2.2507	91.2710	-88.3473	2.1376	-0.1695	2.0665

81. Gd-Model2(iii)-2x2x2 (1st Gd atom)

Central atom: Gd1 at (4.2342, 4.2342, 4.8774)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2987	52.4242	-4.0766	6.0515	4.1047	6.2792
O	2.2987	52.4252	94.0779	4.1047	6.0515	6.2792
O	2.4536	58.6508	-95.7381	4.0247	2.1493	6.1539
O	2.4536	58.6510	-174.2627	2.1493	4.0247	6.1539
O	2.5034	105.8164	45.0004	5.9374	5.9373	4.1951
O	2.7486	104.4663	-48.9350	5.9826	2.2276	4.1908
O	2.7487	104.4660	138.9358	2.2275	5.9825	4.1908

◈ **Local site symmetry around Gd1**: Low symmetry (C1 or Cs)

82. Gd-Model2(iii)-2x2x2 (2nd Gd atom)

Central atom: Gd2 at (2.0557, 2.0557, 2.1436)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)

O	2.1996	94.7481	93.7525	1.9122	4.2431	1.9616
O	2.1997	94.7466	-3.7530	4.2431	1.9122	1.9616
O	2.2543	89.7848	-178.0158	-0.1973	1.9777	2.1521
O	2.2543	89.7849	-91.9837	1.9777	-0.1973	2.1521
O	2.2705	178.4604	-134.9905	2.0126	2.0126	-0.1261

◈ **Local site symmetry around Gd2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

83. Gd-Model2(iv)a-2x2x2

Central atom: Gd at (3.7001, 3.7002, 4.0845)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2982	90.2435	-134.9994	2.0751	2.0751	4.0747
O	2.4767	40.4488	168.1008	2.1279	4.0315	5.9692
O	2.4767	40.4495	-78.0999	4.0315	2.1279	5.9692
O	2.4982	139.9562	168.1279	2.1272	4.0308	2.1720
O	2.4982	139.9554	-78.1269	4.0308	2.1272	2.1720
O	2.7719	90.4077	124.4658	2.1315	5.9854	4.0648
O	2.7720	90.4077	-34.4660	5.9854	2.1315	4.0648
O	3.1634	48.9371	80.3348	4.1006	6.0515	6.1625
O	3.1634	48.9374	9.6642	6.0515	4.1006	6.1625
O	3.1838	131.3353	80.3081	4.1026	6.0566	1.9817
O	3.1838	131.3350	9.6910	6.0566	4.1026	1.9817

◈ **Local site symmetry around Gd**: Low symmetry (C1 or Cs)

84. Gd-Model2(iv)b-2x2x2

Central atom: Gd at (2.0762, 2.0777, 2.1000)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2450	91.9191	178.5615	-0.1668	2.1341	2.0248
O	2.2459	91.8868	-88.5629	2.1325	-0.1662	2.0261
O	2.2697	91.8017	1.3961	4.3441	2.1330	2.0287
O	2.2708	91.7674	88.5905	2.1321	4.3468	2.0300
O	2.2744	0.8943	45.7332	2.1010	2.1032	4.3741
O	2.3084	178.7379	45.7679	2.1117	2.1142	-0.2078

◈ **Local site symmetry around Gd**: Octahedral (Oh)

85. Model3a-Gd-Ti-2x2x2

Central atom: Gd at (2.0635, 2.0635, 2.2144)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1964	95.9039	94.0074	1.9108	4.2428	1.9885
O	2.1964	95.9037	-4.0068	4.2429	1.9108	1.9885
O	2.2455	4.6323	-135.0019	1.9352	1.9352	4.4526
O	2.2595	94.7139	-92.2980	1.9732	-0.1866	2.0287
O	2.2595	94.7138	-177.7020	-0.1866	1.9732	2.0287
O	2.4105	178.0575	-134.9952	2.0057	2.0057	-0.1947

◈ **Local site symmetry around Gd**: Octahedral (Oh)

86. Gd-Model3b-2x2x2

Central atom: Gd at (4.4011, 3.7904, 4.1477)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2985	90.1678	-44.9866	6.0267	2.1655	4.1410
O	2.3359	138.7645	18.0956	5.8646	4.2686	2.3911
O	2.3362	138.7896	-108.0578	3.9240	2.3271	2.3902
O	2.4460	43.8469	-101.7956	4.0547	2.1318	5.9117
O	2.4463	43.8581	11.8219	6.0601	4.1377	5.9117
O	2.8332	92.5862	-144.2457	2.1042	2.1366	4.0199
O	2.8341	92.5897	54.2439	6.0554	6.0880	4.0197
O	2.9583	53.0135	170.5349	2.0702	4.1790	5.9275
O	2.9601	53.0239	99.4333	4.0135	6.1232	5.9282
O	3.2695	131.6256	169.6586	1.9968	4.2291	1.9759
O	3.2705	131.6183	100.3141	3.9633	6.1959	1.9756

◈ **Local site symmetry around Gd**: Low symmetry (C1 or Cs)

87. Tb-Model0a-2x2x2

Central atom: Tb at (3.9746, 3.9744, 4.8957)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3542	53.3164	-0.0083	5.8625	3.9741	6.3021
O	2.3543	53.3187	90.0130	3.9742	5.8625	6.3021
O	2.3546	53.3266	-90.0133	3.9741	2.0859	6.3020
O	2.3547	53.3289	-179.9914	2.0859	3.9741	6.3020
O	2.6248	106.4238	45.0025	5.7548	5.7547	4.1536
O	2.6253	106.4197	-45.0123	5.7549	2.1934	4.1536
O	2.6257	106.4177	135.0122	2.1933	5.7549	4.1536
O	2.6264	106.4149	-135.0027	2.1931	2.1931	4.1535
O	3.5294	145.5141	-0.0438	5.9729	3.9729	1.9866
O	3.5297	145.5052	90.0627	3.9724	5.9734	1.9866
O	3.5308	145.4727	-90.0550	3.9727	1.9731	1.9868
O	3.5311	145.4638	-179.9676	1.9727	3.9733	1.9869

◈ **Local site symmetry around Tb**: Low symmetry (C1 or Cs)

88. Tb-Model0b-2x2x2

Central atom: Tb at (2.0622, 2.0662, 2.0765)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2249	91.7098	-91.8352	1.9910	-0.1566	2.0102
O	2.2281	2.1330	135.6463	2.0029	2.1241	4.3031
O	2.2290	91.5916	1.5144	4.2896	2.1250	2.0146
O	2.2554	91.7094	91.7979	1.9915	4.3195	2.0093
O	2.2616	177.6650	137.1976	1.9946	2.1288	-0.1831
O	2.2646	91.6090	178.4730	-0.2007	2.1265	2.0130

◈ **Local site symmetry around Tb**: Octahedral (Oh)

89. Tb-Model1-2x2x2 (1st Tb atom)

Central atom: Tb1 at (3.9462, 3.9462, 5.2630)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3615	52.1703	-87.5856	4.0248	2.0827	6.7114
O	2.3615	52.1704	177.5854	2.0827	4.0248	6.7114
O	2.3985	55.5544	1.4283	5.9235	3.9955	6.6197
O	2.3985	55.5543	88.5718	3.9955	5.9235	6.6197
O	2.4348	107.1374	-135.0002	2.3010	2.3010	4.5456
O	2.5243	110.9799	-43.7930	5.6475	2.3151	4.3593
O	2.5243	110.9798	133.7931	2.3151	5.6475	4.3593
O	2.6502	108.4956	45.0000	5.7234	5.7234	4.4223
O	3.7949	147.8516	1.6598	5.9647	4.0047	2.0500
O	3.7949	147.8515	88.3404	4.0047	5.9647	2.0500
O	3.9865	149.2860	173.0751	1.9249	4.1917	1.8357
O	3.9865	149.2860	-83.0752	4.1917	1.9249	1.8357

◈ **Local site symmetry around Tb1**: Low symmetry (C1 or Cs)

90. Tb-Model1-2x2x2 (2nd Tb atom)

Central atom: Tb2 at (2.0589, 2.0589, 2.3732)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1992	8.9561	45.0006	2.3010	2.3010	4.5456
O	2.2036	104.1179	93.5939	1.9249	4.1917	1.8357
O	2.2036	104.1179	-3.5942	4.1917	1.9249	1.8357
O	2.2651	90.5714	-92.5539	1.9580	-0.2038	2.3506
O	2.2651	90.5716	-177.4462	-0.2038	1.9580	2.3506
O	2.6533	174.6211	-134.9993	1.8830	1.8830	-0.2684

◈ **Local site symmetry around Tb2**: Octahedral (Oh)

91. Tb-Model2(i)-2x2x2

Central atom: Tb at (4.6178, 4.0365, 4.1153)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3458	38.5408	0.0201	6.0795	4.0370	5.9501
O	2.3781	91.6485	-53.6055	6.0283	2.1231	4.0469
O	2.3785	91.6500	53.6194	6.0281	5.9507	4.0468
O	2.4080	144.7568	0.0328	6.0073	4.0373	2.1487
O	2.5850	46.5503	-110.0533	3.9743	2.2737	5.8930
O	2.5856	46.5659	110.0840	3.9731	5.7999	5.8929
O	2.8302	134.4842	-107.2071	4.0205	2.1077	2.1321
O	2.8330	134.4642	107.1863	4.0204	5.9681	2.1309

◈ **Local site symmetry around Tb**: Low symmetry (C1 or Cs)

92. Tb-Model2(ii)-2x2x2

Central atom: Tb at (2.0753, 2.0596, 2.0831)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1725	179.4404	104.2931	2.0701	2.0802	-0.0893
O	2.2110	89.8979	-1.6198	4.2855	1.9971	2.0871

O	2.2183	89.7133	91.5679	2.0147	4.2770	2.0942
O	2.2240	90.7099	-91.3316	2.0237	-0.1636	2.0556
O	2.2314	90.0650	-178.5143	-0.1553	2.0018	2.0806

◈ **Local site symmetry around Tb**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

93. Tb-Model2(iii)-2x2x2 (1st Tb atom)

Central atom: Tb1 at (4.2102, 4.2105, 4.9925)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2837	53.3275	93.2899	4.1051	6.0391	6.3564
O	2.2837	53.3384	-3.2981	6.0391	4.1051	6.3561
O	2.4066	58.9689	-95.2363	4.0220	2.1569	6.2331
O	2.4068	58.9597	-174.7650	2.1566	4.0223	6.2335
O	2.5094	107.7682	44.9969	5.9001	5.9002	4.2267
O	2.6767	106.7304	138.4458	2.2920	5.9108	4.2219
O	2.6778	106.7245	-48.4448	5.9113	2.2914	4.2219

◈ **Local site symmetry around Tb1**: Low symmetry (C1 or Cs)

94. Tb-Model2(iii)-2x2x2 (2nd Tb atom)

Central atom: Tb2 at (2.0397, 2.0396, 2.0982)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1946	93.7238	-2.7790	4.2271	1.9335	1.9557
O	2.1947	93.7277	92.7797	1.9334	4.2271	1.9555
O	2.2247	177.8239	-134.8623	1.9801	1.9798	-0.1249
O	2.2312	86.9707	-178.3675	-0.1875	1.9762	2.2161
O	2.2312	86.9566	-91.6310	1.9762	-0.1876	2.2167

◈ **Local site symmetry around Tb2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

95. Tb-Model2(iv)a-2x2x2

Central atom: Tb at (3.6712, 3.6712, 4.0750)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2684	89.9678	-134.9999	2.0672	2.0672	4.0762
O	2.4642	140.2310	167.0320	2.1350	4.0249	2.1809
O	2.4642	140.2309	-77.0318	4.0249	2.1350	2.1809
O	2.4685	39.6881	167.0699	2.1347	4.0239	5.9746
O	2.4685	39.6881	-77.0698	4.0239	2.1347	5.9746
O	2.7306	89.9321	123.2895	2.1724	5.9537	4.0782
O	2.7306	89.9321	-33.2895	5.9537	2.1724	4.0782

◈ **Local site symmetry around Tb**: Low symmetry (C1 or Cs)

96. Tb-Model2(iv)b-2x2x2

Central atom: Tb at (2.0576, 2.0775, 2.0958)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2332	91.6092	178.7909	-0.1742	2.1246	2.0331

O	2.2370	91.7383	-88.2434	2.1261	-0.1574	2.0280
O	2.2406	91.7463	1.0461	4.2968	2.1184	2.0275
O	2.2502	91.5892	88.4304	2.1192	4.3260	2.0334
O	2.2578	1.4429	162.5352	2.0034	2.0946	4.3530
O	2.2888	178.7126	146.5140	2.0147	2.1059	-0.1924

◈ **Local site symmetry around Tb**: Octahedral (Oh)

97. Model3a-Tb-Ti-2x2x2

Central atom: Tb at (2.0676, 2.0676, 2.2191)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1939	96.0955	94.0398	1.9140	4.2437	1.9862
O	2.1939	96.0964	-4.0401	4.2438	1.9139	1.9861
O	2.2242	4.7399	-134.9970	1.9377	1.9377	4.4357
O	2.2508	94.7987	-177.6846	-0.1734	1.9770	2.0308
O	2.2508	94.7992	-92.3150	1.9770	-0.1735	2.0308
O	2.4056	178.1390	-135.0067	2.0124	2.0124	-0.1852

◈ **Local site symmetry around Tb**: Octahedral (Oh)

98. Tb-Model3b-2x2x2

Central atom: Tb at (4.4670, 3.7235, 4.1812)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2546	90.0058	-44.9969	6.0613	2.1293	4.1810
O	2.3104	139.3159	-111.7357	3.9092	2.3244	2.4292
O	2.3105	139.3078	21.7371	5.8663	4.2814	2.4293
O	2.3963	43.3793	-104.0015	4.0688	2.1265	5.9229
O	2.3967	43.3855	14.0018	6.0644	4.1218	5.9230
O	2.8187	93.2772	-145.9397	2.1356	2.1474	4.0201
O	2.8190	93.2768	55.9328	6.0435	6.0549	4.0201
O	3.0096	54.0988	100.5700	4.0198	6.1200	5.9460
O	3.0098	54.0968	169.4278	2.0704	4.1708	5.9462

◈ **Local site symmetry around Tb**: Low symmetry (C1 or Cs)

99. Dy-Model0a-2x2x2

Central atom: Dy at (3.9716, 3.9720, 4.9418)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3317	53.8929	179.9996	2.0878	3.9720	6.3159
O	2.3319	53.8972	-89.9903	3.9719	2.0879	6.3158
O	2.3319	53.8976	89.9905	3.9719	5.8560	6.3158
O	2.3321	53.9021	0.0005	5.8560	3.9720	6.3158
O	2.6252	107.3091	-134.9948	2.1995	2.1995	4.1607
O	2.6253	107.3093	134.9945	2.1995	5.7444	4.1607
O	2.6259	107.3052	-44.9944	5.7446	2.1994	4.1607
O	2.6259	107.3046	44.9949	5.7446	5.7446	4.1607
O	3.5713	145.9815	-179.9998	1.9736	3.9720	1.9817
O	3.5719	145.9635	-89.9579	3.9731	1.9727	1.9819
O	3.5719	145.9618	89.9546	3.9732	5.9713	1.9819
O	3.5725	145.9440	0.0041	5.9722	3.9721	1.9820

◈ **Local site symmetry around Dy**: Low symmetry (C1 or Cs)

100. Dy-Model0b-2x2x2

Central atom: Dy at (2.0652, 2.0752, 2.0685)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2133	91.5307	178.3778	-0.1465	2.1378	2.0094
O	2.2182	1.9280	46.0456	2.1170	2.1289	4.2854
O	2.2210	91.3727	-88.7520	2.1135	-0.1447	2.0153
O	2.2401	91.5941	1.6505	4.3035	2.1397	2.0062
O	2.2500	177.8831	48.4806	2.1203	2.1374	-0.1800
O	2.2558	91.4704	88.6503	2.1183	4.3296	2.0106

◈ **Local site symmetry around Dy**: Octahedral (Oh)

101. Dy-Model1-2x2x2 (1st Dy atom)

Central atom: Dy1 at (3.9281, 3.9281, 5.2739)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3433	52.2841	-87.4661	4.0101	2.0762	6.7074
O	2.3433	52.2845	177.4660	2.0762	4.0100	6.7074
O	2.3803	56.0379	1.5289	5.9016	3.9808	6.6036
O	2.3803	56.0381	88.4715	3.9808	5.9016	6.6036
O	2.4105	107.8987	-135.0000	2.3061	2.3061	4.5330
O	2.5309	111.3664	-43.6169	5.6345	2.3022	4.3518
O	2.5309	111.3667	133.6169	2.3022	5.6345	4.3518
O	2.6733	108.8390	45.0000	5.7171	5.7171	4.4107
O	3.8111	147.7785	1.9326	5.9590	3.9966	2.0497
O	3.8111	147.7786	88.0672	3.9966	5.9590	2.0497
O	3.9852	149.6055	-82.9512	4.1755	1.9270	1.8364
O	3.9852	149.6054	172.9512	1.9270	4.1755	1.8364

◈ **Local site symmetry around Dy1**: Low symmetry (C1 or Cs)

102. Dy-Model1-2x2x2 (2nd Dy atom)

Central atom: Dy2 at (2.0578, 2.0578, 2.3860)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1755	9.2885	44.9997	2.3061	2.3061	4.5330
O	2.1918	104.5229	93.5333	1.9270	4.1755	1.8364
O	2.1918	104.5227	-3.5331	4.1755	1.9270	1.8364
O	2.2517	90.6650	-92.3775	1.9644	-0.1918	2.3599
O	2.2517	90.6648	-177.6226	-0.1918	1.9644	2.3599
O	2.6638	174.6417	-135.0016	1.8819	1.8819	-0.2662

◈ **Local site symmetry around Dy2**: Octahedral (Oh)

103. Dy-Model2(i)-2x2x2

Central atom: Dy at (4.6346, 4.0359, 4.1331)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3219	38.5100	-0.0066	6.0804	4.0357	5.9500

O	2.3531	91.9920	53.9939	6.0171	5.9383	4.0513
O	2.3532	91.9922	-53.9983	6.0171	2.1333	4.0513
O	2.3918	145.4682	-0.0106	5.9905	4.0357	2.1627
O	2.5645	46.8039	110.7284	3.9729	5.7844	5.8885
O	2.5647	46.8081	-110.7328	3.9727	2.2872	5.8885
O	2.8586	134.6413	107.5539	4.0212	5.9751	2.1245
O	2.8592	134.6338	-107.5502	4.0211	2.0960	2.1243

◈ **Local site symmetry around Dy**: Low symmetry (C1 or Cs)

104. Dy-Model2(ii)-2x2x2

Central atom: Dy at (2.0640, 2.0596, 2.0581)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1674	179.4890	-147.8031	2.0476	2.0493	-0.1093
O	2.1953	88.8894	-88.6050	2.1174	-0.1347	2.1007
O	2.1962	88.8267	178.6813	-0.1311	2.1101	2.1031
O	2.2028	89.7812	88.6546	2.1157	4.2617	2.0665
O	2.2034	89.7612	1.3232	4.2668	2.1105	2.0673

◈ **Local site symmetry around Dy**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

105. Dy-Model2(iii)-2x2x2 (1st Dy atom)

Central atom: Dy1 at (4.4853, 4.4852, 4.3762)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2815	95.6173	45.0006	6.0908	6.0907	4.1529
O	2.2968	44.5141	-13.1137	6.0535	4.1199	6.0141
O	2.2969	44.5144	103.1148	4.1199	6.0535	6.0141
O	2.6423	143.2940	-14.3366	6.0154	4.0941	2.2579
O	2.6423	143.2933	104.3372	4.0942	6.0154	2.2579
O	2.8722	95.1958	-56.4030	6.0680	2.1027	4.1161
O	2.8722	95.1959	146.4029	2.1027	6.0680	4.1161
O	2.9079	55.9341	-100.8337	4.0325	2.1193	6.0051
O	2.9080	55.9341	-169.1681	2.1192	4.0325	6.0051

◈ **Local site symmetry around Dy1**: Low symmetry (C1 or Cs)

106. Dy-Model2(iii)-2x2x2 (2nd Dy atom)

Central atom: Dy2 at (2.0473, 2.0473, 2.0620)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1772	179.7240	-135.0117	2.0399	2.0399	-0.1152
O	2.1868	91.8382	92.2944	1.9598	4.2313	1.9918
O	2.1869	91.8381	-2.2945	4.2313	1.9598	1.9918
O	2.2256	89.4820	-90.6414	2.0224	-0.1780	2.0821
O	2.2256	89.4818	-179.3586	-0.1780	2.0224	2.0821

◈ **Local site symmetry around Dy2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

107. Dy-Model2(iv)a-2x2x2

Central atom: Dy at (3.6532, 3.6532, 4.0924)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2430	90.3453	-135.0001	2.0672	2.0672	4.0789
O	2.4294	39.8753	-76.3585	4.0206	2.1396	5.9568
O	2.4294	39.8755	166.3582	2.1396	4.0206	5.9568
O	2.4597	140.6636	-76.2692	4.0233	2.1386	2.1899
O	2.4597	140.6635	166.2690	2.1386	4.0233	2.1899
O	2.7362	90.3025	-32.7358	5.9549	2.1736	4.0779
O	2.7363	90.3026	122.7359	2.1736	5.9549	4.0779

◈ **Local site symmetry around Dy**: Low symmetry (C1 or Cs)

108. Dy-Model2(iv)b-2x2x2

Central atom: Dy at (2.0739, 2.0336, 2.0942)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2181	91.6449	88.8297	2.1192	4.2503	2.0305
O	2.2259	91.5275	-178.9331	-0.1508	1.9922	2.0348
O	2.2353	91.5510	-88.8752	2.1177	-0.2004	2.0337
O	2.2435	91.4338	-1.0655	4.3163	1.9919	2.0380
O	2.2472	0.6241	-47.5385	2.0904	2.0155	4.3412
O	2.2759	179.1548	-41.0871	2.0992	2.0115	-0.1815

◈ **Local site symmetry around Dy**: Octahedral (Oh)

109. Model3a-Dy-Ti-2x2x2

Central atom: Dy at (2.0607, 2.0606, 2.2107)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1851	95.6223	-3.4976	4.2312	1.9280	1.9967
O	2.1851	95.6205	93.4976	1.9280	4.2312	1.9967
O	2.2174	4.2312	-135.0071	1.9450	1.9450	4.4221
O	2.2364	94.5034	-92.0285	1.9817	-0.1675	2.0351
O	2.2364	94.5042	-177.9716	-0.1675	1.9817	2.0351
O	2.3893	178.2454	-135.0051	2.0089	2.0089	-0.1774

◈ **Local site symmetry around Dy**: Octahedral (Oh)

110. Dy-Model3b-2x2x2

Central atom: Dy at (4.4854, 3.7068, 4.1833)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2411	90.0979	-45.0008	6.0701	2.1221	4.1795
O	2.2982	139.5549	22.6429	5.8614	4.2808	2.4343
O	2.2984	139.5524	-112.6643	3.9109	2.3309	2.4343
O	2.3733	43.2971	-104.6448	4.0739	2.1321	5.9106
O	2.3744	43.2957	14.6181	6.0610	4.1177	5.9114
O	2.8200	93.3681	56.5368	6.0377	6.0553	4.0176
O	2.8214	93.3690	-146.5523	2.1353	2.1544	4.0175
O	3.0235	54.3865	100.8783	4.0216	6.1206	5.9439
O	3.0251	54.3973	169.1386	2.0699	4.1703	5.9444

◈ **Local site symmetry around Dy**: Low symmetry (C1 or Cs)

111. Ho-Model0a-2x2x2

Central atom: Ho at (3.9709, 3.9704, 4.9779)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3123	54.3824	-89.9992	3.9709	2.0907	6.3245
O	2.3126	54.3881	179.9871	2.0908	3.9709	6.3245
O	2.3126	54.3890	0.0128	5.8510	3.9709	6.3245
O	2.3129	54.3947	89.9991	3.9709	5.8509	6.3244
O	2.6361	107.8931	-135.0064	2.1969	2.1968	4.1680
O	2.6362	107.8927	-44.9927	5.7450	2.1968	4.1680
O	2.6370	107.8873	134.9926	2.1966	5.7452	4.1679
O	2.6371	107.8868	45.0065	5.7453	5.7452	4.1679
O	3.5989	146.2721	-89.9967	3.9710	1.9722	1.9848
O	3.5997	146.2455	179.9348	1.9708	3.9727	1.9850
O	3.5998	146.2420	0.0659	5.9713	3.9727	1.9850
O	3.6006	146.2153	89.9951	3.9711	5.9727	1.9853

◈ **Local site symmetry around Ho**: Low symmetry (C1 or Cs)

112. Ho-Model0b-2x2x2

Central atom: Ho at (2.0578, 2.0410, 2.0848)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2102	91.7947	-91.4968	2.0001	-0.1674	2.0156
O	2.2121	91.6128	91.7397	1.9907	4.2512	2.0225
O	2.2122	91.3736	-1.7973	4.2682	1.9717	2.0318
O	2.2148	2.1885	125.0850	2.0092	2.1102	4.2979
O	2.2428	91.4814	-178.3375	-0.1833	1.9760	2.0268
O	2.2525	177.8363	131.0189	2.0020	2.1052	-0.1661

◈ **Local site symmetry around Ho**: Octahedral (Oh)

113. Ho-Model1-2x2x2 (1st Ho atom)

Central atom: Ho1 at (3.9200, 3.9200, 5.2698)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3275	52.3670	177.3293	2.0788	4.0059	6.6910
O	2.3275	52.3669	-87.3294	4.0059	2.0788	6.6910
O	2.3730	56.3093	1.7128	5.8936	3.9790	6.5861
O	2.3731	56.3097	88.2874	3.9790	5.8936	6.5861
O	2.3940	108.4123	-135.0003	2.3138	2.3139	4.5136
O	2.5249	111.5880	133.3372	2.3087	5.6276	4.3408
O	2.5249	111.5882	-43.3371	5.6276	2.3087	4.3408
O	2.6865	108.9280	45.0000	5.7170	5.7170	4.3983
O	3.8213	147.7161	87.8819	3.9954	5.9596	2.0392
O	3.8213	147.7163	2.1183	5.9596	3.9954	2.0392
O	3.9727	149.6543	-82.9454	4.1665	1.9281	1.8414
O	3.9727	149.6544	172.9454	1.9281	4.1665	1.8414

◈ **Local site symmetry around Ho1**: Low symmetry (C1 or Cs)

114. Ho-Model1-2x2x2 (2nd Ho atom)

Central atom: Ho2 at (2.0554, 2.0554, 2.3752)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1695	9.6998	45.0016	2.3138	2.3139	4.5136
O	2.1813	104.1651	-3.4496	4.1665	1.9281	1.8414
O	2.1813	104.1652	93.4494	1.9281	4.1665	1.8414
O	2.2401	90.4249	-92.2705	1.9666	-0.1829	2.3585
O	2.2401	90.4257	-177.7293	-0.1829	1.9666	2.3585
O	2.6460	174.6507	-135.0014	1.8809	1.8810	-0.2593

◈ **Local site symmetry around Ho2**: Octahedral (Oh)

115. Ho-Model2(i)-2x2x2

Central atom: Ho at (4.6784, 4.0359, 4.1591)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2961	38.2807	0.0080	6.1009	4.0361	5.9616
O	2.3333	92.4657	-54.6523	6.0270	2.1345	4.0587
O	2.3335	92.4661	54.6583	6.0270	5.9376	4.0587
O	2.3731	146.6747	0.0125	5.9822	4.0362	2.1763
O	2.5493	47.3726	-112.0552	3.9741	2.2974	5.8856
O	2.5496	47.3780	112.0601	3.9738	5.7746	5.8856
O	2.9057	134.7025	-108.5697	4.0207	2.0782	2.1152
O	2.9063	134.6961	108.5700	4.0205	5.9943	2.1150

◈ **Local site symmetry around Ho**: Low symmetry (C1 or Cs)

116. Ho-Model2(ii)-2x2x2

Central atom: Ho at (2.0563, 2.0577, 2.0420)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1420	179.5224	-70.7222	2.0622	2.0409	-0.0999
O	2.1875	88.6071	-88.5026	2.1134	-0.1284	2.0952
O	2.1908	88.6729	178.6720	-0.1333	2.1085	2.0928
O	2.1973	89.6638	88.6647	2.1075	4.2544	2.0549
O	2.2129	88.9334	1.1401	4.2683	2.1017	2.0832

◈ **Local site symmetry around Ho**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

117. Ho-Model2(iii)-2x2x2 (1st Ho atom)

Central atom: Ho1 at (4.5350, 4.5350, 4.2698)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2378	93.2882	45.0002	6.1147	6.1147	4.1414
O	2.3168	42.4998	-15.5359	6.0430	4.1157	5.9780
O	2.3168	42.5002	105.5361	4.1157	6.0430	5.9779
O	2.5175	142.3849	-16.2959	6.0098	4.1038	2.2757
O	2.5175	142.3846	106.2962	4.1038	6.0098	2.2757
O	2.8664	93.2395	-58.3864	6.0351	2.0979	4.1078
O	2.8664	93.2396	148.3863	2.0979	6.0351	4.1078
O	3.0880	54.5208	-101.8934	4.0167	2.0743	6.0621
O	3.0880	54.5209	-168.1069	2.0743	4.0167	6.0621

◈ **Local site symmetry around Ho1**: Low symmetry (C1 or Cs)

118. Ho-Model2(iii)-2x2x2 (2nd Ho atom)

Central atom: Ho2 at (2.0489, 2.0489, 2.0608)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1595	178.4701	-135.0043	2.0081	2.0081	-0.0979
O	2.1782	92.4540	-2.0614	4.2236	1.9706	1.9675
O	2.1782	92.4540	92.0616	1.9706	4.2236	1.9675
O	2.2219	88.9107	-179.4393	-0.1725	2.0272	2.1030
O	2.2219	88.9109	-90.5604	2.0272	-0.1725	2.1030

◈ **Local site symmetry around Ho2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

119. Ho-Model2(iv)a-2x2x2

Central atom: Ho at (3.6313, 3.6313, 4.0746)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2284	90.0338	-135.0006	2.0556	2.0556	4.0733
O	2.4249	39.3784	-75.2791	4.0223	2.1434	5.9489
O	2.4249	39.3793	165.2781	2.1434	4.0223	5.9489
O	2.4263	140.6062	-75.3271	4.0214	2.1416	2.1995
O	2.4264	140.6053	165.3260	2.1416	4.0214	2.1995
O	2.7477	89.9891	-31.9665	5.9624	2.1766	4.0751
O	2.7478	89.9891	121.9668	2.1766	5.9624	4.0751

◈ **Local site symmetry around Ho**: Low symmetry (C1 or Cs)

120. Ho-Model2(iv)b-2x2x2

Central atom: Ho at (2.0542, 2.0416, 2.0960)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2106	91.6048	-178.7348	-0.1550	1.9928	2.0341
O	2.2166	91.5268	88.4070	2.1158	4.2566	2.0369
O	2.2225	91.6603	-0.9585	4.2754	2.0045	2.0316
O	2.2358	91.4229	-88.5995	2.1088	-0.1928	2.0405
O	2.2383	1.2631	-160.7789	2.0076	2.0254	4.3337
O	2.2686	178.8663	-142.9361	2.0184	2.0146	-0.1722

◈ **Local site symmetry around Ho**: Octahedral (Oh)

121. Model3a-Ho-Ti-2x2x2

Central atom: Ho at (2.0622, 2.0622, 2.2075)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1773	95.5173	93.3637	1.9350	4.2256	1.9982
O	2.1773	95.5168	-3.3632	4.2256	1.9350	1.9982
O	2.2078	4.0730	-134.9960	1.9513	1.9513	4.4098
O	2.2294	94.2447	-91.9718	1.9857	-0.1598	2.0425
O	2.2294	94.2444	-178.0288	-0.1598	1.9857	2.0425
O	2.3738	178.1384	-134.9936	2.0077	2.0076	-0.1650

◈ **Local site symmetry around Ho**: Octahedral (Oh)

122. Ho-Model3b-2x2x2

Central atom: Ho at (4.5129, 3.6799, 4.1835)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2154	90.1302	-44.9996	6.0795	2.1134	4.1784
O	2.2802	139.7649	24.2642	5.8557	4.2851	2.4427
O	2.2802	139.7655	-114.2620	3.9077	2.3371	2.4427
O	2.3491	43.1123	15.8732	6.0572	4.1190	5.8984
O	2.3492	43.1116	-105.8721	4.0738	2.1356	5.8984
O	2.8351	93.3520	-147.4048	2.1285	2.1552	4.0177
O	2.8351	93.3524	57.4055	6.0376	6.0644	4.0177
O	3.0590	54.6679	168.5842	2.0667	4.1738	5.9525
O	3.0590	54.6682	101.4148	4.0190	6.1261	5.9525

◈ **Local site symmetry around Ho**: Low symmetry (C1 or Cs)

123. Er-Model0a-2x2x2

Central atom: Er at (3.9684, 3.9688, 5.0031)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2975	54.7555	179.9994	2.0921	3.9688	6.3289
O	2.2977	54.7603	-89.9892	3.9688	2.0922	6.3289
O	2.2977	54.7607	89.9894	3.9688	5.8454	6.3289
O	2.2979	54.7655	0.0003	5.8453	3.9688	6.3289
O	2.6307	108.4488	-134.9948	2.2040	2.2041	4.1706
O	2.6308	108.4490	134.9943	2.2040	5.7336	4.1706
O	2.6315	108.4437	44.9948	5.7337	5.7338	4.1706
O	2.6315	108.4444	-44.9943	5.7337	2.2038	4.1706
O	3.6242	146.5388	-179.9991	1.9701	3.9688	1.9796
O	3.6249	146.5157	-89.9489	3.9702	1.9689	1.9798
O	3.6250	146.5134	89.9419	3.9704	5.9688	1.9798
O	3.6257	146.4903	0.0061	5.9701	3.9690	1.9801

◈ **Local site symmetry around Er**: Low symmetry (C1 or Cs)

124. Er-Model0b-2x2x2

Central atom: Er at (2.0538, 2.0605, 2.0731)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2043	91.2897	-1.8954	4.2563	1.9876	2.0235
O	2.2051	2.0625	125.1443	2.0081	2.1254	4.2768
O	2.2089	91.2379	91.4492	1.9979	4.2682	2.0254
O	2.2137	91.5100	-91.2554	2.0053	-0.1518	2.0148
O	2.2317	91.3297	-178.1932	-0.1762	1.9902	2.0213
O	2.2330	177.9536	130.7374	2.0017	2.1209	-0.1584

◈ **Local site symmetry around Er**: Octahedral (Oh)

125. Er-Model1-2x2x2 (1st Er atom)

Central atom: Er1 at (3.9146, 3.9146, 5.2931)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3180	52.5681	177.4801	2.0758	3.9955	6.7020
O	2.3180	52.5677	-87.4801	3.9955	2.0758	6.7020
O	2.3601	56.3302	88.3929	3.9697	5.8780	6.6016
O	2.3601	56.3303	1.6072	5.8780	3.9697	6.6016
O	2.3875	108.9631	-135.0000	2.3180	2.3180	4.5173
O	2.5108	112.1343	133.3464	2.3182	5.6059	4.3471
O	2.5108	112.1343	-43.3466	5.6059	2.3182	4.3471
O	2.6771	109.3530	45.0001	5.7006	5.7007	4.4060
O	3.8420	147.9328	87.8045	3.9927	5.9529	2.0373
O	3.8420	147.9327	2.1954	5.9529	3.9927	2.0373
O	3.9825	149.8749	-83.1059	4.1545	1.9303	1.8485
O	3.9825	149.8749	173.1058	1.9303	4.1545	1.8485

◈ **Local site symmetry around Er1**: Low symmetry (C1 or Cs)

126. Er-Model1-2x2x2 (2nd Er atom)

Central atom: Er2 at (2.0559, 2.0559, 2.4005)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1490	9.9336	44.9997	2.3180	2.3180	4.5173
O	2.1737	104.7101	-3.4246	4.1545	1.9303	1.8485
O	2.1737	104.7103	93.4247	1.9303	4.1545	1.8485
O	2.2334	90.6741	-177.7184	-0.1756	1.9670	2.3742
O	2.2334	90.6739	-92.2814	1.9670	-0.1756	2.3742
O	2.6768	174.6196	-134.9994	1.8784	1.8784	-0.2645

◈ **Local site symmetry around Er2**: Octahedral (Oh)

127. Er-Model2(i)-2x2x2

Central atom: Er at (4.7015, 4.0353, 4.1653)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2718	37.9909	0.0052	6.0999	4.0355	5.9558
O	2.3134	92.5930	-55.2001	6.0204	2.1377	4.0607
O	2.3135	92.5935	55.2037	6.0204	5.9332	4.0606
O	2.3478	147.3969	0.0088	5.9666	4.0355	2.1875
O	2.5517	47.5500	-112.7410	3.9737	2.2989	5.8876
O	2.5519	47.5533	112.7467	3.9734	5.7719	5.8876
O	2.9306	134.6495	-109.1292	4.0183	2.0656	2.1058
O	2.9310	134.6452	109.1296	4.0181	6.0055	2.1056

◈ **Local site symmetry around Er**: Low symmetry (C1 or Cs)

128. Er-Model2(ii)-2x2x2

Central atom: Er at (2.0454, 2.0819, 2.0448)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1321	179.7020	-167.0074	2.0346	2.0794	-0.0872
O	2.1734	88.3602	-178.2456	-0.1261	2.0154	2.1070
O	2.1764	89.2786	-1.5902	4.2208	2.0215	2.0722
O	2.1844	87.9539	89.1475	2.0779	4.2647	2.1228
O	2.2115	88.9610	-89.2013	2.0762	-0.1290	2.0849

◈ **Local site symmetry around Er**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

129. Er-Model2(iii)-2x2x2 (1st Er atom)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2140	92.2384	44.9911	6.1392	6.1394	4.1293
O	2.3177	41.7390	106.8484	4.1274	6.0520	5.9451
O	2.3178	41.7531	-16.8691	6.0517	4.1274	5.9449
O	2.4464	141.7475	108.0477	4.1054	6.0154	2.2946
O	2.4467	141.7297	-18.0684	6.0153	4.1053	2.2949
O	2.9131	92.1633	149.1051	2.0766	6.0700	4.1058
O	2.9146	92.1618	-59.1004	6.0703	2.0761	4.1058

◈ **Local site symmetry around Er1**: Low symmetry (C1 or Cs)

130. Er-Model2(iii)-2x2x2 (2nd Er atom)

Central atom: Er2 at (2.0511, 2.0511, 2.0469)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1307	178.4844	-135.0263	2.0112	2.0112	-0.0831
O	2.1758	91.7328	91.8058	1.9825	4.2247	1.9811
O	2.1758	91.7325	-1.8083	4.2247	1.9824	1.9811
O	2.2132	88.6908	-179.4335	-0.1615	2.0292	2.0975
O	2.2133	88.6878	-90.5680	2.0291	-0.1615	2.0976

◈ **Local site symmetry around Er2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

131. Er-Model2(iv)a-2x2x2

Central atom: Er at (3.6200, 3.6211, 4.0746)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2091	89.9910	-134.9809	2.0584	2.0585	4.0749
O	2.4029	140.6385	164.5968	2.1507	4.0259	2.2167
O	2.4037	140.6116	-74.5651	4.0259	2.1508	2.2168
O	2.4046	39.3351	164.5810	2.1506	4.0263	5.9344
O	2.4054	39.3620	-74.5486	4.0264	2.1507	5.9343
O	2.7636	89.9782	121.4118	2.1796	5.9797	4.0756
O	2.7661	89.9790	-31.4222	5.9804	2.1790	4.0756

◈ **Local site symmetry around Er**: Low symmetry (C1 or Cs)

132. Er-Model2(iv)b-2x2x2

Central atom: Er at (2.0646, 2.0622, 2.0898)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2010	91.5159	-88.8595	2.1084	-0.1376	2.0316
O	2.2019	91.4807	178.8991	-0.1361	2.1045	2.0329
O	2.2241	91.4480	88.8856	2.1079	4.2852	2.0336
O	2.2262	91.4479	1.0727	4.2897	2.1039	2.0336
O	2.2306	0.6255	45.2930	2.0817	2.0795	4.3203
O	2.2587	179.1804	42.4508	2.0885	2.0840	-0.1687

◈ **Local site symmetry around Er**: Octahedral (Oh)

133. Model3a-Er-Ti-2x2x2

Central atom: Er at (2.0640, 2.0640, 2.1917)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1701	95.1294	-3.3396	4.2217	1.9381	1.9977
O	2.1701	95.1299	93.3398	1.9381	4.2217	1.9977
O	2.1896	3.9204	-135.0007	1.9581	1.9581	4.3762
O	2.2246	93.8093	-91.9824	1.9872	-0.1544	2.0439
O	2.2246	93.8094	-178.0180	-0.1544	1.9872	2.0439
O	2.3475	178.1559	-135.0033	2.0106	2.0106	-0.1545

◈ **Local site symmetry around Er**: Octahedral (Oh)

134. Er-Model3b-2x2x2

Central atom: Er at (4.5489, 3.6467, 4.1662)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1894	89.7404	-45.0023	6.0970	2.0985	4.1761
O	2.2595	139.6910	25.9960	5.8627	4.2874	2.4432
O	2.2595	139.6873	-116.0026	3.9080	2.3329	2.4433
O	2.3323	42.6032	17.4643	6.0549	4.1205	5.8829
O	2.3323	42.6064	-107.4708	4.0749	2.1407	5.8828
O	2.8491	92.9886	58.6343	6.0298	6.0761	4.0177
O	2.8493	92.9881	-148.6357	2.1192	2.1657	4.0177
O	3.1285	54.7881	102.0872	4.0137	6.1461	5.9701
O	3.1288	54.7897	167.9187	2.0492	4.1818	5.9702

◈ **Local site symmetry around Er**: Low symmetry (C1 or Cs)

135. Tm-Model0a-2x2x2

Central atom: Tm at (3.9654, 3.9652, 5.0247)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2934	54.6134	-90.0014	3.9653	2.0955	6.3528
O	2.2934	54.6139	0.0026	5.8352	3.9653	6.3528
O	2.2935	54.6157	179.9969	2.0955	3.9653	6.3527
O	2.2935	54.6160	90.0016	3.9653	5.8351	6.3528
O	2.6090	108.9028	-44.9993	5.7107	2.2199	4.1795
O	2.6090	108.9013	-135.0020	2.2199	2.2199	4.1795
O	2.6091	108.9009	45.0022	5.7108	5.7107	4.1795
O	2.6093	108.9007	134.9994	2.2198	5.7108	4.1794
O	3.6446	146.7587	-90.0125	3.9649	1.9674	1.9764
O	3.6447	146.7554	0.0204	5.9635	3.9659	1.9765
O	3.6449	146.7486	179.9910	1.9668	3.9655	1.9766
O	3.6450	146.7454	90.0023	3.9653	5.9640	1.9766

◈ **Local site symmetry around Tm**: Low symmetry (C1 or Cs)

136. Tm-Model0b-2x2x2

Central atom: Tm at (2.0442, 2.0577, 2.0698)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1866	91.2742	-1.3692	4.2296	2.0054	2.0212
O	2.1915	1.6347	-133.6615	2.0010	2.0124	4.2604
O	2.1936	91.1066	91.0488	2.0040	4.2504	2.0275
O	2.2104	91.3139	-178.6066	-0.1651	2.0039	2.0191
O	2.2205	178.2167	-131.0387	1.9988	2.0056	-0.1496
O	2.2242	91.2130	-91.1040	2.0013	-0.1657	2.0227

◈ **Local site symmetry around Tm**: Octahedral (Oh)

137. Tm-Model1-2x2x2 (1st Tm atom)

Central atom: Tm1 at (3.9174, 3.9175, 5.2408)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2913	52.7214	-87.0580	4.0110	2.0967	6.6286
O	2.2913	52.7214	177.0578	2.0967	4.0110	6.6286
O	2.3535	57.0452	2.1054	5.8909	3.9900	6.5211
O	2.3535	57.0451	87.8947	3.9900	5.8909	6.5211
O	2.3672	109.0934	-134.9999	2.3357	2.3357	4.4665
O	2.5306	111.5086	-42.9839	5.6398	2.3123	4.3130
O	2.5306	111.5091	132.9836	2.3123	5.6398	4.3130
O	2.7130	109.1024	45.0000	5.7302	5.7302	4.3530
O	3.8202	147.4627	2.2696	5.9705	3.9988	2.0202
O	3.8202	147.4628	87.7300	3.9988	5.9705	2.0202
O	3.9309	149.4680	173.2005	1.9345	4.1539	1.8550
O	3.9309	149.4680	-83.2002	4.1539	1.9345	1.8550

◈ **Local site symmetry around Tm1**: Low symmetry (C1 or Cs)

138. Tm-Model1-2x2x2 (2nd Tm atom)

Central atom: Tm2 at (2.0557, 2.0557, 2.3534)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1498	10.6133	44.9994	2.3357	2.3357	4.4665
O	2.1600	103.3429	93.3055	1.9345	4.1539	1.8550
O	2.1600	103.3430	-3.3055	4.1539	1.9345	1.8550
O	2.2218	90.2560	-92.2412	1.9688	-0.1644	2.3435
O	2.2218	90.2556	-177.7587	-0.1644	1.9688	2.3435
O	2.5976	174.7906	-135.0009	1.8889	1.8889	-0.2334

◈ **Local site symmetry around Tm2**: Octahedral (Oh)

139. Tm-Model2(i)-2x2x2

Central atom: Tm at (4.7266, 4.0345, 4.1777)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2499	38.0589	0.0043	6.1135	4.0346	5.9492
O	2.3020	92.8124	-55.5291	6.0279	2.1390	4.0648
O	2.3021	92.8135	55.5330	6.0278	5.9302	4.0647
O	2.3382	147.8522	0.0081	5.9707	4.0347	2.1980
O	2.5200	47.9019	-113.8005	3.9720	2.3237	5.8671
O	2.5201	47.9050	113.8057	3.9718	5.7454	5.8671

O	2.9405	134.6711	-109.7109	4.0213	2.0659	2.1104
O	2.9412	134.6658	109.7114	4.0210	6.0038	2.1101

◈ **Local site symmetry around Tm**: Low symmetry (C1 or Cs)

140. Tm-Model2(ii)-2x2x2

Central atom: Tm at (2.0490, 2.0529, 2.0234)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1128	179.8953	-25.7565	2.0524	2.0512	-0.0894
O	2.1684	88.0813	88.8809	2.0913	4.2197	2.0960
O	2.1692	87.9970	-178.8807	-0.1186	2.0106	2.0992
O	2.1840	88.0713	-88.9254	2.0899	-0.1294	2.0969
O	2.1853	88.0509	-1.0880	4.2326	2.0114	2.0978

◈ **Local site symmetry around Tm**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

141. Tm-Model2(iii)-2x2x2 (1st Tm atom)

Central atom: Tm1 at (4.5846, 4.5844, 4.1976)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1949	91.9255	45.0018	6.1357	6.1356	4.1238
O	2.3072	41.2000	-17.8937	6.0308	4.1175	5.9336
O	2.3072	41.2027	107.8982	4.1175	6.0307	5.9335
O	2.4195	141.7565	-18.4348	6.0054	4.1108	2.2974
O	2.4195	141.7530	108.4389	4.1108	6.0053	2.2974
O	2.8861	91.9579	-59.9656	6.0283	2.0873	4.0990
O	2.8864	91.9583	149.9641	2.0872	6.0283	4.0990

◈ **Local site symmetry around Tm1**: Low symmetry (C1 or Cs)

142. Tm-Model2(iii)-2x2x2 (2nd Tm atom)

Central atom: Tm2 at (2.0437, 2.0437, 2.0242)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1130	178.0867	-135.0135	1.9938	1.9939	-0.0876
O	2.1646	91.2943	-1.5142	4.2070	1.9865	1.9753
O	2.1646	91.2950	91.5151	1.9865	4.2070	1.9753
O	2.2040	87.7341	-90.3425	2.0306	-0.1585	2.1114
O	2.2040	87.7319	-179.6566	-0.1585	2.0305	2.1114

◈ **Local site symmetry around Tm2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

143. Tm-Model2(iv)a-2x2x2

Central atom: Tm at (3.6017, 3.6015, 4.0713)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1968	89.9289	-135.0029	2.0482	2.0482	4.0740
O	2.3736	140.6316	-73.5854	4.0271	2.1573	2.2363
O	2.3737	140.6273	163.5804	2.1573	4.0271	2.2363
O	2.3779	39.2695	-73.5941	4.0268	2.1576	5.9121

O	2.3780	39.2738	163.5890	2.1577	4.0268	5.9121
O	2.7928	89.9349	-30.8402	5.9995	2.1698	4.0744
O	2.7932	89.9350	120.8419	2.1697	5.9996	4.0744

◈ **Local site symmetry around Tm**: Low symmetry (C1 or Cs)

144. Tm-Model2(iv)b-2x2x2

Central atom: Tm at (2.0488, 2.0661, 2.0861)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1938	91.3747	178.7591	-0.1439	2.1136	2.0335
O	2.1994	91.2289	-88.6628	2.1001	-0.1322	2.0389
O	2.2040	91.4937	0.8662	4.2517	2.0994	2.0286
O	2.2178	91.3562	88.7874	2.0957	4.2828	2.0336
O	2.2234	1.1807	161.7963	2.0052	2.0804	4.3090
O	2.2477	179.0347	150.0425	2.0160	2.0850	-0.1613

◈ **Local site symmetry around Tm**: Octahedral (Oh)

145. Model3a-Tm-Ti-2x2x2

Central atom: Tm at (2.0637, 2.0637, 2.1704)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1633	94.5572	93.1362	1.9458	4.2169	1.9985
O	2.1633	94.5572	-3.1374	4.2169	1.9457	1.9985
O	2.1821	3.8572	-135.0024	1.9599	1.9600	4.3475
O	2.2095	93.2754	-91.7445	1.9966	-0.1411	2.0441
O	2.2095	93.2754	-178.2532	-0.1411	1.9965	2.0441
O	2.3115	178.1900	-135.0054	2.0121	2.0121	-0.1399

◈ **Local site symmetry around Tm**: Octahedral (Oh)

146. Tm-Model3b-2x2x2

Central atom: Tm at (4.5935, 3.5992, 4.1925)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1521	89.5305	-45.0045	6.1151	2.0774	4.2101
O	2.2447	139.9997	-119.0843	3.8921	2.3383	2.4729
O	2.2448	140.0101	29.0670	5.8544	4.3001	2.4726
O	2.2963	42.6675	-109.6938	4.0690	2.1339	5.8810
O	2.2964	42.6599	19.6806	6.0587	4.1233	5.8812
O	2.8615	93.7052	59.8906	6.0260	6.0695	4.0076
O	2.8621	93.7060	-149.8892	2.1228	2.1664	4.0075
O	3.1613	55.8459	102.8561	4.0114	6.1497	5.9673
O	3.1616	55.8495	167.1527	2.0425	4.1810	5.9673

◈ **Local site symmetry around Tm**: Low symmetry (C1 or Cs)

147. Yb-Model0a-2x2x2

Central atom: Yb at (3.9708, 3.9707, 4.8986)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3785	54.1192	-89.9965	3.9709	2.0436	6.2927
O	2.3785	54.1204	179.9932	2.0436	3.9710	6.2927

O	2.3787	54.1238	0.0060	5.8982	3.9709	6.2926
O	2.3788	54.1250	89.9960	3.9709	5.8983	6.2926
O	2.7542	105.8621	-135.0007	2.0974	2.0974	4.1458
O	2.7543	105.8619	-44.9974	5.8443	2.0974	4.1458
O	2.7544	105.8618	134.9972	2.0974	5.8443	4.1458
O	2.7545	105.8617	45.0006	5.8443	5.8443	4.1458
O	3.5011	145.2954	-89.9871	3.9712	1.9774	2.0204
O	3.5012	145.2926	179.9805	1.9772	3.9714	2.0204
O	3.5016	145.2827	0.0173	5.9650	3.9713	2.0204
O	3.5017	145.2799	89.9895	3.9711	5.9652	2.0204

◈ **Local site symmetry around Yb**: Low symmetry (C1 or Cs)

148. Yb-Model0b-2x2x2

Central atom: Yb at (2.0381, 2.0705, 2.0649)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2482	91.3385	-91.2719	1.9882	-0.1766	2.0124
O	2.2519	91.3101	1.0771	4.2890	2.1128	2.0134
O	2.2535	91.6208	91.5344	1.9777	4.3224	2.0012
O	2.2585	91.6581	178.6638	-0.2189	2.1232	1.9996
O	2.2616	1.4189	135.6570	1.9980	2.1097	4.3259
O	2.2696	178.0662	136.6349	1.9824	2.1231	-0.2034

◈ **Local site symmetry around Yb**: Octahedral (Oh)

149. Yb-Model1-2x2x2 (1st Yb atom)

Central atom: Yb1 at (3.9571, 3.9571, 5.2198)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3758	55.3765	0.7920	5.9120	3.9841	6.5696
O	2.3758	55.3766	89.2088	3.9841	5.9120	6.5697
O	2.3789	53.5255	-88.9387	3.9926	2.0445	6.6340
O	2.3789	53.5258	178.9378	2.0445	3.9926	6.6340
O	2.5955	104.2618	-135.0004	2.1783	2.1783	4.5804
O	2.5961	109.2468	-44.7457	5.6979	2.2317	4.3640
O	2.5961	109.2467	134.7450	2.2318	5.6979	4.3640
O	2.6975	108.3156	45.0000	5.7679	5.7679	4.3721
O	3.7355	147.1465	2.0533	5.9823	4.0297	2.0817
O	3.7355	147.1466	87.9478	4.0297	5.9823	2.0817
O	3.9217	148.7867	-83.0484	4.2031	1.9397	1.8657
O	3.9218	148.7865	173.0476	1.9397	4.2031	1.8657

◈ **Local site symmetry around Yb1**: Low symmetry (C1 or Cs)

150. Yb-Model1-2x2x2 (2nd Yb atom)

Central atom: Yb2 at (2.0481, 2.0481, 2.2926)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1995	101.1906	-2.8797	4.2031	1.9397	1.8657
O	2.1996	101.1912	92.8800	1.9397	4.2031	1.8657
O	2.2574	90.4312	-91.9095	1.9729	-0.2080	2.2756
O	2.2575	90.4305	-178.0903	-0.2080	1.9729	2.2757

O	2.2951	4.6031	45.0007	2.1783	2.1783	4.5804
O	2.5795	175.7197	-135.0021	1.9120	1.9120	-0.2797

◈ **Local site symmetry around Yb2**: Octahedral (Oh)

151. Yb-Model2(i)-2x2x2

Central atom: Yb at (4.5629, 4.0018, 4.1123)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4254	39.6392	0.8951	6.1100	4.0259	5.9800
O	2.4442	92.0847	-52.0170	6.0662	2.0765	4.0234
O	2.4674	92.0727	52.6243	6.0598	5.9613	4.0230
O	2.5078	143.8158	0.7815	6.0433	4.0220	2.0882
O	2.6293	46.1065	-108.1033	3.9742	2.2008	5.9352
O	2.6472	46.5404	108.1345	3.9649	5.8278	5.9331
O	2.8461	135.2519	-105.8855	4.0145	2.0747	2.0910
O	2.8849	134.7638	105.7011	4.0086	5.9737	2.0807
O	3.2278	91.1561	-143.1158	1.9818	2.0649	4.0471

◈ **Local site symmetry around Yb**: Low symmetry (C1 or Cs)

152. Yb-Model2(ii)-2x2x2

Central atom: Yb at (2.0616, 2.0734, 2.0784)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1800	179.8623	35.0378	2.0659	2.0764	-0.1016
O	2.2182	89.9233	-1.8888	4.2786	2.0003	2.0813
O	2.2242	89.6395	91.6422	1.9979	4.2966	2.0924
O	2.2399	90.1526	-178.2018	-0.1771	2.0031	2.0724
O	2.2519	90.0388	-91.5836	1.9994	-0.1776	2.0769

◈ **Local site symmetry around Yb**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

153. Yb-Model2(iii)-2x2x2 (1st Yb atom)

Central atom: Yb1 at (4.4435, 4.4436, 4.3918)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3545	96.1186	44.9998	6.0989	6.0989	4.1408
O	2.3701	45.2649	101.8458	4.0979	6.0914	6.0599
O	2.3701	45.2652	-11.8463	6.0914	4.0979	6.0599
O	2.7151	143.0725	103.0485	4.0752	6.0327	2.2213
O	2.7152	143.0722	-13.0488	6.0327	4.0752	2.2213
O	2.8038	55.0215	-171.8106	2.1696	4.1163	5.9991
O	2.8038	55.0217	-98.1889	4.1163	2.1696	5.9991
O	2.9421	94.7495	144.6590	2.0518	6.1396	4.1482
O	2.9422	94.7495	-54.6591	6.1396	2.0518	4.1482

◈ **Local site symmetry around Yb1**: Low symmetry (C1 or Cs)

154. Yb-Model2(iii)-2x2x2 (2nd Yb atom)

Central atom: Yb2 at (2.0532, 2.0532, 2.0856)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2048	91.3378	92.8135	1.9450	4.2547	2.0341
O	2.2048	91.3380	-2.8135	4.2547	1.9450	2.0341
O	2.2079	179.9850	-135.3431	2.0528	2.0528	-0.1223
O	2.2474	90.7178	-178.5468	-0.1932	1.9962	2.0574
O	2.2474	90.7180	-91.4531	1.9963	-0.1932	2.0574

◈ **Local site symmetry around Yb2**: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

155. Yb-Model2(iv)a-2x2x2

Central atom: Yb at (3.9138, 3.9138, 4.7418)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3985	51.7588	-88.1989	3.9730	2.0310	6.2264
O	2.3985	51.7587	178.1989	2.0310	3.9730	6.2264
O	2.5114	52.7261	2.4434	5.9105	3.9990	6.2628
O	2.5114	52.7261	87.5566	3.9990	5.9105	6.2628
O	2.6142	104.5126	-135.0000	2.1243	2.1243	4.0867
O	2.7099	104.1472	132.6797	2.1325	5.8456	4.0794
O	2.7099	104.1472	-42.6797	5.8456	2.1325	4.0794
O	2.8126	101.9930	45.0001	5.8593	5.8593	4.1573

◈ **Local site symmetry around Yb**: Low symmetry (C1 or Cs)

156. Yb-Model2(iv)b-2x2x2

Central atom: Yb at (2.0273, 2.0825, 2.0894)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2465	91.5662	1.1138	4.2725	2.1262	2.0280
O	2.2512	91.3358	-90.9118	1.9915	-0.1678	2.0369
O	2.2590	91.6192	178.6876	-0.2302	2.1343	2.0256
O	2.2694	0.7861	135.9342	2.0050	2.1042	4.3585
O	2.2701	91.3316	91.0488	1.9858	4.3517	2.0366
O	2.3074	179.0518	132.3734	2.0016	2.1107	-0.2177

◈ **Local site symmetry around Yb**: Octahedral (Oh)

157. Model3a-Yb-Ti-2x2x2

Central atom: Yb at (2.0775, 2.0775, 2.1216)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2191	94.2184	-4.0902	4.2850	1.9197	1.9584
O	2.2191	94.2183	94.0903	1.9197	4.2850	1.9584
O	2.2307	5.2885	-135.0016	1.9321	1.9322	4.3428
O	2.2712	92.5217	-92.2824	1.9872	-0.1897	2.0217
O	2.2712	92.5216	-177.7175	-0.1897	1.9872	2.0217
O	2.3052	177.1946	-135.0019	1.9978	1.9978	-0.1809

◈ **Local site symmetry around Yb**: Octahedral (Oh)

158. Yb-Model3b-2x2x2

Central atom: Yb at (4.4272, 3.7578, 4.2560)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3142	91.6639	-45.0001	6.0629	2.1221	4.1888
O	2.3428	139.3628	-111.5337	3.8671	2.3385	2.4781
O	2.3429	139.3610	21.5359	5.8465	4.3179	2.4781
O	2.4153	44.7702	-101.8511	4.0778	2.0930	5.9707
O	2.4154	44.7732	11.8513	6.0920	4.1072	5.9706
O	2.8025	94.9990	-144.4903	2.1546	2.1362	4.0118
O	2.8026	94.9990	54.4898	6.0488	6.0304	4.0118
O	2.9390	54.4127	99.4823	4.0334	6.1152	5.9663
O	2.9391	54.4126	170.5170	2.0697	4.1516	5.9664

◈ **Local site symmetry around Yb**: Low symmetry (C1 or Cs)

159. Lu-Model0a-2x2x2

Central atom: Lu at (3.9652, 3.9642, 5.0683)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2563	55.5339	0.0074	5.8254	3.9645	6.3452
O	2.2564	55.5372	-90.0146	3.9647	2.1038	6.3452
O	2.2567	55.5447	90.0153	3.9647	5.8251	6.3451
O	2.2569	55.5482	179.9920	2.1041	3.9645	6.3451
O	2.6242	109.7696	-45.0031	5.7113	2.2179	4.1807
O	2.6246	109.7653	45.0100	5.7114	5.7111	4.1808
O	2.6251	109.7617	-135.0101	2.2179	2.2176	4.1808
O	2.6259	109.7590	135.0032	2.2176	5.7116	4.1806
O	3.6825	147.1598	0.0521	5.9622	3.9661	1.9744
O	3.6830	147.1398	-90.0951	3.9619	1.9659	1.9746
O	3.6842	147.0982	90.0805	3.9624	5.9655	1.9751
O	3.6847	147.0779	179.9629	1.9625	3.9655	1.9753

◈ **Local site symmetry around Lu**: Low symmetry (C1 or Cs)

160. Lu-Model0b-2x2x2

Central atom: Lu at (2.0455, 2.0604, 2.0629)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1758	91.0911	1.0503	4.2205	2.1003	2.0214
O	2.1764	1.4715	135.3186	2.0057	2.0997	4.2386
O	2.1772	91.0440	-91.0042	2.0073	-0.1161	2.0232
O	2.1998	91.1087	178.9257	-0.1535	2.1016	2.0203
O	2.2011	178.4017	134.8439	2.0022	2.1039	-0.1374
O	2.2017	91.1145	91.0357	2.0057	4.2613	2.0200

◈ **Local site symmetry around Lu**: Octahedral (Oh)

161. Y-Model0a-2x2x2

Central atom: Y at (3.9742, 3.9760, 4.9235)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3500	53.5710	90.0034	3.9741	5.8668	6.3190

O	2.3508	53.5897	-0.0472	5.8661	3.9745	6.3189
O	2.3510	53.5939	-179.9516	2.0821	3.9744	6.3188
O	2.3518	53.6143	-90.0047	3.9740	2.0827	6.3187
O	2.6379	106.7543	44.9743	5.7611	5.7614	4.1631
O	2.6381	106.7525	135.0306	2.1870	5.7613	4.1631
O	2.6415	106.7349	-45.0318	5.7619	2.1864	4.1629
O	2.6420	106.7338	-134.9729	2.1860	2.1862	4.1628
O	3.5460	145.8291	90.0258	3.9733	5.9677	1.9897
O	3.5495	145.7275	-0.2659	5.9730	3.9668	1.9903
O	3.5500	145.7113	-179.7483	1.9743	3.9673	1.9904
O	3.5535	145.6088	-90.0123	3.9738	1.9689	1.9912

◈ **Local site symmetry around Y**: Low symmetry (C1 or Cs)

162. Y-Model0b-2x2x2

Central atom: Y at (2.0531, 2.0478, 2.0826)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2275	91.4720	-178.0263	-0.1724	1.9711	2.0253
O	2.2282	91.5211	87.7098	2.1421	4.2734	2.0234
O	2.2287	91.7783	-87.8904	2.1351	-0.1783	2.0134
O	2.2304	2.6664	133.9423	1.9811	2.1225	4.3105
O	2.2358	91.7537	-1.7671	4.2868	1.9788	2.0141
O	2.2672	177.5146	131.9645	1.9873	2.1209	-0.1825

◈ **Local site symmetry around Y**: Octahedral (Oh)

163. La-Model0a-3x3x3

Central atom: La at (4.1136, 4.1155, 4.3518)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.5131	47.1154	-3.4918	5.9515	4.0034	6.0620
O	2.5143	47.1449	93.4627	4.0022	5.9554	6.0619
O	2.6153	96.4352	45.0003	5.9512	5.9532	4.0587
O	2.6637	49.9657	-176.7140	2.0774	3.9986	6.0652
O	2.6658	49.9917	-93.2525	3.9977	2.0770	6.0656
O	2.7622	96.2640	137.6619	2.0840	5.9647	4.0504
O	2.7626	96.2441	-47.6852	5.9623	2.0848	4.0513
O	2.9199	96.1199	-134.9853	2.0612	2.0621	4.0405
O	2.9455	140.4933	-3.5662	5.9838	3.9990	2.0792
O	2.9482	140.4879	93.5390	3.9978	5.9877	2.0773
O	3.1164	137.6729	-176.7801	2.0184	3.9977	2.0478
O	3.1179	137.6483	-93.2012	3.9963	2.0184	2.0476

◈ **Local site symmetry around La**: Low symmetry (C1 or Cs)

164. La-Model0b-3x3x3

Central atom: La at (6.1056, 6.1094, 6.2693)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2994	93.3826	-2.1563	8.3994	6.0230	6.1337
O	2.3011	93.3616	92.1472	6.0196	8.4049	6.1344

O	2.3226	92.9890	-178.2479	3.7873	6.0385	6.1482
O	2.3246	92.9669	-91.7520	6.0347	3.7890	6.1490
O	2.3274	2.2410	-135.9228	6.0402	6.0461	8.5950
O	2.3804	178.5574	-135.4423	6.0629	6.0673	3.8897

◈ **Local site symmetry around La**: Octahedral (Oh)

165. Ce-Model0a-3x3x3

Central atom: Ce at (4.0572, 4.0257, 4.6554)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3592	52.0941	0.2456	5.9186	4.0337	6.1048
O	2.3817	52.5403	-91.3418	4.0129	2.1356	6.1039
O	2.3914	52.8374	91.2852	4.0144	5.9310	6.1000
O	2.4110	53.3046	179.5935	2.1240	4.0394	6.0961
O	2.7084	102.3724	-45.6854	5.9053	2.1328	4.0751
O	2.7100	102.5103	45.4963	5.9117	5.9126	4.0683
O	2.7783	102.3164	-135.5416	2.1198	2.1246	4.0627
O	2.7861	102.2864	135.5213	2.1148	5.9331	4.0625
O	3.2636	143.6083	-0.6643	5.9933	4.0033	2.0282
O	3.3083	142.8654	92.0412	3.9860	6.0216	2.0180
O	3.3164	142.7089	-91.7635	3.9953	2.0174	2.0169
O	3.3508	141.9741	179.5062	1.9931	4.0435	2.0158

□ **Local site symmetry around Ce**: Low symmetry (C1 or Cs)

166. Ce-Model0b-3x3x3

Central atom: Ce at (6.1765, 6.0212, 6.1926)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1739	91.8188	-88.2525	6.2428	3.8494	6.1236
O	2.1757	92.0842	87.9809	6.2531	8.1941	6.1135
O	2.2169	90.9294	-179.4645	3.9600	6.0005	6.1566
O	2.2179	0.8107	29.5262	6.2038	6.0367	8.4102
O	2.2521	91.0626	0.4871	8.4282	6.0404	6.1508
O	2.2572	178.7634	-8.3294	6.2247	6.0142	3.9359

◈ **Local site symmetry around Ce**: Octahedral (Oh)

167. Pr-Model0a-3x3x3

Central atom: Pr at (4.0865, 4.1039, 4.4365)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4766	48.0555	92.4028	4.0093	5.9444	6.0919
O	2.4919	48.4209	-3.1615	5.9477	4.0011	6.0903
O	2.5896	50.5177	-177.0030	2.0905	3.9994	6.0831
O	2.6018	50.8342	-92.4299	4.0010	2.0885	6.0797
O	2.6162	98.1039	44.8371	5.9232	5.9302	4.0677
O	2.7265	97.8773	137.1270	2.1072	5.9414	4.0628

O	2.7510	97.9007	-47.2076	5.9376	2.1044	4.0584
O	2.8770	97.7223	-134.7969	2.0778	2.0809	4.0499
O	3.0309	141.5037	92.8363	3.9931	5.9882	2.0644
O	3.0384	141.3600	-3.2372	5.9807	3.9968	2.0633
O	3.1692	139.0383	-176.9977	2.0118	3.9951	2.0433
O	3.1836	138.8482	-92.6160	3.9909	2.0111	2.0393

◈ **Local site symmetry around Pr**: Low symmetry (C1 or Cs)

168. Pr-Model0b-3x3x3

Central atom: Pr at (6.1182, 6.1072, 6.2147)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2971	91.9849	-91.7914	6.0465	3.8126	6.1351
O	2.2972	92.2151	1.6372	8.4128	6.1728	6.1259
O	2.3112	1.5094	130.1604	6.0790	6.1537	8.5251
O	2.3143	92.3425	178.2983	3.8069	6.1759	6.1201
O	2.3162	92.2543	91.8360	6.0441	8.4205	6.1236
O	2.3457	178.1173	133.7861	6.0649	6.1628	3.8702

◈ **Local site symmetry around Pr**: Octahedral (Oh)

169. Nd-Model0a-3x3x3

Central atom: Nd at (4.0189, 4.0431, 4.5719)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.4541	50.6831	179.9992	2.1203	4.0431	6.1268
O	2.4676	50.9326	89.0224	4.0516	5.9587	6.1271
O	2.4724	51.0943	-89.2915	4.0427	2.1193	6.1246
O	2.4848	51.2957	-0.1273	5.9579	4.0388	6.1256
O	2.6985	100.7987	135.1917	2.1383	5.9112	4.0663
O	2.7145	100.7606	44.4411	5.9229	5.9103	4.0651
O	2.7389	100.5307	-134.6089	2.1278	2.1260	4.0713
O	2.7459	100.6789	-45.2947	5.9171	2.1253	4.0631
O	3.2027	142.5997	89.2131	4.0456	5.9882	2.0276
O	3.2317	142.0365	-178.3747	2.0317	3.9867	2.0240
O	3.2443	141.8678	-1.3798	6.0216	3.9948	2.0199
O	3.2676	141.3195	-90.4037	4.0045	2.0010	2.0211

◈ **Local site symmetry around Nd**: Low symmetry (C1 or Cs)

170. Nd-Model0b-3x3x3

Central atom: Nd at (6.2301, 6.0169, 6.2378)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2681	93.0357	-93.0776	6.1085	3.7552	6.1177
O	2.2692	92.9553	93.0766	6.1085	8.2797	6.1208
O	2.2941	1.9281	154.0224	6.1607	6.0507	8.5307
O	2.2953	91.6033	-0.7904	8.5243	5.9852	6.1736
O	2.3414	178.2947	162.7243	6.1636	6.0375	3.8975
O	2.3444	91.6753	-179.4153	3.8869	5.9929	6.1693

◈ **Local site symmetry around Nd**: Octahedral (Oh)

171. Sm-Model0a-3x3x3

Central atom: Sm at (3.9999, 3.9942, 4.6900)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3887	51.9720	179.3225	2.1184	4.0165	6.1615
O	2.3958	52.1731	-89.1264	4.0287	2.1020	6.1593
O	2.4202	52.8515	89.0758	4.0310	5.9231	6.1515
O	2.4207	52.7655	0.7595	5.9269	4.0198	6.1547
O	2.6773	103.1496	-135.0559	2.1545	2.1525	4.0809
O	2.7036	103.1178	-44.3809	5.8817	2.1526	4.0764
O	2.7195	103.0112	134.3207	2.1486	5.8899	4.0777
O	2.7561	103.0303	45.0990	5.8953	5.8962	4.0685
O	3.3230	144.0432	-88.8595	4.0387	2.0434	2.0002
O	3.3277	143.8496	178.4451	2.0376	4.0475	2.0030
O	3.3767	142.9127	1.4947	6.0354	4.0473	1.9963
O	3.3875	142.6566	88.8819	4.0400	6.0487	1.9968

◈ **Local site symmetry around Sm**: Low symmetry (C1 or Cs)

172. Sm-Model0b-3x3x3

Central atom: Sm at (6.0717, 6.0816, 6.2783)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2584	92.5991	-91.6996	6.0048	3.8265	6.1758
O	2.2606	92.5184	1.4504	8.3294	6.1388	6.1789
O	2.2668	92.6585	178.7096	3.8079	6.1326	6.1731
O	2.2691	92.4811	91.4634	6.0138	8.3479	6.1800
O	2.2822	1.4220	20.7434	6.1247	6.1017	8.5598
O	2.3446	178.7930	-29.4018	6.1147	6.0574	3.9342

◈ **Local site symmetry around Sm**: Octahedral (Oh)

173. Eu-Model0a-3x3x3

Central atom: Eu at (4.0870, 4.0122, 4.4073)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.5535	47.2528	-0.9755	5.9619	3.9802	6.1405
O	2.5906	48.0011	92.7046	3.9961	5.9353	6.1408
O	2.6339	48.7537	-92.6560	3.9952	2.0339	6.1438
O	2.6762	49.5285	-179.0547	2.0514	3.9786	6.1443
O	2.7091	96.9912	-45.9286	5.9573	2.0802	4.0776
O	2.7100	96.9243	46.1459	5.9509	5.9522	4.0806
O	2.8248	96.7763	-136.1825	2.0630	2.0700	4.0740
O	2.8283	96.7838	135.9533	2.0683	5.9647	4.0732
O	3.0144	140.9655	1.2883	5.9850	4.0549	2.0658
O	3.0465	140.2202	-92.9124	3.9880	2.0654	2.0661
O	3.1100	139.1822	92.7882	3.9881	6.0426	2.0537
O	3.1507	138.5023	178.8009	1.9998	4.0559	2.0475

◈ **Local site symmetry around Eu**: Low symmetry (C1 or Cs)

174. Eu-Model0b-3x3x3

Central atom: Eu at (6.0862, 6.0894, 6.2538)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2500	92.2774	-1.3574	8.3338	6.0362	6.1644
O	2.2518	92.2393	91.3789	6.0321	8.3389	6.1658
O	2.2674	92.2150	-178.7574	3.8210	6.0403	6.1662
O	2.2692	92.1984	-91.2737	6.0358	3.8224	6.1668
O	2.2853	1.2651	-135.7481	6.0501	6.0542	8.5386
O	2.3404	179.0061	-134.8588	6.0576	6.0606	3.9137

◈ **Local site symmetry around Eu**: Octahedral (Oh)

175. Gd-Model0a-3x3x3

Central atom: Gd at (4.0419, 4.0233, 4.7021)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3506	52.7412	0.7003	5.9127	4.0462	6.1252
O	2.3625	52.9880	-91.3902	3.9962	2.1374	6.1243
O	2.3880	53.6917	91.3226	3.9975	5.9472	6.1161
O	2.3974	53.9133	179.0695	2.1047	4.0548	6.1142
O	2.7145	103.2754	-45.3357	5.8991	2.1443	4.0787
O	2.7317	103.4208	45.3503	5.9093	5.9137	4.0680
O	2.7562	103.4127	-135.4157	2.1324	2.1413	4.0627
O	2.7766	103.4315	135.2988	2.1224	5.9230	4.0571

◈ **Local site symmetry around Gd**: Low symmetry (C1 or Cs)

176. Gd-Model0b-3x3x3

Central atom: Gd at (6.0984, 6.0735, 6.2323)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2281	92.5187	88.1075	6.1720	8.2983	6.1344
O	2.2342	91.9641	-178.8500	3.8660	6.0287	6.1558
O	2.2427	1.3095	-29.2368	6.1432	6.0484	8.4744
O	2.2514	92.6150	-87.9555	6.1787	3.8259	6.1296
O	2.2802	92.3211	-1.0894	8.3764	6.0302	6.1400
O	2.3174	178.3880	-33.8754	6.1526	6.0371	3.9158

◈ **Local site symmetry around Gd**: Octahedral (Oh)

177. Tb-Model0a-3x3x3

Central atom: Tb at (3.9864, 4.0238, 4.8081)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3101	53.4723	-179.7897	2.1301	4.0170	6.1831
O	2.3295	54.0803	88.5228	4.0350	5.9097	6.1747
O	2.3296	54.4177	-88.5598	4.0340	2.1298	6.1636
O	2.3528	55.1880	-0.1532	5.9181	4.0187	6.1512
O	2.6578	105.6767	134.7790	2.1839	5.8403	4.0899
O	2.7010	105.5175	-134.4369	2.1642	2.1655	4.0855
O	2.7449	105.5932	44.3547	5.8768	5.8721	4.0702
O	2.7770	105.3664	-44.6435	5.8915	2.1422	4.0722
O	3.4343	145.4302	-179.8080	2.0377	4.0173	1.9802
O	3.4609	144.8732	88.3634	4.0432	6.0144	1.9775
O	3.4752	144.4098	-88.0719	4.0544	2.0025	1.9820
O	3.5071	143.7706	-0.8280	6.0589	3.9939	1.9790

◈ **Local site symmetry around Tb**: Low symmetry (C1 or Cs)

178. Tb-Model0b-3x3x3

Central atom: Tb at (6.0953, 6.1233, 6.2165)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2269	91.7436	88.3957	6.1576	8.3483	6.1488
O	2.2307	91.8588	-178.4703	3.8665	6.0638	6.1442
O	2.2353	91.9780	-1.3671	8.3286	6.0700	6.1394
O	2.2398	1.6563	-144.2821	6.0427	6.0855	8.4553
O	2.2533	91.7798	-88.6627	6.1478	3.8717	6.1465
O	2.2833	178.5059	-137.0126	6.0517	6.0827	3.9340

◈ **Local site symmetry around Tb**: Octahedral (Oh)

179. Dy-Model0a-3x3x3

Central atom: Dy at (3.9933, 4.0469, 4.8493)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2896	54.4106	89.7756	4.0006	5.9088	6.1818
O	2.2990	54.7267	-178.8020	2.1168	4.0077	6.1769
O	2.3085	54.8950	-1.2195	5.8815	4.0067	6.1769
O	2.3276	55.6710	-89.7298	4.0024	2.1248	6.1619
O	2.7021	106.1886	135.0303	2.1574	5.8809	4.0959
O	2.7121	106.1005	44.6220	5.8480	5.8772	4.0972
O	2.7453	106.2114	-134.3581	2.1503	2.1621	4.0829
O	2.7700	106.1327	-45.2613	5.8663	2.1568	4.0796
O	3.4730	145.5101	89.0719	4.0252	6.0133	1.9867
O	3.4787	145.3705	-178.5208	2.0171	3.9959	1.9869
O	3.5124	144.5565	-1.4649	6.0295	3.9948	1.9878
O	3.5350	144.2378	-89.0563	4.0273	1.9813	1.9808

 Local site symmetry around Dy: Low symmetry (C1 or Cs)

180. Dy-Model0b-3x3x3

Central atom: Dy at (6.1100, 6.1073, 6.2085)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2148	91.6814	-0.8103	8.3236	6.0759	6.1435
O	2.2214	91.5513	91.2643	6.0610	8.3273	6.1484
O	2.2298	1.3465	-129.2977	6.0768	6.0667	8.4377
O	2.2310	91.6072	-91.2538	6.0612	3.8777	6.1460
O	2.2383	91.6120	179.1913	3.8728	6.1388	6.1456
O	2.2720	178.6499	-136.0926	6.0714	6.0701	3.9371

 Local site symmetry around Dy: Octahedral (Oh)

181. Ho-Model0a-3x3x3

Central atom: Ho at (4.0481, 3.9797, 4.8667)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2688	54.6059	-91.1149	4.0121	2.1306	6.1808
O	2.2708	54.8309	1.2674	5.9039	4.0208	6.1747
O	2.3024	56.3936	91.2682	4.0056	5.8968	6.1411
O	2.3039	56.3456	178.7074	2.1308	4.0230	6.1435
O	2.6731	106.7792	-44.9322	5.8599	2.1721	4.0951
O	2.7316	106.6694	-135.8263	2.1712	2.1562	4.0832
O	2.7498	106.5968	45.7832	5.8858	5.8684	4.0813
O	2.8343	106.4252	134.9658	2.1268	5.9032	4.0653
O	3.4881	145.9563	-91.6386	3.9922	2.0278	1.9765
O	3.4924	145.8364	1.7750	6.0083	4.0405	1.9770
O	3.5522	144.2894	91.6266	3.9892	6.0522	1.9825
O	3.5530	144.3435	178.2268	1.9779	4.0438	1.9798

 Local site symmetry around Ho: Low symmetry (C1 or Cs)

182. Ho-Model0b-3x3x3

Central atom: Ho at (6.0805, 6.0762, 6.2339)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2089	92.0679	90.8869	6.0464	8.2834	6.1541
O	2.2099	91.9991	178.9935	3.8723	6.1150	6.1568
O	2.2115	91.9657	-89.1961	6.1115	3.8663	6.1580
O	2.2176	91.8951	-0.5501	8.2969	6.0549	6.1605
O	2.2249	1.2441	-36.3906	6.1194	6.0475	8.4582
O	2.2820	179.0061	-35.2266	6.1129	6.0534	3.9522

 Local site symmetry around Ho: Octahedral (Oh)

183. Er-Model0a-3x3x3

Central atom: Er at (4.0521, 3.9707, 4.9045)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2558	55.1223	0.5527	5.9026	3.9886	6.1944

O	2.2621	55.4003	-91.1593	4.0144	2.1091	6.1890
O	2.2758	56.3355	91.3092	4.0088	5.8643	6.1661
O	2.2860	56.8220	179.3741	2.1389	3.9916	6.1555
O	2.6709	107.6056	-44.9503	5.8538	2.1721	4.0967
O	2.7231	107.2848	45.7770	5.8656	5.8341	4.0954
O	2.7346	107.4000	-135.8618	2.1794	2.1535	4.0868
O	2.8335	106.9456	135.0208	2.1348	5.8866	4.0787
O	3.5224	146.3809	-91.7809	3.9915	2.0214	1.9713
O	3.5249	146.3180	1.7559	6.0061	4.0306	1.9713
O	3.5824	144.6457	91.7799	3.9877	6.0426	1.9827
O	3.5862	144.6116	178.2180	1.9763	4.0353	1.9809

 Local site symmetry around Er: Low symmetry (C1 or Cs)

184. Er-Model0b-3x3x3

Central atom: Er at (6.1049, 6.1169, 6.1627)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2028	91.2170	1.1917	8.3067	6.1627	6.1159
O	2.2063	91.1330	-90.9206	6.0695	3.9113	6.1191
O	2.2100	1.2388	132.5335	6.0726	6.1521	8.3722
O	2.2225	91.2721	178.8703	3.8834	6.1607	6.1134
O	2.2301	91.1970	90.9206	6.0691	8.3463	6.1161
O	2.2412	178.7360	133.1533	6.0711	6.1530	3.9220

 Local site symmetry around Er: Octahedral (Oh)

185. Tm-Model0a-3x3x3

Central atom: Tm at (3.9977, 4.0049, 4.9219)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2507	55.6496	179.4978	2.1396	4.0211	6.1918
O	2.2515	55.7073	-89.6806	4.0080	2.1448	6.1904
O	2.2590	56.2633	0.6178	5.8761	4.0251	6.1765
O	2.2656	56.5456	89.5610	4.0121	5.8951	6.1709
O	2.7190	107.7976	-134.9306	2.1692	2.1720	4.0908
O	2.7217	107.7924	-44.9589	5.8315	2.1737	4.0902
O	2.7247	107.7782	134.8393	2.1682	5.8446	4.0900
O	2.7667	107.8807	45.0547	5.8577	5.8685	4.0724
O	3.5658	145.9034	179.2330	1.9989	4.0316	1.9690
O	3.5732	145.8735	-89.2704	4.0232	2.0003	1.9639
O	3.5758	145.6606	-0.1489	6.0147	3.9996	1.9693
O	3.5826	145.5856	90.1779	3.9914	6.0297	1.9663

 Local site symmetry around Tm: Low symmetry (C1 or Cs)

186. Tm-Model0b-3x3x3

Central atom: Tm at (6.0956, 6.0887, 6.2059)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1906	91.5447	-178.9227	3.9061	6.0475	6.1468
O	2.1910	91.4805	88.9104	6.1372	8.2786	6.1493
O	2.2016	91.7150	-88.9750	6.1349	3.8884	6.1400
O	2.2020	1.0159	43.9587	6.1237	6.1158	8.4075
O	2.2113	91.5197	-0.9940	8.3057	6.0504	6.1472
O	2.2500	179.2023	-32.5537	6.1220	6.0718	3.9561

◈ **Local site symmetry around Tm**: Octahedral (Oh)

187. Yb-Model0a-3x3x3

Central atom: Yb at (4.0378, 4.0399, 4.7603)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3577	53.5583	91.5134	3.9877	5.9359	6.1608
O	2.3591	53.6124	-1.5860	5.9362	3.9874	6.1599
O	2.4222	54.8431	-178.4169	2.0582	3.9852	6.1551
O	2.4243	54.8822	-91.4965	3.9860	2.0576	6.1549
O	2.7777	103.9346	44.9790	5.9448	5.9455	4.0914
O	2.8147	103.8443	135.7831	2.0791	5.9458	4.0868
O	2.8179	103.8523	-45.7779	5.9460	2.0792	4.0857
O	2.8648	103.7740	-134.9677	2.0714	2.0713	4.0782
O	3.3658	144.2267	91.3818	3.9904	6.0069	2.0296
O	3.3676	144.2069	-1.4350	6.0068	3.9906	2.0288
O	3.4220	143.1004	-178.6301	1.9838	3.9908	2.0238
O	3.4233	143.0827	-91.3226	3.9904	1.9842	2.0234

 Local site symmetry around Yb: Low symmetry (C1 or Cs)

188. Yb-Model0b-3x3x3

Central atom: Yb at (6.0568, 6.0455, 6.2863)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2406	91.9000	-178.9789	3.8178	6.0056	6.2120
O	2.2407	92.1006	89.0472	6.0940	8.2844	6.2042
O	2.2443	92.2177	-0.8990	8.2991	6.0103	6.1995
O	2.2453	91.9282	-89.1984	6.0882	3.8017	6.2108
O	2.3068	0.7414	-159.9604	6.0287	6.0353	8.5929
O	2.3429	179.2303	62.3826	6.0714	6.0734	3.9437

 Local site symmetry around Yb: Octahedral (Oh)

189. Lu-Model0a-3x3x3

Central atom: Lu at (3.9802, 4.0130, 4.9850)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2103	56.8779	89.4108	3.9993	5.8641	6.1927
O	2.2120	56.8968	-179.4841	2.1273	3.9964	6.1931
O	2.2226	57.6769	-0.5149	5.8584	3.9962	6.1734

O	2.2227	57.6522	-89.5335	3.9955	2.1354	6.1742
O	2.7142	108.8753	134.6947	2.1739	5.8387	4.1069
O	2.7552	108.9219	-134.5921	2.1505	2.1570	4.0915
O	2.7854	108.5600	44.6715	5.8581	5.8695	4.0984
O	2.8064	108.5713	-44.7007	5.8711	2.1418	4.0912
O	3.5903	146.9305	179.7973	2.0212	4.0200	1.9763
O	3.6184	146.1836	88.6131	4.0290	6.0262	1.9787
O	3.6234	146.1823	-88.2809	4.0407	1.9973	1.9746
O	3.6425	145.4379	-0.3882	6.0466	3.9990	1.9853

◈ **Local site symmetry around Lu**: Low symmetry (C1 or Cs)

190. Lu-Model0b-3x3x3

Central atom: Lu at (6.0200, 6.1386, 6.1911)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1612	91.8483	1.7801	8.1791	6.2057	6.1214
O	2.1660	91.8150	178.2219	3.8561	6.2058	6.1225
O	2.1831	90.8881	-90.2706	6.0097	3.9558	6.1573
O	2.1853	0.8895	106.0004	6.0107	6.1712	8.3762
O	2.2301	91.2709	90.2142	6.0117	8.3681	6.1417
O	2.2367	178.8758	106.3870	6.0076	6.1807	3.9549

◈ **Local site symmetry around Lu**: Octahedral (Oh)

191. Y-Model0a-3x3x3

Central atom: Y at (4.0421, 3.9952, 4.8183)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.3118	53.8965	0.6678	5.9098	4.0170	6.1805
O	2.3160	54.0834	-91.0739	4.0069	2.1199	6.1769
O	2.3422	54.7750	91.1846	4.0025	5.9081	6.1693
O	2.3486	55.0995	179.2635	2.1161	4.0200	6.1620
O	2.6947	105.6479	-45.0055	5.8767	2.1602	4.0915
O	2.7128	105.5932	45.5084	5.8733	5.8592	4.0891
O	2.7333	105.6782	-135.5939	2.1621	2.1538	4.0797
O	2.7702	105.6272	135.1238	2.1516	5.8776	4.0721
O	3.4496	145.2531	1.1317	6.0078	4.0340	1.9838
O	3.4562	145.1568	-91.4390	3.9925	2.0212	1.9817
O	3.4969	144.2070	91.3978	3.9922	6.0398	1.9818
O	3.5083	144.0487	178.8994	1.9827	4.0348	1.9783

◈ **Local site symmetry around Y**: Low symmetry (C1 or Cs)

192. Y-Model0b-3x3x3

Central atom: Y at (6.1205, 6.1160, 6.1511)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.2203	91.3844	-88.7787	6.1678	3.8969	6.0974
O	2.2218	91.2515	178.7760	3.8997	6.1635	6.1026
O	2.2268	1.4300	42.9645	6.1611	6.1539	8.3772
O	2.2445	91.3426	88.8292	6.1663	8.3594	6.0985

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O          2.2477   91.3367    1.1638      8.3671      6.1617      6.0987
O          2.2593  178.5251   43.1823      6.1629      6.1558      3.8925
```

◈ **Local site symmetry around Y**: Octahedral (Oh)

S2. Additional data regarding Size Effects

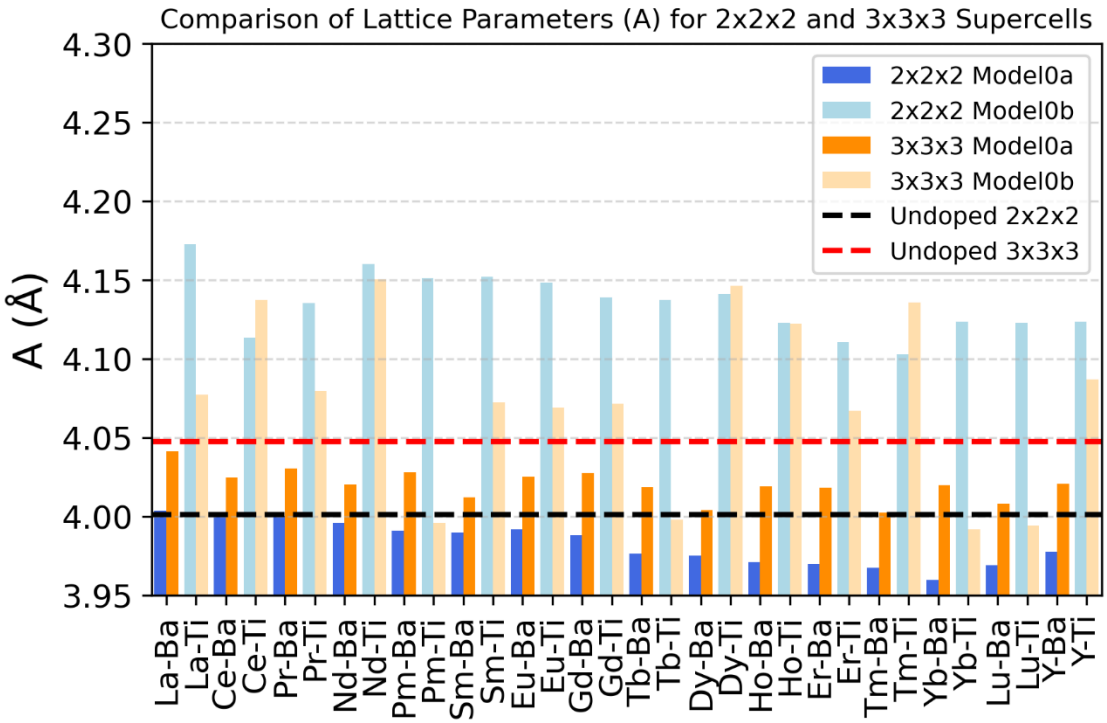
Table S2.1 Structural and energetic parameters for undoped and RE doped tetragonal BaTiO3 (2×2×2 supercell). Calculated values include force convergence criterion (*f*max), total energy, unit cell volume, lattice constants (*a*, *b*, *c*), and formation energy. Dopant ions are substituted either at the Ba site (Model0a) or the Ti site (Model0b). Undoped $BaTiO_3$ is included as a reference for comparison.

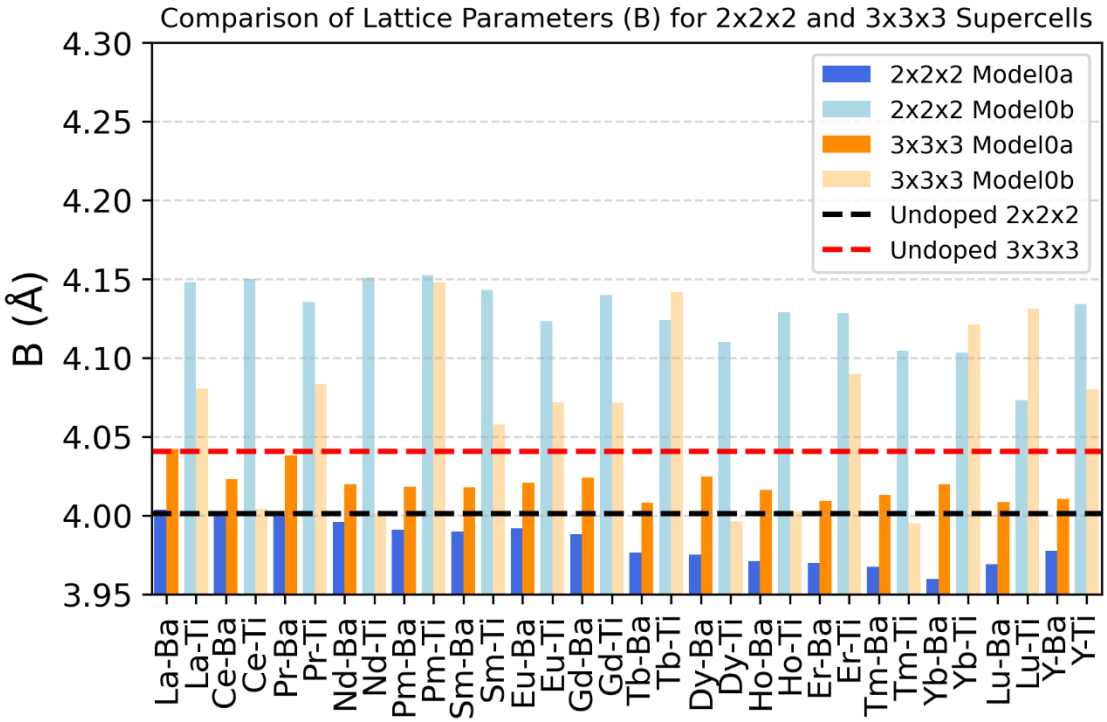
Sample - 2x2x2	fmax(eV/Å)	energy(eV)	volume(Å³)	A (Å)	b(Å)	c (Å)	Formation Energy(eV)
Undoped			538.1	8.0029	8.0029	8.4017	
La-Ba_Model0a	0.0174	-341.1279	532.16	8.0074	8.0074	8.2996	-1.509
La-Ti_Model0b	0.0178	-332.0094	579.58	8.3456	8.2964	8.3708	1.709
Ce-Ba_Model0a	0.0141	-341.5040	532.91	8.0061	8.0061	8.3139	-0.915
Ce-Ti_Model0b	0.0182	-334.9043	566.45	8.2269	8.3003	8.2954	-0.215
Pr-Ba_Model0a	0.0196	-340.5848	532.30	8.0006	8.0006	8.3159	-1.106
Pr-Ti_Model0b	0.0165	-331.4448	577.27	8.2712	8.2713	8.4380	2.134
Nd-Ba_Model0a	0.0131	-340.5815	532.65	7.9923	7.9923	8.3387	-1.123
Nd-Ti_Model0b	0.0190	-331.7446	575.12	8.3202	8.3021	8.3261	1.814
Pm-Ba_Model0a	0.0189	-340.5542	533.91	7.9819	7.9819	8.3802	-1.095
Pm-Ti_Model0b	0.0170	-332.1495	572.45	8.3030	8.3055	8.3013	1.409
Sm-Ba_Model0a	0.0116	-340.5262	533.79	7.9799	7.9799	8.3825	-1.107
Sm-Ti_Model0b	0.0188	-332.1588	570.50	8.3040	8.2861	8.2913	1.360
Eu-Ba_Model0a	0.0184	-345.1828	532.44	7.9837	7.9837	8.3534	-0.204
Eu-Ti_Model0b	0.0159	-335.8916	567.41	8.2973	8.2469	8.2923	3.187
Gd-Ba_Model0a	0.0170	-349.9500	533.94	7.9769	7.9769	8.3912	-1.171
Gd-Ti_Model0b	0.0187	-341.7988	566.78	8.2784	8.2798	8.2691	1.080
Tb-Ba_Model0a	0.0172	-340.5387	536.01	7.9531	7.9531	8.4742	-1.220
Tb-Ti_Model0b	0.0193	-332.6079	564.42	8.2748	8.2480	8.2699	0.811
Dy-Ba_Model0a	0.0122	-340.5199	536.23	7.9508	7.9508	8.4827	-1.211
Dy-Ti_Model0b	0.0182	-332.7295	562.74	8.2824	8.2206	8.2653	0.679
Ho-Ba_Model0a	0.0161	-340.4674	536.53	7.9421	7.9421	8.5060	-1.179
Ho-Ti_Model0b	0.0193	-332.8645	561.44	8.2454	8.2577	8.2459	0.524
Er-Ba_Model0a	0.0144	-340.4484	537.07	7.9403	7.9403	8.5183	-1.170
Er-Ti_Model0b	0.0192	-332.9393	560.05	8.2217	8.2568	8.2501	0.439
Tm-Ba_Model0a	0.0168	-340.3537	537.16	7.9353	7.9353	8.5306	-1.165
Tm-Ti_Model0b	0.0171	-332.9305	557.58	8.2058	8.2090	8.2775	0.358
Yb-Ba_Model0a	0.0169	-336.7789	534.36	7.9193	7.9193	8.5204	-0.700
Yb-Ti_Model0b	0.0154	-326.6536	559.19	8.2477	8.2067	8.2616	3.525
Lu-Ba_Model0a	0.0186	-340.3342	537.78	7.9380	7.9380	8.5346	-1.105
Lu-Ti_Model0b	0.0183	-333.1914	555.09	8.2455	8.1469	8.2635	0.137
Y-Ba_Model0a	0.0139	-342.2384	536.46	7.9552	7.9552	8.4768	-1.070
Y-Ti_Model0b	0.0185	-334.5205	563.40	8.2470	8.2688	8.2620	0.748

Table S2.2 Structural and energetic parameters for undoped and RE doped tetragonal BaTiO3 (3×3×3 supercell). Calculated values include force convergence criterion (*f*max), total energy, unit cell volume, lattice

constants (*a*, *b*, *c*), and formation energy. Dopant ions are substituted either at the Ba site (Model0a) or the Ti site (Model0b). Undoped $BaTiO_3$ is included as a reference for comparison.

Sample 3x3x3	fmax(eV/Å)	energy(eV)	volume(Å³)	A (Å)	b(Å)	c (Å)	Formation Energy(eV)
Undoped			1824.95	12.143	12.122	12.398	
La-Ba_Model0a	0.0170	-1136.9037	1854.93	12.2274	12.2274	12.4069	-0.540
La-Ti_Model0b	0.0174	-1131.9355	1862.25	12.2321	12.2420	12.4363	1.418
Ce-Ba_Model0a	0.0192	-1137.6779	1854.55	12.2253	12.2253	12.4085	-0.344
Ce-Ti_Model0b	0.0193	-1134.5332	1852.05	12.4127	12.0120	12.4216	-0.210
Pr-Ba_Model0a	0.0159	-1136.3361	1854.26	12.2241	12.2241	12.4091	-0.113
Pr-Ti_Model0b	0.0180	-1131.4934	1859.71	12.2392	12.2504	12.4035	1.720
Nd-Ba_Model0a	0.0193	-1136.3147	1853.71	12.2217	12.2217	12.4103	-0.111
Nd-Ti_Model0b	0.0172	-1131.8107	1859.82	12.4513	12.0053	12.4420	1.383
Pm-Ba_Model0a	0.0186	-1140.4968	1818.67	12.0844	12.0554	12.4839	-1.403
Pm-Ti_Model0b	0.0161	-1132.2445	1856.39	11.9879	12.4441	12.4442	0.949
Sm-Ba_Model0a	0.0196	-1136.2307	1854.90	12.2207	12.2207	12.4204	-0.067
Sm-Ti_Model0b	0.0194	-1132.0658	1852.22	12.2174	12.1734	12.4540	1.088
Eu-Ba_Model0a	0.0199	-1140.4069	1854.62	12.2241	12.2241	12.4115	1.317
Eu-Ti_Model0b	0.0161	-1135.9976	1850.10	12.2074	12.2167	12.4058	2.716
Gd-Ba_Model0a	0.0152	-1141.8484	1852.23	12.3512	12.1283	12.3651	0.665
Gd-Ti_Model0b	0.0197	-1145.5970	1855.26	12.2145	12.2145	12.4353	-0.074
Tb-Ba_Model0a	0.0176	-1136.1697	1856.74	12.2112	12.2112	12.4520	-0.106
Tb-Ti_Model0b	0.0200	-1132.7223	1849.23	11.9939	12.4256	12.4085	0.331
Dy-Ba_Model0a	0.0187	-1136.1533	1853.91	12.1427	12.1427	12.5735	-0.100
Dy-Ti_Model0b	0.0184	-1132.8413	1847.99	12.4391	11.9891	12.3916	0.202
Ho-Ba_Model0a	0.0200	-1136.1144	1855.04	12.1366	12.1366	12.5940	-0.081
Ho-Ti_Model0b	0.0198	-1132.8555	1844.60	12.3676	12.0094	12.4194	0.168
Er-Ba_Model0a	0.0174	-1136.1052	1855.32	12.1353	12.1352	12.5986	-0.082
Er-Ti_Model0b	0.0174	-1132.9672	1845.45	12.2020	12.2695	12.3269	0.046
Tm-Ba_Model0a	0.0197	-1136.0096	1855.34	12.1292	12.1293	12.6112	-0.076
Tm-Ti_Model0b	0.0143	-1133.1093	1843.60	12.4079	11.9857	12.3968	-0.186
Yb-Ba_Model0a	0.0186	-1131.7522	1854.02	12.1940	12.1939	12.4692	1.071
Yb-Ti_Model0b	0.0194	-1127.6389	1846.55	11.9754	12.3633	12.4721	2.175
Lu-Ba_Model0a	0.0188	-1136.0253	1855.88	12.1243	12.1243	12.6251	-0.052
Lu-Ti_Model0b	0.0151	-1133.3220	1842.42	11.9830	12.3948	12.4048	-0.358
Y-Ba_Model0a	0.0186	-1137.9025	1858.06	12.2129	12.2129	12.4575	-6.429
Y-Ti_Model0b	0.0187	-1134.5562	1849.04	12.2609	12.2402	12.3209	-6.093


Comparison of Lattice Parameters (A) for 2x2x2 and 3x3x3 Supercells
A (Å)
4.30
4.25
4.20
4.15
4.10
4.05
4.00
3.95
2x2x2 Model0a
2x2x2 Model0b
3x3x3 Model0a
3x3x3 Model0b
Undoped 2x2x2
Undoped 3x3x3
La-Ba
La-Ti
Ce-Ba
Ce-Ti
Pr-Ba
Pr-Ti
Nd-Ba
Nd-Ti
Pm-Ba
Pm-Ti
Sm-Ba
Sm-Ti
Eu-Ba
Eu-Ti
Gd-Ba
Gd-Ti
Tb-Ba
Tb-Ti
Dy-Ba
Dy-Ti
Ho-Ba
Ho-Ti
Er-Ba
Er-Ti
Tm-Ba
Tm-Ti
Yb-Ba
Yb-Ti
Lu-Ba
Lu-Ti
Y-Ba
Y-Ti


Comparison of Lattice Parameters (B) for 2x2x2 and 3x3x3 Supercells
B (Å)
4.30
4.25
4.20
4.15
4.10
4.05
4.00
3.95
2x2x2 Model0a
2x2x2 Model0b
3x3x3 Model0a
3x3x3 Model0b
Undoped 2x2x2
Undoped 3x3x3
La-Ba
La-Ti
Ce-Ba
Ce-Ti
Pr-Ba
Pr-Ti
Nd-Ba
Nd-Ti
Pm-Ba
Pm-Ti
Sm-Ba
Sm-Ti
Eu-Ba
Eu-Ti
Gd-Ba
Gd-Ti
Tb-Ba
Tb-Ti
Dy-Ba
Dy-Ti
Ho-Ba
Ho-Ti
Er-Ba
Er-Ti
Tm-Ba
Tm-Ti
Yb-Ba
Yb-Ti
Lu-Ba
Lu-Ti
Y-Ba
Y-Ti

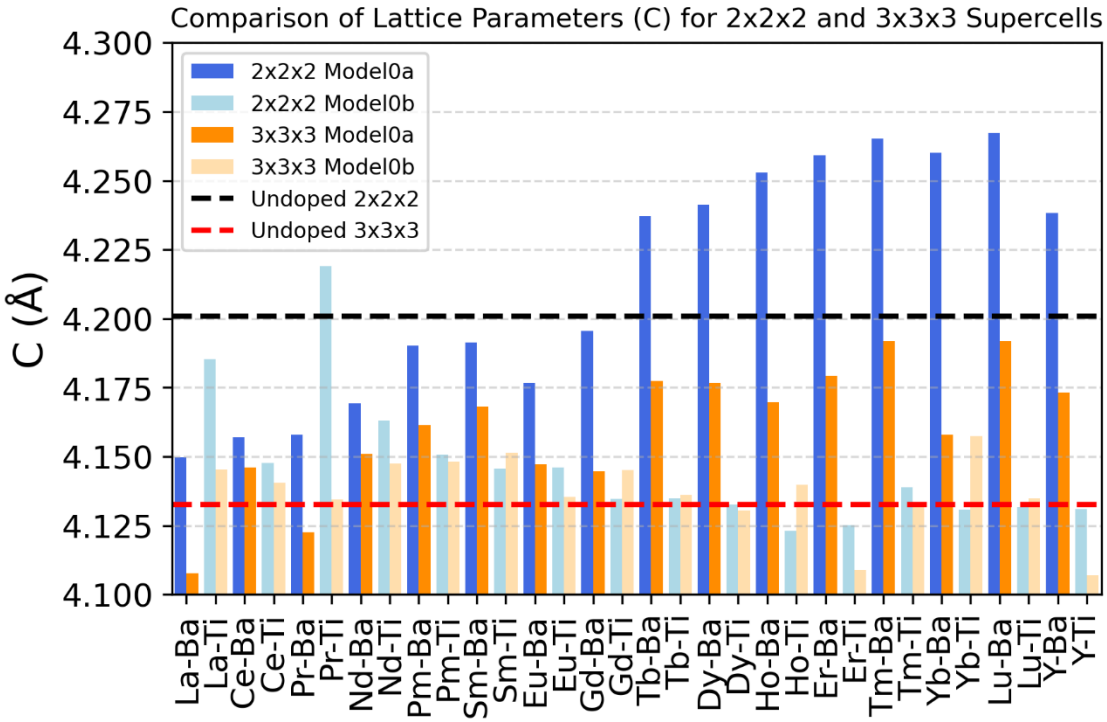


Figure S2. Variation of lattice Parameters in all RE doped BaTiO3 in Model0a and Model0b of 2x2x2 and 3x3x3 supercells.

Table S3. Structural, energetic, and stability parameters of RE-doped models evaluated using CHGNet relaxation for 2x2x2 supercells. The tables below list the maximum residual force (fmax), total energy, relaxed unit cell volume, lattice parameters (*a*, *b*, *c*), and formation energy for each model configuration (Model0–Model3). Negative formation energies indicate thermodynamic stability with respect to the reference phases.

(0) Model-La-4f^0	fmax(eV/Å)	energy(eV)	volume(Å^3)	A (Å)	b(Å)	c (Å)	Formation Energy(eV)
Model0a	0.0174	-341.1279	532.16	8.0074	8.0074	8.2996	-1.509
Model0b	0.0178	-332.0094	579.58	8.3456	8.2964	8.3708	1.709
Model1	0.0138	-337.4103	576.75	8.1905	8.1905	8.5975	-0.681
Model2(i)	0.0191	-330.2547	527.30	8.0620	8.0886	8.0862	4.434
Model2(ii)	0.0183	-323.7487	570.96	8.3506	8.3828	8.1564	5.040
Model2(iii)	0.0193	-327.2898	560.49	8.2559	8.2559	8.2231	4.509
Model2(iv)a	0.0174	-330.1861	528.14	8.0580	8.0580	8.1339	4.503
Model2(iv)b	0.0185	-323.5326	584.37	8.3075	8.2885	8.4867	5.256
Model3a	0.0182	-322.4213	577.98	8.1022	8.1022	8.8045	9.418
Model3b	0.0188	-322.6492	540.65	8.1112	8.1112	8.2177	9.190

(1) Model-Ce-4f^1	fmax(eV/Å)	energy(eV)	volume(Å^3)	A (Å)	b(Å)	c (Å)	Formation Energy(eV)
Model0a	0.0141	-341.5040	532.91	8.0061	8.0061	8.3139	-0.915
Model0b	0.0182	-334.9043	566.45	8.2269	8.3003	8.2954	-0.215

Model1	0.0179	-339.7733	563.05	8.1480	8.1480	8.4811	-1.104
Model2(i)	0.0189	-330.7687	526.33	8.0616	8.0968	8.0636	4.890
Model2(ii)	0.0172	-324.8662	565.51	8.2915	8.3018	8.2156	4.893
Model2(iii)	0.0186	-328.9421	553.55	8.2226	8.2226	8.1873	4.797
Model2(iv)a	0.0194	-330.6521	526.86	8.0520	8.0520	8.1262	5.007
Model2(iv)b	0.0181	-324.8714	568.18	8.2114	8.2204	8.4174	4.887
Model3a	0.0175	-326.3346	558.39	8.1933	8.1933	8.3181	6.474
Model3b	0.0178	-325.4971	547.69	8.2969	8.2968	7.9571	7.312

(2) Model-Pr-4f^2	**fmax(eV/Å)**	**energy(eV)**	**volume(Å^3)**	**A (Å)**	**b(Å)**	**c (Å)**	**Formation Energy(eV)**
Model0a	0.0196	-340.5848	532.30	8.0006	8.0006	8.3159	-1.106
Model0b	0.0165	-331.4448	577.27	8.2712	8.2713	8.4380	2.134
Model1	0.0155	-336.4836	580.39	8.0526	8.0526	8.9507	-0.035
Model2(i)	0.0197	-329.6656	526.83	8.0613	8.0863	8.0819	4.883
Model2(ii)	0.0195	-323.2927	570.78	8.4091	8.2809	8.1969	5.356
Model2(iii)	0.0191	-326.2611	559.01	8.2510	8.2510	8.2113	5.258
Model2(iv)a	0.0152	-329.5760	527.82	8.0568	8.0568	8.1313	4.973
Model2(iv)b	0.0179	-323.1498	582.39	8.2982	8.2980	8.4577	5.499
Model3a	0.0172	-321.7935	576.31	8.0957	8.0956	8.7934	9.905
Model3b	0.0163	-322.0336	540.00	8.1110	8.1110	8.2083	9.665

(3) Model-Nd-4f^3	**fmax(eV/Å)**	**energy(eV)**	**volume(Å^3)**	**A (Å)**	**b(Å)**	**c (Å)**	**Formation Energy(eV)**
Model0a	0.0131	-340.5815	532.65	7.9923	7.9923	8.3387	-1.123
Model0b	0.0190	-331.7446	575.12	8.3202	8.3021	8.3261	1.814
Model1	0.0179	-336.7231	578.18	8.0303	8.0303	8.9662	-0.314
Model2(i)	0.0199	-329.6509	526.35	8.0613	8.0870	8.0738	4.878
Model2(ii)	0.0134	-323.4637	569.11	8.3612	8.3328	8.1684	5.165
Model2(iii)	0.0168	-326.5692	558.95	8.2513	8.2513	8.2097	4.910
Model2(iv)a	0.0179	-329.5595	527.34	8.0545	8.0545	8.1285	4.969
Model2(iv)b	0.0189	-323.3539	579.02	8.2726	8.2840	8.4492	5.275
Model3a	0.0172	-321.9615	572.18	8.0742	8.0741	8.7769	9.717
Model3b	0.0175	-322.0253	539.29	8.1126	8.1126	8.1942	9.654

(4) Model-Pm-4f^4	**fmax(eV/Å)**	**energy(eV)**	**volume(Å^3)**	**A (Å)**	**b(Å)**	**c (Å)**	**Formation Energy(eV)**
Model0a	0.0189	-340.5542	533.91	7.9819	7.9819	8.3802	-1.095
Model0b	0.0170	-332.1495	572.45	8.3030	8.3055	8.3013	1.409
Model1	0.0179	-337.1503	574.77	8.0223	8.0223	8.9311	-0.741
Model2(i)	0.0193	-329.5748	526.91	8.0648	8.0954	8.0707	4.954
Model2(ii)	0.0162	-323.8217	567.06	8.3399	8.2931	8.1989	4.807
Model2(iii)	0.0181	-326.8897	556.43	8.2376	8.2376	8.1999	4.589
Model2(iv)a	0.0177	-329.4746	528.04	8.0590	8.0590	8.1304	5.054
Model2(iv)b	0.0155	-323.7461	575.22	8.2654	8.2593	8.4262	4.883

Model3a	0.0172	-322.2796	569.62	8.0609	8.0616	8.7656	9.399
Model3b	0.0184	-322.1138	542.61	8.2386	8.2387	7.9945	9.565

(5) Model-Sm-4f[5]	fmax(eV/Å)	energy(eV)	volume(Å³)	A (Å)	b(Å)	c (Å)	Formation Energy(eV)
Model0a	0.0116	-340.5262	533.79	7.9799	7.9799	8.3825	-1.107
Model0b	0.0188	-332.1588	570.50	8.3040	8.2861	8.2913	1.360
Model1	0.0172	-337.0880	574.39	7.9933	7.9933	8.9900	-0.759
Model2(i)	0.0196	-329.5509	525.80	8.0605	8.0853	8.0680	4.938
Model2(ii)	0.0169	-323.7811	565.60	8.2895	8.3251	8.1959	4.808
Model2(iii)	0.0163	-326.8524	560.46	8.1858	8.1858	8.3643	4.546
Model2(iv)a	0.0193	-329.4561	527.35	8.0552	8.0552	8.1273	5.033
Model2(iv)b	0.0154	-323.7608	573.79	8.2564	8.2613	8.4122	4.828
Model3a	0.0152	-322.2249	562.04	8.1263	8.1262	8.5113	9.414
Model3b	0.0178	-322.0599	544.13	8.2497	8.2497	7.9954	9.579

(6) Model-Eu-4f[6]	fmax(eV/Å)	energy(eV)	volume(Å³)	A (Å)	b(Å)	c (Å)	Formation Energy(eV)
Model0a	0.0184	-345.1828	532.44	7.9837	7.9837	8.3534	-0.204
Model0b	0.0159	-335.8916	567.41	8.2973	8.2469	8.2923	3.187
Model1	0.0192	-344.7548	564.18	8.1502	8.1501	8.4937	2.694
Model2(i)	0.0157	-334.8516	528.46	8.0551	8.0789	8.1206	5.197
Model2(ii)	0.0191	-328.1887	565.04	8.3015	8.3197	8.1812	5.960
Model2(iii)	0.0191	-336.6298	558.80	8.2727	8.2727	8.1652	5.889
Model2(iv)a	0.0183	-334.8439	532.27	8.0272	8.0272	8.2606	5.205
Model2(iv)b	0.0177	-327.9000	573.89	8.2616	8.2489	8.4211	6.249
Model3a	0.0167	-326.1625	558.13	8.1126	8.1127	8.4803	11.036
Model3b	0.0180	-325.8747	543.92	8.2460	8.2459	7.9997	11.324

(7) Model-Gd-4f[7]	fmax(eV/Å)	energy(eV)	volume(Å³)	A (Å)	b(Å)	c (Å)	Formation Energy(eV)
Model0a	0.0170	-349.9500	533.94	7.9769	7.9769	8.3912	-1.171
Model0b	0.0187	-341.7988	566.78	8.2784	8.2798	8.2691	1.080
Model1	0.0177	-356.0710	562.55	8.0748	8.0748	8.6279	-1.022
Model2(i)	0.0164	-346.0899	558.90	8.1612	8.1612	8.3913	4.029
Model2(ii)	0.0188	-338.9814	526.28	8.0631	8.0883	8.0699	4.867
Model2(iii)	0.0192	-333.4896	563.41	8.2718	8.2991	8.2072	4.459
Model2(iv)a	0.0165	-333.4360	570.29	8.2398	8.2449	8.3945	4.513
Model2(iv)b	0.0187	-338.9124	527.62	8.0587	8.0587	8.1244	4.936
Model3a	0.0189	-331.8245	556.73	8.0992	8.0992	8.4871	9.174
Model3b	0.0156	-331.4451	543.07	8.2446	8.2447	7.9896	9.554

(8) Model-Tb-4f[8]	fmax(eV/Å)	energy(eV)	volume(Å³)	A (Å)	b(Å)	c (Å)	Formation

							Energy (eV)
Model0a	0.0172	-340.5387	536.01	7.9531	7.9531	8.4742	-1.220
Model0b	0.0193	-332.6079	564.42	8.2748	8.2480	8.2699	0.811
Model1	0.0161	-337.5850	568.06	7.9869	7.9869	8.9051	-1.456
Model2(i)	0.0187	-329.5411	528.47	8.1393	8.0742	8.0415	4.848
Model2(ii)	0.0157	-324.1900	561.74	8.2744	8.2613	8.2177	4.299
Model2(iii)	0.0170	-327.3394	559.94	8.1289	8.1289	8.4738	3.859
Model2(iv)a	0.0197	-329.4010	527.62	8.0573	8.0573	8.1271	4.988
Model2(iv)b	0.0168	-324.2482	567.09	8.2165	8.2358	8.3803	4.241
Model3a	0.0181	-322.6226	555.74	8.0988	8.0988	8.4729	8.916
Model3b	0.0196	-322.0517	544.98	8.2513	8.2511	8.0053	9.487

(9) Model-Dy-4f[9]	fmax(eV/Å)	energy(eV)	volume(Å³)	A (Å)	b(Å)	c (Å)	Formation Energy(eV)
Model0a	0.0122	-340.5199	536.23	7.9508	7.9508	8.4827	-1.211
Model0b	0.0182	-332.7295	562.74	8.2824	8.2206	8.2653	0.679
Model1	0.0171	-337.6643	566.58	7.9765	7.9765	8.9051	-1.556
Model2(i)	0.0174	-329.5121	528.05	8.1356	8.0715	8.0413	4.867
Model2(ii)	0.0170	-324.2414	560.37	8.2193	8.2130	8.3011	4.237
Model2(iii)	0.0174	-327.2116	548.99	8.1944	8.1943	8.1760	3.967
Model2(iv)a	0.0185	-329.3664	527.32	8.0557	8.0557	8.1257	5.012
Model2(iv)b	0.0193	-324.3740	565.30	8.2368	8.2006	8.3691	4.105
Model3a	0.0192	-322.7198	554.31	8.0948	8.0949	8.4593	8.809
Model3b	0.0175	-322.0255	544.94	8.2539	8.2536	7.9998	9.503

(10) Model-Ho-4f[10]	fmax(eV/Å)	energy(eV)	volume(Å³)	A (Å)	b(Å)	c (Å)	Formation Energy (eV)
Model0a	0.0161	-340.4674	536.53	7.9421	7.9421	8.5060	-1.179
Model0b	0.0193	-332.8645	561.44	8.2454	8.2577	8.2459	0.524
Model1	0.0157	-337.7328	564.58	7.9734	7.9734	8.8805	-1.664
Model2(i)	0.0174	-329.4769	528.65	8.1444	8.0722	8.0411	4.882
Model2(ii)	0.0121	-324.3797	559.24	8.2589	8.2153	8.2424	4.079
Model2(iii)	0.0181	-327.2570	548.09	8.1881	8.1881	8.1751	3.882
Model2(iv)a	0.0193	-329.3203	527.26	8.0558	8.0558	8.1247	5.039
Model2(iv)b	0.0180	-324.4805	563.70	8.1946	8.2244	8.3640	3.978
Model3a	0.0189	-322.8320	553.09	8.0925	8.0924	8.4457	8.677
Model3b	0.0173	-321.9988	545.11	8.2549	8.2550	7.9999	9.510

(11) Model-Er-4f[11]	fmax(eV/Å)	energy(eV)	volume(Å³)	A (Å)	b(Å)	c (Å)	Formation Energy (eV)
Model0a	0.0144	-340.4484	537.07	7.9403	7.9403	8.5183	-1.170
Model0b	0.0192	-332.9393	560.05	8.2217	8.2568	8.2501	0.439
Model1	0.0169	-337.7784	564.25	7.9598	7.9598	8.9056	-1.730

Model2(i)	0.0169	-329.4495	528.49	8.1431	8.0710	8.0412	4.899
Model2(ii)	0.0154	-324.4477	558.53	8.1670	8.2763	8.2633	4.001
Model2(iii)	0.0162	-327.2756	548.59	8.1919	8.1919	8.1749	3.843
Model2(iv)a	0.0180	-329.2869	527.09	8.0587	8.0586	8.1165	5.062
Model2(iv)b	0.0170	-324.5569	562.20	8.2077	8.1971	8.3563	3.892
Model3a	0.0183	-322.8984	551.48	8.1013	8.1012	8.4028	8.600
Model3b	0.0163	-321.9993	545.48	8.2591	8.2590	7.9973	9.500

(12) Model-Tm-4f^{12}	**fmax(eV/Å)**	**energy(eV)**	**volume(Å^3)**	**A (Å)**	**b(Å)**	**c (Å)**	**Formation Energy (eV)**
Model0a	0.0168	-340.3537	537.16	7.9353	7.9353	8.5306	-1.165
Model0b	0.0171	-332.9305	557.58	8.2058	8.2090	8.2775	0.358
Model1	0.0190	-337.7209	559.76	7.9765	7.9765	8.7980	-1.852
Model2(i)	0.0194	-329.3448	528.81	8.1540	8.0694	8.0369	4.914
Model2(ii)	0.0176	-324.4983	557.11	8.2119	8.2058	8.2675	3.861
Model2(iii)	0.0179	-327.2010	546.37	8.1788	8.1788	8.1680	3.738
Model2(iv)a	0.0194	-329.1729	527.23	8.0604	8.0604	8.1150	5.086
Model2(iv)b	0.0128	-324.6183	560.76	8.1785	8.2136	8.3478	3.740
Model3a	0.0165	-322.9293	549.42	8.1054	8.1054	8.3630	8.480
Model3b	0.0185	-321.9101	547.41	8.2755	8.2754	7.9943	9.499

(13) Model-Yb-4f^{13}	**fmax(eV/Å)**	**energy(eV)**	**volume(Å^3)**	**A (Å)**	**b(Å)**	**c (Å)**	**Formation Energy (eV)**
Model0a	0.0169	-336.7789	534.36	7.9193	7.9193	8.5204	-0.700
Model0b	0.0154	-326.6536	559.19	8.2477	8.2067	8.2616	3.525
Model1	0.0151	-326.6395	561.28	7.9684	7.9683	8.8399	3.009
Model2(i)	0.0154	-326.7628	529.09	8.1837	8.0371	8.0441	4.386
Model2(ii)	0.0185	-320.3070	557.90	8.2249	8.2619	8.2102	4.942
Model2(iii)	0.0155	-320.3371	550.20	8.1865	8.1865	8.2098	4.382
Model2(iv)a	0.0192	-326.8103	532.99	7.9795	7.9795	8.3709	4.339
Model2(iv)b	0.0175	-320.0811	564.98	8.2070	8.2430	8.3515	5.168
Model3a	0.0167	-316.4173	549.61	8.1631	8.1631	8.2479	11.881
Model3b	0.0194	-316.0337	543.30	8.2299	8.2299	8.0217	12.265

(14) Model-Lu-4f^{14}	**fmax(eV/Å)**	**energy(eV)**	**volume(Å^3)**	**A (Å)**	**b(Å)**	**c (Å)**	**Formation Energy (eV)**
Model0a	0.0186	-340.3342	537.78	7.9380	7.9380	8.5346	-1.105
Model0b	0.0183	-333.1914	555.09	8.2455	8.1469	8.2635	0.137
Model1	0.0178	-337.8828	553.43	8.0109	8.0109	8.6239	-1.934
Model2(i)	0.0197	-329.3320	529.51	8.1650	8.0705	8.0357	4.967
Model2(ii)	0.0161	-324.7093	554.74	8.2034	8.1578	8.2894	3.690
Model2(iii)	0.0166	-327.4045	544.70	8.1689	8.1689	8.1627	3.614
Model2(iv)a	0.0169	-329.1417	527.40	8.0628	8.0628	8.1128	5.157
Model2(iv)b	0.0179	-324.8206	558.15	8.1649	8.2008	8.3358	3.578
Model3a	0.0168	-323.0957	546.02	8.1246	8.1246	8.2719	8.353

Model3b	0.0179	-321.9209	547.18	8.2784	8.2784	7.9855	9.528

(15) Model-Y-4f^0	fmax(eV/Å)	energy(eV)	volume(Å^3)	A (Å)	b(Å)	c (Å)	Formation Energy (eV)
Model0a	0.0139	-342.2384	536.46	7.9552	7.9552	8.4768	-1.070
Model0b	0.0185	-334.5205	563.40	8.2470	8.2688	8.2620	0.748
Model1	0.0188	-341.0966	558.53	8.0566	8.0566	8.6050	-1.268
Model2(i)	0.0188	-331.2735	528.72	8.1372	8.0805	8.0410	4.965
Model2(ii)	0.0170	-326.1307	560.97	8.2919	8.2263	8.2240	4.208
Model2(iii)	0.0183	-330.8336	550.28	8.2020	8.2020	8.1799	4.065
Model2(iv)a	0.0177	-331.1372	527.66	8.0572	8.0572	8.1280	5.102
Model2(iv)b	0.0170	-326.1564	566.03	8.2114	8.2308	8.3750	4.182
Model3a	0.0179	-324.5061	554.74	8.0944	8.0944	8.4668	8.883
Model3b	0.0169	-323.7632	545.55	8.2593	8.2590	7.9982	9.626

S4. Calculated CFPs (in cm^{-1}) for the dopant RE ions in all structural models.

Ce ($4f^1$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-394.82	-84.83	-278.12	-26.17	-1101.097	-81.45	-614.39	-835.83	2.29	-106.86	-59.80	540.64
B_{21}	-21.68	7.55	-0.01	-14.43	-6.689	-100.01	0.86	140.21	5.94	5.02	51.34	-129.33
B_{2-1}	-7.73	3.49	-0.01	6.87	6.647	0.01	0.94	-140.20	-5.94	0.39	-51.34	-129.36
B_{22}	2.86	-95.29	-0.00	34.22	-0.012	-150.36	3.05	-0.00	-0.00	10.59	-0.00	-0.05
B_{2-2}	0.89	-15.75	-0.00	14.22	-112.097	0.01	-6.03	127.38	-39.52	-7.15	48.49	-218.89
B_{40}	-1467.54	1315.47	-1042.93	1326.70	-343.387	-610.77	936.59	136.23	-503.99	1298.79	1290.56	-858.57
B_{41}	-45.58	3.85	0.01	-3.17	-4.092	62.54	1.04	-156.67	6.53	2.19	11.49	243.08
B_{4-1}	-10.84	11.50	0.01	-1.93	4.785	0.00	0.38	156.67	-6.53	1.23	-11.49	243.16
B_{42}	9.26	47.66	0.00	-15.33	0.060	-16.40	-1.36	0.00	0.00	-4.32	0.00	0.09
B_{4-2}	3.24	6.61	0.01	-3.50	175.795	0.02	2.65	167.26	222.70	2.36	-28.26	-1904.09
B_{43}	-147.95	-3.88	0.01	-2.08	318.701	151.84	-5.15	-291.48	20.99	-4.08	34.18	569.32
B_{4-3}	24.66	2.77	-0.01	0.26	317.764	0.02	5.20	-291.47	20.99	4.77	34.18	-569.28
B_{44}	54.28	825.61	-276.78	802.98	733.527	-411.96	807.27	721.33	-619.22	828.12	802.86	-888.59
B_{4-4}	0.22	-9.65	0.00	-0.37	0.098	-0.01	0.05	-0.01	0.00	-1.76	-0.01	-0.18
B_{60}	1933.65	365.88	-93.85	476.28	3564.599	-1686.75	-231.98	-435.49	-2961.62	328.74	431.53	-5228.10
B_{61}	405.77	16.32	-0.01	-41.84	-877.776	-490.98	0.76	860.37	-58.52	14.56	159.60	-1852.97
B_{6-1}	61.13	14.79	-0.01	12.65	874.438	-0.02	0.43	-860.36	58.52	-1.15	-159.60	-1852.94
B_{62}	-7.06	-117.18	-0.00	44.11	0.365	224.03	3.15	-0.00	-0.00	14.31	0.00	-0.24
B_{6-2}	4.84	-10.08	-0.03	18.86	-564.355	0.01	-4.57	-43.03	-136.88	-7.65	5.54	-353.06
B_{63}	-255.17	11.66	-0.01	5.10	-13.146	277.87	13.98	-533.74	40.49	11.11	-94.22	1084.55
B_{6-3}	88.28	-6.97	0.01	-2.20	-14.216	0.02	-14.31	-533.75	40.49	-13.18	-94.22	-1084.84
B_{64}	7151.40	-1057.14	5233.79	-1009.24	7495.802	3379.13	-1004.85	2174.23	3805.33	-1051.35	-984.34	538.36
B_{6-4}	27.01	11.53	0.00	1.33	0.438	0.04	-0.13	0.02	0.00	1.98	0.02	0.27

B_{65}	-1.49	15.49	0.02	-18.71	-52.470	-30.37	9.39	50.67	6.72	14.25	12.98	-483.75
B_{6-5}	30.23	-5.72	0.02	15.47	53.204	0.07	10.58	-50.66	-6.72	7.64	-12.98	-483.30
B_{66}	32.83	-175.22	0.00	67.57	0.197	345.33	5.30	-0.01	0.00	24.39	-0.01	0.96
B_{6-6}	7.95	-44.45	0.01	41.61	810.095	0.05	-20.87	663.34	728.58	-23.29	170.59	-3322.49

Pr ($4f^2$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	1517.07	114.17	1997.90	194.16	9613.492	-801.13	-4334.23	-1865.94	619.95	141.67	642.45	394.65
B_{21}	-235.07	-59.57	-0.97	201.81	1307.105	-2572.11	-79.68	516.20	38.59	6.34	60.60	-673.66
B_{2-1}	248.50	-61.27	-0.00	-187.44	-1306.899	-0.01	17.54	-516.14	-38.55	5.90	-60.42	-673.71
B_{22}	-28.05	-2.27	0.56	-2.14	-0.101	-1049.03	93.43	0.00	0.01	0.60	-0.01	-0.08
B_{2-2}	-72.59	17.76	-0.00	68.85	532.635	-0.01	-24.52	2957.38	-462.76	12.55	861.03	608.10
B_{40}	-16167.85	19710.22	-16234.89	19169.82	-16969.677	-9806.23	14087.28	-6172.29	-8177.83	19640.96	18136.59	-8897.56
B_{41}	-1173.50	-19.48	-0.18	207.86	1033.792	562.24	68.57	-3561.48	233.21	133.88	1164.23	1359.91
B_{4-1}	1549.91	33.31	0.00	-294.81	-1032.525	-0.29	20.85	3561.54	-233.17	119.26	-1165.07	1359.91
B_{42}	-209.10	-11.16	-18.03	-3.66	0.451	-1534.12	245.62	-0.01	0.03	-1.17	0.48	0.10
B_{4-2}	847.83	31.97	-0.00	-225.13	6295.716	0.01	42.47	3660.20	3415.81	40.65	-1032.07	-6640.40
B_{43}	-3203.20	62.58	16.82	-120.91	6633.422	1878.39	220.23	-7953.26	650.13	-188.46	541.36	-353.87
B_{4-3}	-4053.00	-41.52	-0.00	-170.32	6631.804	-0.09	-132.60	-7953.19	650.31	180.54	541.28	353.83
B_{44}	-4625.97	12278.23	-4504.79	12206.74	2809.480	-5821.63	11736.66	11700.57	-9395.11	12297.06	11773.68	-10215.54
B_{4-4}	25.23	8.93	-0.00	-4.39	0.865	0.02	-30.63	0.02	-0.06	6.02	-1.28	0.18
B_{60}	-4068.23	1988.65	-3481.37	1516.39	24743.914	-6744.51	-167.36	-5396.97	-13936.38	1948.39	1786.14	-17752.09
B_{61}	2434.33	-29.01	-18.95	428.18	-5887.534	-1771.80	-26.24	5789.99	-533.95	-57.79	710.15	271.37
B_{6-1}	-3087.77	-19.37	0.00	-415.88	5886.389	0.02	86.01	-5789.98	533.92	-60.05	-710.08	271.39
B_{62}	-84.93	-0.28	6.57	2.55	-1.211	327.68	-118.52	0.00	0.01	2.40	-0.76	-0.05
B_{6-2}	-151.14	18.99	0.00	-64.65	-6236.501	0.03	-23.55	-498.12	-771.14	3.18	200.02	921.47
B_{63}	-1666.15	-56.46	16.20	100.64	649.976	1234.70	-189.41	-6123.99	407.90	159.28	-489.84	36.80
B_{6-3}	-2312.81	40.50	-0.00	139.22	650.162	0.14	111.28	-6123.93	408.07	-153.29	-489.71	-36.82
B_{64}	24980.58	-4869.52	24929.62	-4788.03	52605.466	16257.24	-4368.87	20773.88	18815.40	-4864.22	-4192.97	21642.33
B_{6-4}	55.51	-4.75	-0.00	-0.86	-0.091	0.01	13.98	0.05	-0.14	-2.54	0.59	-0.14
B_{65}	-268.35	-59.93	14.15	246.27	-406.853	124.23	-210.72	1427.17	124.82	5.52	-842.96	645.45
B_{6-5}	341.54	-73.15	-0.00	-216.08	408.400	0.08	-34.88	-1427.15	-124.78	7.64	843.70	645.37

B_{66}	-127.31	23.48	-4.74	-13.00	0.429	345.92	-270.81	-0.00	0.01	1.89	0.37	0.18
B_{6-6}	839.07	-38.72	-0.00	284.30	7246.641	-0.02	-114.17	3113.32	3208.17	-87.08	1845.72	-5569.14

Nd ($4f^3$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-363.58	-64.71	-309.55	-2.41	-1373.931	-258.88	-855.28	-1058.51	102.36	-95.57	-211.96	240.61
B_{21}	16.46	-1.04	0.00	-5.97	224.383	-244.08	4.90	364.94	-1.38	14.40	15.28	-10.76
B_{2-1}	-16.73	10.01	-0.00	5.86	-224.402	-0.00	9.02	-364.95	1.38	-2.97	-15.26	-10.75
B_{22}	1.88	-85.71	-0.00	-2.09	0.000	-208.57	-7.14	0.03	-0.00	23.74	0.00	0.01
B_{2-2}	-1.47	5.63	-0.00	14.89	-72.481	-0.00	-17.58	291.85	-17.84	-16.50	166.34	-52.60
B_{40}	-1827.94	2052.99	-1658.31	2067.24	-1113.645	-1046.87	1483.10	291.05	-843.26	2033.53	1885.80	-900.52
B_{41}	25.80	10.84	-0.00	0.33	-19.908	64.52	1.27	-186.96	7.49	17.64	108.63	129.21
B_{4-1}	14.45	7.17	0.00	-0.62	19.904	-0.03	-24.96	187.01	-7.49	11.66	-108.64	129.23
B_{42}	1.84	57.57	0.00	1.19	-0.002	-143.11	1.98	-0.03	0.00	-13.35	-0.01	0.00
B_{4-2}	-12.10	-0.34	-0.00	-17.97	484.360	0.00	8.00	393.02	422.58	4.42	-83.94	-668.42
B_{43}	98.56	18.39	0.00	-19.56	577.555	213.13	-17.25	-409.54	25.10	-15.71	37.54	-10.02
B_{4-3}	-29.08	0.29	-0.00	-17.03	577.584	-0.01	3.58	-409.56	25.10	16.73	37.52	10.04
B_{44}	-316.40	1266.24	-436.83	1234.29	433.223	-570.42	1214.29	1026.33	-955.00	1273.18	1248.66	-989.09
B_{4-4}	1.67	6.39	-0.00	0.83	-0.002	0.00	3.55	0.00	0.00	7.18	0.02	0.00
B_{60}	243.31	328.03	-128.57	396.69	3657.963	-918.91	-20.07	-558.88	-2356.33	286.97	265.13	-2777.26
B_{61}	-97.11	10.72	0.00	-20.72	-747.840	-308.67	1.40	550.66	-34.52	23.94	75.93	8.32
B_{6-1}	-57.26	16.36	0.00	19.91	747.900	0.01	0.04	-550.70	34.52	-6.69	-75.91	8.31
B_{62}	1.22	-57.56	-0.00	-0.09	0.017	74.56	-0.37	-0.04	-0.00	20.89	0.02	-0.01
B_{6-2}	-1.09	5.66	0.00	-8.18	-735.072	0.01	-6.61	-73.18	-87.86	-11.27	33.13	38.03
B_{63}	127.83	-24.71	0.00	26.05	50.957	180.00	22.49	-329.76	16.47	19.98	-54.60	35.48
B_{6-3}	55.79	-0.07	-0.00	22.88	51.020	0.03	-5.53	-329.82	16.47	-21.75	-54.58	-35.45
B_{64}	4205.85	-768.11	3934.67	-737.79	5960.130	2622.53	-699.78	1511.48	2953.02	-773.33	-690.90	3181.10
B_{6-4}	29.53	-4.44	-0.00	-0.58	-0.017	0.00	-1.75	0.06	0.00	-4.90	-0.01	0.02
B_{65}	-23.24	-24.58	-0.00	7.99	-28.292	-22.80	17.10	40.25	4.14	14.84	-118.86	111.31
B_{6-5}	24.90	4.50	-0.00	-5.74	28.296	0.01	28.98	-40.37	-4.14	2.87	118.85	111.29
B_{66}	-2.94	-84.45	0.00	0.69	0.018	79.58	-7.97	-0.06	0.00	37.82	0.01	0.01

B_{6-6}	-15.81	8.41	-0.00	39.66	829.641	-0.00	-29.00	587.60	613.69	-28.15	243.42	-852.66

Pm ($4f^4$)										
	2x2x2									
CFPs/Model	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-395.75	-26.17	-1009.436	-201.71	-697.24	-748.38	163.14	-77.61	-174.86	308.80
B_{21}	0.01	-14.43	169.788	-225.38	-4.62	307.25	1.53	13.69	27.13	15.68
B_{2-1}	0.01	6.87	-169.806	-0.00	-5.82	-307.25	-1.25	13.63	-27.28	15.58
B_{22}	0.01	34.22	-0.013	-198.53	-10.37	-0.03	0.17	-1.87	0.64	0.92
B_{2-2}	-0.00	14.22	-42.897	0.00	-9.09	264.25	32.57	-4.45	114.68	-329.78
B_{40}	-5613.74	1326.70	-5286.945	-2735.72	3235.48	307.48	-1715.53	4331.42	3997.47	-2924.74
B_{41}	-0.00	-3.17	496.422	609.42	-1.63	-549.44	0.06	19.86	186.75	445.43
B_{4-1}	0.13	-1.93	-496.267	0.00	66.54	549.22	-0.03	21.09	-185.98	447.13
B_{42}	-0.07	-15.33	0.021	245.46	22.83	0.12	0.60	5.20	-1.55	-2.10
B_{4-2}	-0.00	-3.50	1529.749	0.00	11.38	1611.93	2617.84	18.34	-165.41	-3680.67
B_{43}	-0.00	-2.08	2085.591	1572.48	21.73	-1393.44	15.13	-15.22	122.70	985.55
B_{4-3}	0.04	0.26	2085.515	-0.00	12.10	-1393.25	14.32	14.75	123.76	-987.42
B_{44}	-596.39	802.98	837.004	-1287.97	2617.43	2068.06	-3016.33	2773.73	2839.52	-2335.40
B_{4-4}	-0.00	-0.37	0.009	0.00	-0.13	0.02	-0.11	-1.39	0.07	-1.55
B_{60}	1011.84	476.28	4779.537	-1186.70	-53.26	-959.83	-3948.46	294.15	239.31	-3478.33
B_{61}	-0.00	-41.84	-1152.398	-753.20	-5.35	763.62	-7.69	28.95	103.34	-440.21
B_{6-1}	-0.05	12.65	1152.291	0.00	1.81	-763.61	7.49	29.10	-104.02	-438.92
B_{62}	-0.08	44.11	0.081	275.62	-9.04	0.15	-0.05	-2.42	0.55	-2.41
B_{6-2}	0.00	18.86	-900.352	-0.00	-4.95	-144.69	-143.84	6.37	29.37	72.83
B_{63}	-0.00	5.10	8.101	427.63	-14.39	-508.25	10.91	9.95	-84.02	675.70
B_{6-3}	-0.09	-2.20	8.105	-0.00	-7.29	-508.13	10.55	-9.60	-84.83	-677.03
B_{64}	5681.91	-1009.24	7604.804	3429.80	-827.30	1759.56	4041.42	-898.49	-825.18	3418.04
B_{6-4}	-0.00	1.33	-0.034	0.00	0.08	-0.14	-0.13	0.48	0.04	-2.06
B_{65}	0.00	-18.71	58.285	-32.81	-14.83	42.77	-0.81	18.67	-111.91	-93.19
B_{6-5}	-0.04	15.47	-58.336	-0.00	-27.38	-42.60	0.82	17.88	111.51	-93.26
B_{66}	0.03	67.57	-0.007	411.21	-19.31	0.11	0.03	-3.38	1.30	-3.71

B_{6-6}	-0.00	41.61	1110.050	0.00	-30.43	939.63	1486.65	-15.99	259.41	-1576.78

Sm (4f^5)

	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-233.31	-64.16	-228.80	-0.28	-566.37	-156.97	-523.25	-1144.64	102.60	-45.37	-83.36	204.17
B_{21}	3.42	-7.39	0.02	-1.29	126.22	-170.17	5.17	106.79	-0.92	0.26	43.26	37.99
B_{2-1}	3.50	12.73	0.03	0.63	-126.20	0.00	3.32	-106.78	0.92	-8.49	-43.27	38.15
B_{22}	-0.92	-0.03	0.00	-3.58	0.01	-138.21	4.43	0.00	-0.01	-5.63	0.00	0.24
B_{2-2}	2.00	-5.20	0.00	-0.12	-26.38	-0.00	-5.18	176.54	-2.67	5.54	42.51	-276.04
B_{40}	-14253.56	6544.99	-12418.77	6826.59	-15833.03	-4988.81	5011.57	278.09	-2496.91	6623.62	6227.59	-6256.40
B_{41}	257.85	-27.20	0.25	13.88	1808.86	1035.45	-95.49	-1083.66	150.52	35.31	135.58	636.49
B_{4-1}	-313.76	65.54	0.24	-21.62	-1809.16	-0.00	-0.58	1083.65	-150.50	-36.92	-135.63	637.44
B_{42}	165.60	7.28	0.00	28.67	0.01	158.65	-28.07	0.01	0.07	29.53	-0.01	-1.36
B_{4-2}	3.53	14.11	-0.00	-40.58	3226.38	-0.00	15.31	166.70	5177.66	-9.91	-182.32	-9084.60
B_{43}	1107.55	19.03	-0.00	33.22	4726.95	2871.23	23.19	-1752.11	400.06	-40.31	280.08	1386.78
B_{4-3}	971.18	-33.04	0.01	28.06	4726.76	0.00	23.88	-1752.00	400.05	-26.17	280.07	-1387.95
B_{44}	2600.59	4387.57	926.08	4081.70	1615.86	-1652.64	3976.87	5160.69	-5634.39	4278.95	4450.61	-4384.04
B_{4-4}	-3.61	8.95	0.00	9.06	0.23	-0.00	2.81	0.01	-0.09	19.85	0.07	-1.04
B_{60}	2141.17	295.11	1511.93	513.08	6969.26	-1164.32	-49.80	637.17	-4322.77	350.60	314.25	-4148.71
B_{61}	-278.37	-27.04	-0.06	14.11	-1522.12	-785.40	-0.01	586.26	-128.06	-2.79	189.13	-231.06
B_{6-1}	256.53	40.52	-0.07	-16.36	1522.13	-0.00	4.75	-586.27	128.06	-27.67	-189.16	-230.31
B_{62}	8.37	0.51	-0.00	-8.01	-0.05	231.53	6.82	0.00	0.16	-13.96	-0.00	-0.87

B_{6-2}	6.75	-4.73	-0.00	-14.15	-977.66	0.00	-4.81	61.88	-336.37	9.92	-5.49	139.92
B_{63}	222.83	-9.11	0.08	-16.21	3.12	496.07	-10.40	-374.55	75.99	19.12	-130.53	944.29
B_{6-3}	116.02	15.72	-0.08	-13.76	3.02	0.00	-11.41	-374.52	75.98	12.54	-130.53	-945.02
B_{64}	7746.73	-1037.26	7088.34	-967.79	9617.60	3872.95	-937.60	1100.16	4634.81	-1017.33	-950.17	3974.10
B_{6-4}	-2.75	-2.07	-0.00	-2.11	0.02	-0.00	-0.54	-0.07	-0.10	-4.71	-0.02	-0.58
B_{65}	-16.37	-16.80	-0.10	-9.05	121.85	10.98	27.73	53.15	19.83	1.17	-29.26	-240.89
B_{6-5}	-9.79	-8.12	-0.09	8.15	-121.83	0.00	13.26	-53.13	-19.84	-16.48	29.25	-240.92
B_{66}	6.03	0.43	0.00	-11.30	0.02	289.28	14.77	0.02	0.01	-26.48	0.01	-1.46
B_{6-6}	-5.90	-19.48	-0.00	22.32	1352.49	-0.00	-19.90	200.08	1746.55	22.24	189.95	-2028.28

Eu ($4f^6$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-648.59	-731.22	-877.35	-78.95	-6372.935	-552.96	-2954.01	-2124.85	-437.96	-583.07	-1275.06	1753.35
B_{21}	-220.38	21.48	2.82	42.95	74.205	-988.18	5.23	442.39	204.72	71.11	294.23	659.99
B_{2-1}	264.09	-18.48	1.71	47.94	-74.251	0.02	-1.15	-442.36	-204.72	-17.56	-294.20	645.51
B_{22}	-21.89	19.24	-0.00	-104.43	-0.282	-765.81	28.86	0.01	-0.00	36.93	-0.02	3.23
B_{2-2}	10.57	20.03	0.34	-69.40	-1707.311	-4.39	-84.86	103.04	-231.91	-59.28	317.78	-429.04
B_{40}	-5468.86	9122.41	-5017.84	9324.86	337.536	-3293.90	6413.99	170.57	-3901.78	9142.28	8579.86	-5729.35
B_{41}	-345.98	25.76	2.24	20.62	427.457	-217.00	0.05	-554.77	205.40	55.85	35.53	734.71
B_{4-1}	201.28	-24.92	2.97	26.75	-428.077	-0.02	17.62	554.83	-205.40	29.04	-35.33	728.82
B_{42}	56.19	-11.09	-0.00	61.09	-0.311	-1292.74	-12.02	-0.03	0.00	-17.77	0.05	9.29
B_{4-2}	30.95	-17.67	0.44	77.45	2211.170	2.71	50.23	3023.93	258.67	21.68	-231.44	-6470.10
B_{43}	-946.26	34.27	6.06	70.90	3379.174	-870.35	107.61	-1133.88	696.40	-38.32	354.03	1987.82
B_{4-3}	-397.66	32.55	-7.91	-58.13	3380.326	0.02	-108.28	-1133.82	696.40	61.75	354.17	-1987.75
B_{44}	-2850.16	5885.28	-3225.90	5613.71	2969.708	-3452.03	5583.60	3552.06	-3812.65	5783.07	5920.58	-4233.74
B_{4-4}	3.44	0.89	0.07	-8.61	-0.262	0.42	5.74	-0.09	0.00	14.78	0.22	-0.44
B_{60}	-4406.96	1256.16	-4675.45	1723.44	2598.957	-6079.70	-409.20	-6404.71	-6564.96	1355.60	1001.03	-9543.43
B_{61}	665.35	48.69	-6.38	88.12	-2487.602	627.69	14.57	946.31	-535.36	143.93	509.16	-1350.61
B_{6-1}	-126.74	-43.10	-5.53	98.50	2488.459	0.03	9.37	-946.33	535.36	-27.51	-509.04	-1342.22
B_{62}	52.79	8.93	-0.00	-41.35	-0.120	-120.46	4.37	-0.04	-0.00	46.03	-0.01	3.48
B_{6-2}	-15.04	0.85	0.11	23.43	-1715.464	-2.36	-35.91	245.11	-112.09	-48.96	14.03	-736.37
B_{63}	-335.51	-41.58	-0.20	-85.84	135.287	-607.65	-128.44	-409.93	122.86	46.28	-413.30	1482.29
B_{6-3}	-559.28	-39.58	-2.45	70.87	135.234	-0.02	129.62	-409.81	122.86	-74.93	-413.47	-1482.96
B_{64}	11908.57	-3519.18	11784.79	-	12600.910	9881.60	-	7749.83	11099.24	-	-	9254.26

				3339.69			3140.55			3444.45	3310.85	
B_{6-4}	-2.19	-0.50	0.88	5.08	-0.044	-0.30	-3.73	0.11	0.00	-9.06	-0.12	-7.23
B_{65}	111.65	-24.62	2.11	-29.79	-268.030	-412.87	-99.64	338.61	103.73	89.86	-26.08	-348.50
B_{6-5}	-128.44	26.27	-0.62	-15.10	267.966	-0.03	-121.69	-338.65	-103.73	17.24	26.07	-353.03
B_{66}	96.32	15.55	-0.00	-62.52	-0.634	-132.89	11.31	0.05	0.00	66.04	-0.13	3.11
B_{6-6}	8.95	45.07	0.14	-160.24	2437.001	3.46	-173.10	2412.44	309.54	-114.86	640.68	-3638.10

Gd ($4f^7$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-787.99	-117.41	-892.25	13.36	-2220.670	-264.75	-864.18	-1901.05	563.20	-129.16	-333.79	625.34
B_{21}	-47.86	6.37	-0.02	-2.07	29.487	14.77	1.73	106.30	15.81	1.18	75.70	176.08
B_{2-1}	-30.36	3.50	0.00	2.10	-29.495	0.00	-0.86	-106.30	-15.80	-1.32	-75.69	175.09
B_{22}	7.60	-41.49	-0.02	2.51	-0.007	-318.97	13.41	0.00	-0.05	2.57	0.00	1.68
B_{2-2}	5.61	-1.85	0.01	-1.12	-234.736	-0.00	-14.12	193.37	50.46	4.25	87.35	-315.46
B_{40}	-4561.02	3824.40	-4625.63	3896.45	-1725.188	-2288.41	2834.41	672.95	-1505.89	3825.52	3571.14	-2700.66
B_{41}	-111.08	-11.01	-0.19	5.49	303.291	542.59	-45.23	-664.84	22.33	12.82	56.90	78.61
B_{4-1}	-77.73	3.96	0.10	-5.86	-303.264	0.00	6.42	664.82	-22.41	-13.02	-56.88	80.56
B_{42}	21.38	36.06	0.06	-2.33	0.001	252.61	-10.70	0.03	0.08	-2.19	0.00	-1.14
B_{4-2}	1.01	5.56	-0.02	-13.26	854.998	-0.00	11.13	-49.89	1991.83	-5.82	-87.20	-2841.70
B_{43}	-408.63	-13.30	-0.35	9.00	1780.765	1519.77	8.99	-758.19	83.54	-15.22	118.15	220.06
B_{4-3}	224.02	9.22	-0.17	8.95	1780.777	0.00	13.85	-758.11	83.53	-15.36	118.15	-219.95
B_{44}	349.27	2390.20	156.90	2318.21	1869.223	-1057.93	2287.58	2650.99	-1882.08	2396.67	2459.65	-1527.48
B_{4-4}	9.58	-9.40	0.00	0.32	-0.032	-0.00	-2.85	0.01	0.11	0.63	-0.00	0.30
B_{60}	479.82	72.59	519.14	97.03	841.981	-241.84	-12.40	148.77	-816.69	67.70	40.84	-744.39
B_{61}	64.61	-0.90	0.02	1.43	-341.198	-244.99	-1.46	107.71	-13.58	-0.14	28.78	-18.96
B_{6-1}	34.28	-0.38	-0.01	-1.44	341.196	-0.00	-0.27	-107.71	13.56	0.09	-28.78	-18.38
B_{62}	-1.28	-4.65	0.02	0.33	0.015	92.45	1.59	0.01	0.01	0.30	0.00	-0.68
B_{6-2}	0.91	0.18	0.01	-2.24	-141.553	0.00	-1.16	13.08	-46.44	0.13	1.64	3.25
B_{63}	-55.80	2.80	-0.06	-1.84	28.270	157.70	-1.26	-67.99	12.92	2.66	-21.07	160.97
B_{6-3}	37.02	-1.86	-0.03	-1.83	28.270	0.00	-2.25	-67.98	12.92	2.67	-21.07	-161.30
B_{64}	1368.79	-183.70	1388.26	-176.13	1504.243	769.79	-172.44	190.38	739.56	-185.40	-181.64	668.13
B_{6-4}	6.71	0.74	0.00	-0.03	0.003	-0.00	0.10	0.00	-0.03	-0.05	-0.00	-0.59
B_{65}	13.56	3.20	0.13	-1.38	19.552	-1.72	3.44	15.29	-1.00	0.51	-3.39	-45.96

B_{6-5}	11.21	0.85	-0.06	1.42	-19.551	0.00	0.76	-15.27	1.00	-0.55	3.39	-45.78
B_{66}	2.97	-7.19	-0.01	0.51	-0.012	133.31	2.69	0.00	0.04	0.56	-0.00	-0.74
B_{6-6}	-0.19	-2.22	-0.00	2.36	247.511	-0.00	-5.01	39.38	380.87	2.54	35.58	-356.02

Tb ($4f^8$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-2222.99	-210.75	-2488.08	-5.03	-4829.369	1114.96	-1754.16	-3981.53	417.49	-285.45	-632.11	1041.83
B_{21}	24.05	23.83	0.02	-9.87	178.376	198.70	-14.01	357.27	-8.58	24.99	174.64	507.68
B_{2-1}	-91.78	-0.36	0.48	-10.82	-178.346	1.09	16.41	-358.83	8.58	-4.10	-174.66	509.09
B_{22}	6.51	38.31	-0.19	-19.20	-0.008	-1292.19	0.32	0.44	-0.00	39.78	-0.00	-2.27
B_{2-2}	45.65	-24.98	0.04	3.09	108.680	1.37	19.52	471.58	402.77	19.49	184.14	-843.53
B_{40}	-6388.63	4634.85	-6280.17	4699.78	-3602.900	-1065.68	3476.65	810.54	-337.00	4616.33	4327.59	-2146.88
B_{41}	297.36	12.09	0.14	9.98	-140.004	-35.40	-1.30	-847.14	-2.29	12.01	82.27	37.87
B_{4-1}	117.70	-3.55	-0.10	10.30	139.981	-0.20	-70.03	850.22	2.29	-17.06	-82.31	39.42
B_{42}	-14.35	-17.11	-0.30	9.99	-0.045	1005.58	-1.23	-0.34	0.00	-17.58	-0.00	-5.27
B_{4-2}	-17.63	5.84	-0.02	11.67	728.235	-5.89	-8.53	-105.32	1736.45	-5.72	-104.36	-3409.74
B_{43}	676.27	-6.03	-0.01	7.35	1724.513	-749.21	-4.83	-771.38	-12.95	-6.65	144.97	76.80
B_{4-3}	-121.55	13.40	0.43	-3.71	1724.688	0.38	-33.82	-772.22	-12.95	-14.41	144.97	-75.78
B_{44}	936.07	2871.82	272.43	2809.58	1790.685	-1327.85	2740.51	3287.52	-1571.56	2894.09	2942.76	-1750.88
B_{4-4}	-0.68	9.32	-0.13	0.18	0.017	-0.49	-2.00	0.35	0.00	-2.65	0.00	1.09
B_{60}	2764.08	260.31	2694.15	329.48	4513.245	-1319.46	-2.84	683.89	-1230.90	231.47	180.53	-1908.10
B_{61}	-355.66	14.18	-0.08	2.14	-802.866	147.59	-6.86	331.19	3.80	13.62	108.29	-12.38
B_{6-1}	-66.38	-4.30	0.17	1.22	802.905	0.06	-1.38	-331.96	-3.80	-1.72	-108.31	-12.59
B_{62}	8.12	8.34	-0.06	-3.20	-0.003	440.04	0.45	-0.17	-0.00	10.26	-0.00	-1.81
B_{6-2}	0.08	-6.37	0.04	5.72	-579.621	0.37	2.77	37.70	-51.41	4.21	2.61	-60.57
B_{63}	228.57	2.84	0.10	-4.83	-61.069	-176.30	2.06	-208.63	-5.57	3.31	-73.46	274.24
B_{6-3}	8.06	-7.14	0.36	3.05	-61.085	-0.03	14.28	-209.11	-5.57	6.90	-73.46	-272.74

B_{64}	5651.49	-640.97	5353.73	-620.87	5143.891	1092.24	-598.63	580.79	965.26	-650.16	-622.91	1251.57
B_{6-4}	-4.75	-2.67	0.00	0.01	0.011	0.71	0.03	0.22	-0.00	0.76	0.00	2.97
B_{65}	-64.84	7.12	-0.03	-6.53	61.175	47.84	-2.57	92.13	0.93	7.51	-13.33	-88.01
B_{6-5}	-5.08	4.41	0.69	-5.80	-61.195	-0.33	12.03	-92.32	-0.93	-1.33	13.33	-88.34
B_{66}	9.66	12.85	-0.00	-4.82	-0.040	722.88	-0.17	-0.10	0.00	16.32	0.00	-0.21
B_{6-6}	-26.46	-14.26	-0.01	-6.59	361.086	-1.83	11.62	34.92	601.02	11.23	119.45	-932.94

Dy ($4f^9$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-1640.88	-148.71	-1607.89	-22.93	-2707.3	1538.13	-2268.56	-1870.02	515.50	-185.82	-449.63	701.84
B_{21}	6.54	-0.85	-0.19	-21.14	239.8	304.97	23.17	900.73	36.37	6.39	155.54	742.71
B_{2-1}	16.52	-6.18	0.43	21.22	-239.8	1.71	-29.59	-900.70	-36.35	-0.20	-155.50	739.91
B_{22}	-23.52	-0.26	-0.19	-52.14	0.0	-1806.54	-1.78	-0.06	0.04	-33.31	-0.01	-0.50
B_{2-2}	-19.20	83.72	0.04	-19.33	68.1	0.72	3.58	920.47	1179.21	-4.62	165.21	-1495.88
B_{40}	-2128.77	599.71	-1951.09	611.53	-1875.0	-68.03	453.90	71.45	-24.73	596.49	564.55	-395.17
B_{41}	4.71	-0.58	-0.04	-0.03	193.4	-25.11	-7.95	-141.95	7.45	1.70	8.26	24.69
B_{4-1}	39.56	-1.79	0.19	-0.13	-193.4	0.06	6.52	141.95	-7.45	1.08	-8.25	24.24
B_{42}	30.50	0.11	-0.03	8.52	-0.0	295.75	0.34	0.01	-0.00	5.37	0.00	-0.53
B_{4-2}	0.91	-4.65	0.00	-1.05	207.5	0.31	-0.34	583.28	358.76	0.68	-13.34	-847.46
B_{43}	56.06	2.10	-0.06	1.81	578.7	-160.93	4.63	-355.98	17.72	-1.92	19.28	24.38
B_{4-3}	-213.82	0.12	-0.30	0.72	578.7	-0.13	4.47	-355.96	17.72	1.81	19.28	-24.49
B_{44}	881.76	380.69	565.52	368.99	497.6	-250.61	355.81	65.12	-276.00	384.09	410.30	-377.29
B_{4-4}	-0.89	10.33	-0.00	0.20	-0.0	-0.09	-0.39	0.03	0.00	0.33	-0.00	0.26
B_{60}	1983.26	117.05	1731.79	148.30	2783.9	-685.04	-13.95	-753.96	-615.98	107.10	68.55	-1047.67
B_{61}	-40.58	2.14	0.04	-0.12	-560.8	98.03	0.77	353.53	-15.60	0.31	45.66	6.87
B_{6-1}	-174.77	-3.49	-0.18	0.68	560.9	-0.26	-2.65	-353.53	15.60	-1.12	-45.65	7.72
B_{62}	-9.75	-0.35	-0.02	-7.63	-0.0	234.53	-0.33	-0.00	-0.02	-5.46	-0.01	-0.05
B_{6-2}	0.37	2.96	0.00	-2.43	-260.9	0.11	0.20	-84.26	-50.60	-0.25	2.17	-27.06
B_{63}	17.02	-3.36	-0.08	-2.95	-12.2	-101.25	-7.09	-291.65	16.84	3.04	-30.02	135.38
B_{6-3}	-133.76	-0.24	-0.40	-1.25	-12.2	-0.14	-6.84	-291.63	16.85	-2.88	-30.02	-135.33
B_{64}	3562.27	-300.33	3209.38	-290.52	3194.6	550.81	-280.61	615.87	471.58	-303.52	-300.94	615.61
B_{6-4}	-2.11	-8.11	-0.00	-0.14	-0.0	-0.12	0.31	-0.05	0.01	-0.27	0.00	0.94
B_{65}	6.12	-0.57	0.15	-2.63	74.0	24.46	4.55	28.92	0.56	0.68	-3.23	-54.19

B_{6-5}	-30.91	-0.02	-0.72	1.75	-74.1	-0.03	-4.33	-28.90	-0.56	0.25	3.24	-54.86
B_{66}	4.11	0.79	-0.00	-11.69	-0.0	396.41	-0.36	0.06	-0.00	-8.35	-0.00	0.29
B_{6-6}	5.36	18.17	0.00	0.61	269.6	0.14	1.43	572.53	337.38	-2.57	49.00	-531.67

Ho ($4f^{10}$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-1121.58	-143.42	-1160.85	5.84	-2011.65	464.36	-699.84	-272.26	268.97	-114.20	-258.64	551.59
B_{21}	-12.64	-7.71	-0.01	2.60	3.52	120.15	7.81	130.95	-0.57	7.77	62.26	142.64
B_{2-1}	2.08	-6.51	0.02	2.57	-3.56	-0.82	-9.04	-130.95	0.57	2.07	-62.25	142.64
B_{22}	-2.57	-9.20	-0.00	7.78	0.03	-561.78	-21.02	0.00	0.05	23.98	0.00	-0.03
B_{2-2}	-7.49	59.94	-0.03	-0.48	-2.16	1.14	7.63	94.46	129.91	-11.08	60.75	-365.18
B_{40}	-11743.21	7421.96	-11391.39	7613.98	-6852.73	-1369.45	5635.48	2926.36	-604.87	7468.53	7068.63	-3603.99
B_{41}	-434.43	-16.04	-0.24	-7.14	97.35	-124.15	-2.24	-857.55	4.62	24.67	85.35	6.53
B_{4-1}	-559.30	-12.32	0.26	-4.77	-97.28	-1.04	107.84	857.54	-4.62	25.29	-85.42	6.51
B_{42}	-66.40	19.05	-0.00	-15.62	0.10	2208.79	43.48	0.00	-0.11	-43.77	-0.03	-0.16
B_{4-2}	-24.68	-97.17	-0.19	18.62	1124.08	-6.23	-12.85	5134.50	3360.63	15.46	-134.82	-6668.32
B_{43}	-1015.58	-7.54	-0.43	-10.13	3450.22	-1793.82	25.20	-1348.87	4.15	-12.79	198.81	-130.67
B_{4-3}	1109.61	3.52	-0.58	12.37	3450.46	1.26	67.94	-1348.89	4.15	21.30	198.72	130.59
B_{44}	3194.69	4723.23	1271.94	4537.87	3656.19	-2350.38	4411.26	1447.04	-2548.52	4676.05	4792.81	-3177.84
B_{4-4}	-21.85	-12.18	-0.12	1.37	-0.05	-2.07	4.67	-0.15	-0.08	-6.41	-0.01	0.00
B_{60}	55675.21	2886.41	48921.01	4541.73	69735.15	-19750.45	274.01	-29193.59	-17763.05	3152.28	2277.66	-30054.79
B_{61}	4766.34	-166.07	0.84	-32.10	-14209.66	3461.50	131.59	6269.43	-16.24	144.69	1245.55	498.49
B_{6-1}	5474.65	-130.79	-0.73	-30.50	14210.16	11.17	-26.03	-6269.50	16.24	24.31	-1245.50	498.52
B_{62}	38.07	-58.60	0.00	55.32	-0.69	7399.36	-163.41	0.01	-0.34	182.66	0.08	-0.28
B_{6-2}	-62.60	249.12	0.91	57.98	-6252.11	13.61	34.08	-960.91	-559.43	-66.47	51.08	-1703.72
B_{63}	-3139.68	33.31	-2.02	55.81	-565.88	-2940.50	-97.18	-5630.30	7.05	53.73	-836.30	2768.85
B_{6-3}	3456.27	-14.38	-2.27	-63.79	-565.14	2.14	-242.77	-5630.26	7.05	-88.20	-835.97	-2769.60
B_{64}	91423.11	-8854.36	81546.79	-8364.16	74021.53	14960.35	-7981.23	14732.28	12522.05	-8764.30	-8620.06	15084.41
B_{6-4}	-211.35	23.96	-1.42	-1.89	-0.24	15.01	-12.17	0.28	0.81	8.88	0.03	-0.04
B_{65}	1321.31	-34.94	4.01	49.37	1909.79	908.68	22.82	1376.42	6.38	64.58	-50.19	-1116.96
B_{6-5}	1483.33	-38.15	-5.42	51.19	-1909.02	-2.49	-139.68	-1376.47	-6.38	18.91	50.18	-1116.39

B_{66}	-104.99	-105.17	-0.00	81.49	-0.41	12091.52	-215.04	0.05	-0.98	293.62	0.21	-0.18
B_{6-6}	76.03	1034.90	-0.87	-108.56	6534.91	-19.73	149.00	17915.89	9222.61	-212.92	1298.13	-14844.90

Er ($4f^{11}$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-1170.65	-33.74	-1171.00	-30.62	-2067.939	292.06	-436.21	-58.21	212.73	-107.62	-195.31	621.24
B_{21}	-32.99	0.50	0.04	4.00	-68.873	52.61	6.64	-79.79	-2.08	0.28	47.05	27.85
B_{2-1}	15.47	0.62	-0.06	2.26	68.865	0.11	12.82	78.21	0.59	0.76	-47.06	27.99
B_{22}	-4.77	10.50	0.02	47.69	0.012	-343.10	48.43	0.23	-0.64	-3.26	0.00	-0.13
B_{2-2}	-23.06	-2.17	-0.00	0.95	-23.709	1.77	-3.55	-100.37	-134.14	2.60	44.52	-111.83
B_{40}	-3872.80	586.07	-3552.33	13629.68	-3429.348	11.84	454.95	323.34	-9.07	571.62	557.41	-513.41
B_{41}	-107.93	0.51	-0.08	3.13	406.623	-55.96	-6.91	-78.72	-0.67	1.37	5.04	37.22
B_{4-1}	-81.60	0.74	0.38	-15.85	-406.650	-0.18	-4.52	78.33	0.18	-1.24	-5.04	37.14
B_{42}	-20.90	-3.52	-0.00	-73.40	-0.029	501.36	-16.01	-0.73	0.90	1.10	-0.00	0.14
B_{4-2}	-0.03	1.10	0.00	25.50	302.925	-1.04	0.78	657.69	490.69	-0.94	-12.99	-1519.22
B_{43}	-402.68	0.85	-0.12	-24.41	1019.733	-242.41	4.64	-132.67	-1.02	-1.85	19.45	36.64
B_{4-3}	214.92	-1.07	-0.32	28.98	1019.717	0.07	-5.73	-132.90	-1.03	-1.95	19.45	-36.64
B_{44}	2114.26	360.64	1554.01	8187.08	891.650	-320.39	333.52	-38.89	-343.19	374.85	395.18	-694.54
B_{4-4}	-3.60	-0.46	-0.01	-1.50	-0.007	-0.84	-0.20	-0.11	0.26	0.01	0.00	-0.07
B_{60}	6313.98	319.62	5564.09	3343.13	7268.385	-1823.43	36.64	-1650.77	-1532.32	239.46	199.54	-3115.05
B_{61}	549.56	3.26	0.09	-30.23	-1442.332	367.23	5.25	264.03	1.96	-0.36	102.40	16.79
B_{6-1}	322.89	3.82	-0.59	-52.90	1442.353	0.42	19.26	-263.44	-1.10	2.25	-102.41	16.52
B_{62}	22.28	6.86	-0.00	98.82	-0.053	719.06	34.62	-1.37	1.47	-2.17	0.01	0.46
B_{6-2}	-7.87	0.69	0.00	36.74	-588.402	1.46	-1.65	-85.49	-102.77	1.02	5.56	-134.44
B_{63}	-364.65	-2.93	-0.25	52.81	-23.127	-264.46	-16.84	-252.96	-2.43	6.42	-66.22	219.72
B_{6-3}	144.44	3.68	-1.11	-61.78	-23.060	-0.12	20.67	-253.50	-2.47	6.78	-66.24	-219.69
B_{64}	9667.90	-675.60	8735.28	-6484.43	7647.848	1326.43	-627.24	491.35	1055.90	-698.20	-684.09	1210.33
B_{6-4}	-12.77	0.84	-0.00	1.77	-0.018	0.94	0.39	0.06	-0.55	-0.03	-0.00	0.28
B_{65}	154.35	-1.62	0.40	21.77	254.245	61.90	9.86	47.79	0.03	1.26	1.03	-117.82

B_{6-5}	43.39	-2.52	-1.33	39.07	-254.162	-0.47	10.04	-48.23	-0.51	-0.58	-1.05	-118.01
B_{66}	3.37	9.75	-0.04	149.15	0.044	1144.35	44.56	-1.32	2.29	-3.21	0.00	0.41
B_{6-6}	39.00	-6.92	-0.00	-67.45	620.666	-1.62	-7.87	1078.31	869.13	7.77	105.42	-1609.87

Tm ($4f^{12}$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-642.42	-53.14	-615.51	-43.62	-950.850	519.37	-686.49	-339.52	298.62	-64.13	-102.02	330.49
B_{21}	-2.39	-1.81	0.06	17.46	28.149	136.24	2.07	-4.47	-1.01	7.78	48.01	131.75
B_{2-1}	-1.47	22.98	0.03	13.77	-28.153	-0.07	0.10	5.25	1.00	-4.04	-47.93	131.86
B_{22}	-2.93	-5.69	-0.05	1.22	-0.017	-607.02	-1.35	0.12	0.12	12.77	-0.64	-0.33
B_{2-2}	20.52	-3.30	-0.01	-9.55	2.085	0.02	-2.01	415.40	368.03	9.44	49.45	-533.04
B_{40}	-3093.60	1424.89	-3020.24	1425.79	-2010.651	-186.33	1083.51	804.56	-173.66	1419.60	1373.54	-794.53
B_{41}	45.25	-1.75	0.19	4.58	147.712	-47.34	0.87	-109.97	-1.53	3.86	13.52	3.49
B_{4-1}	-52.60	14.84	0.00	4.94	-147.722	-0.02	0.72	110.58	1.55	0.06	-13.64	3.40
B_{42}	32.88	4.58	-0.07	-0.83	-0.006	616.85	1.17	0.67	-0.09	-9.41	0.50	0.55
B_{4-2}	-9.45	1.32	-0.02	5.92	226.961	-0.16	1.03	1002.57	848.91	-3.17	-25.41	-2012.43
B_{43}	77.71	-3.30	0.11	0.79	960.761	-450.13	3.87	-126.15	-5.23	-1.04	32.58	-90.57
B_{4-3}	119.61	-0.14	-0.01	0.97	960.778	0.05	-3.26	-126.03	-5.23	-1.23	32.47	90.51
B_{44}	1180.81	892.23	796.03	882.44	963.583	-502.65	831.12	294.55	-518.54	896.15	906.52	-912.41
B_{4-4}	-0.05	-0.69	0.03	0.13	0.003	0.03	0.19	0.12	-0.05	3.39	0.05	0.07
B_{60}	-9835.18	-288.24	-8801.55	-306.06	-10085.204	2277.44	-104.26	2019.15	1951.44	-256.76	-214.09	4620.82
B_{61}	274.13	9.33	0.80	-31.39	2532.406	-515.65	-6.59	-273.98	-8.43	-13.40	-109.50	-72.90
B_{6-1}	-397.20	-36.74	-0.03	-25.56	-2532.502	0.08	-3.37	274.94	8.39	2.50	109.18	-71.97
B_{62}	53.65	7.81	0.04	-2.12	-0.019	-935.44	2.14	-1.09	0.20	-19.02	0.87	-1.32
B_{6-2}	-8.68	2.58	-0.09	-0.59	418.069	0.28	1.48	128.33	145.27	-5.68	-7.23	108.73
B_{63}	-221.65	-7.03	-1.30	0.91	-264.095	413.10	7.58	302.15	6.97	-2.43	65.85	-21.25
B_{6-3}	-330.38	0.50	0.01	2.22	-264.061	-0.01	-6.56	301.65	6.97	-3.24	65.53	20.92
B_{64}	-14760.22	792.99	-13323.66	779.94	-11682.246	-1622.65	699.51	-603.08	-1274.74	800.80	790.99	-1276.21
B_{6-4}	0.96	-0.83	-0.24	0.15	-0.035	0.42	0.18	-0.82	-0.35	2.71	0.10	-0.52
B_{65}	98.08	-1.79	1.09	-13.61	-548.644	-68.16	2.09	-72.11	-0.02	-5.37	-4.78	31.81
B_{6-5}	-100.56	-6.77	-0.02	-11.45	548.763	-0.01	3.21	71.65	0.03	4.37	4.53	32.44
B_{66}	-24.41	12.41	0.00	-2.16	-0.008	-	2.76	-0.25	0.36	-28.76	1.37	-1.62

						1458.88						
B_{6-6}	86.60	9.17	0.13	20.64	-1172.018	0.32	6.74	-1367.72	-1146.19	-19.74	-116.09	2536.87

Yb ($4f^{13}$)												
	3x3x3		2x2x2									
CFPs/Model	M0a	M0b	M0a	M0b	M1	M2(i)	M2(ii)	M2(iii)	M2(iv)a	M2(iv)b	M3a	M3b
B_{20}	-1283.71	-512.26	-1467.56	-65.89	-3768.558	583.78	-1278.86	-1121.75	-1472.16	-198.59	-136.61	602.31
B_{21}	-151.43	42.87	0.95	-14.73	314.906	105.16	-2.93	338.57	86.58	-2.45	122.68	409.90
B_{2-1}	157.49	-30.38	2.82	4.77	-314.915	28.24	9.96	-338.58	-86.58	-3.40	-122.67	410.13
B_{22}	2.78	1.90	2.78	-50.38	0.022	-946.59	34.89	0.00	0.00	32.03	-0.00	0.42
B_{2-2}	28.21	-10.00	-2.04	-3.24	291.198	-321.07	10.68	126.55	-41.34	8.91	130.19	-739.71
B_{40}	-2428.97	1889.66	-2340.50	1963.44	-1282.351	-545.16	1466.58	543.33	-998.94	1945.78	1904.65	-938.66
B_{41}	-45.15	14.12	-0.53	8.30	-126.643	-33.86	6.38	-201.30	55.15	0.43	19.29	-9.88
B_{4-1}	49.57	-15.40	0.18	-0.89	126.600	-6.73	-8.57	201.30	-55.15	-1.96	-19.29	-10.06
B_{42}	-0.14	-0.32	1.42	15.46	0.017	297.62	-10.24	0.01	-0.00	-8.71	0.00	-0.13
B_{4-2}	15.37	2.14	0.37	-3.06	169.895	2.01	-2.89	784.64	16.78	-1.37	-48.22	-1192.50
B_{43}	-263.63	1.81	-0.53	-0.13	306.611	-372.26	-3.68	-464.59	246.89	2.09	48.70	-28.81
B_{4-3}	-277.02	6.27	-2.96	3.16	306.792	12.64	-5.68	-464.59	246.89	-4.14	48.71	28.87
B_{44}	407.63	1272.04	-53.67	1191.77	1280.710	-707.00	1146.69	710.99	-166.12	1216.79	1173.62	-611.24
B_{4-4}	0.09	0.65	-0.02	6.64	-0.041	-52.04	0.51	-0.01	-0.00	1.50	-0.02	-0.27
B_{60}	1535.56	65.14	1337.92	215.72	2882.263	-1122.52	6.76	-794.62	304.59	170.86	186.11	-1077.59
B_{61}	202.96	19.82	0.51	-0.98	-140.848	151.47	0.10	369.67	-107.18	0.37	65.69	52.01
B_{6-1}	-214.51	-14.64	-2.88	-1.06	140.978	4.29	2.71	-369.70	107.18	-0.29	-65.69	52.17
B_{62}	-3.19	0.28	-1.93	-10.11	-0.053	320.16	7.68	-0.01	0.00	6.38	0.00	-0.08
B_{6-2}	-8.63	-1.53	0.03	-2.96	-293.774	-10.93	1.80	-70.06	-7.34	1.36	-2.08	-61.51
B_{63}	-170.48	-1.22	0.43	-1.22	-53.109	-149.35	2.65	-242.63	48.28	-1.96	-40.10	216.90
B_{6-3}	-180.13	-4.96	-1.55	-3.13	-53.024	2.84	4.13	-242.62	48.28	3.58	-40.10	-217.05
B_{64}	3568.89	-497.65	3314.76	-449.53	4033.116	1050.97	-425.57	750.83	1022.08	-465.33	-432.34	857.36
B_{6-4}	-0.68	-0.21	-0.06	-2.60	0.005	1.23	-0.18	0.02	-0.00	-0.61	0.01	0.06
B_{65}	15.80	6.19	-0.44	-7.07	-80.314	32.90	-1.57	43.52	31.23	-1.74	1.05	-83.42
B_{6-5}	-18.63	1.43	1.79	2.70	80.339	0.71	3.65	-43.51	-31.23	-2.18	-1.04	-83.44
B_{66}	0.40	0.41	0.95	-14.65	0.020	534.57	10.02	0.00	-0.00	9.93	-0.00	-0.21

B_{6-6}	14.94	-5.38	0.91	2.62	16.750	-29.48	8.02	599.47	18.23	3.03	78.42	-493.59