A Quantitatively Constrained Framework for Defect Identification in Oxides: Application to Cr^{3+} Centers in $PbTiO_3$

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S1: Mapping of experimental EPR centers to atomistic models

The C1 center, which is observed across single crystals, ceramics, and nanopowders, represents the most stable and prevalent Cr^{3+} environment. Its moderate axial zero-field splitting and near-axial symmetry are consistent with Cr^{3+} substitution at the Ti^{4+} (B) site in a tetragonally elongated oxygen octahedron, with charge compensation occurring at longer range rather than via a nearest-neighbor oxygen vacancy. Accordingly, C1 is most directly represented by the isolated Ti-site substitution model (Cr–Ti_ M0-Ti) and, where explicit compensation is included, by the Ti-site model with a distant oxygen vacancy (Cr–Ti_ M2d-Ti).

The C2 and C3 centers, observed primarily in nanopowder samples, exhibit significantly enhanced axial ZFS parameters and reduced local symmetry. Superposition-model analysis attributes these centers to off-centered Cr^{3+} ions within the TiO_6 octahedron, with estimated displacements of approximately 0.16 Å (C2) and 0.26 Å (C3), respectively. Importantly, both experimental studies explicitly exclude oxygen vacancies in the first coordination shell for these centers. In the present work, such environments are naturally captured by relaxed Ti-site substitution models—either without explicit vacancies or with only distant charge-compensating defects—where structural relaxation allows spontaneous off-centering of the Cr^{3+} ion.

The C4 center, characterized by an almost vanishing ZFS parameter and near-isotropic g-values, appears only in ultrafine nanopowders and is interpreted as arising from a nearly regular octahedral coordination corresponding to a locally cubic or paraelectric-like environment. This center can be qualitatively associated with the high-symmetry limit of the Ti-site substitution model, where the tetragonal distortion of the host lattice is strongly reduced.

Finally, configurations involving nearest-neighbor oxygen vacancies or cation-vacancy complexes—explicitly included in the present model set—are expected to produce much larger symmetry breaking and ZFS magnitudes than those observed for the dominant experimental centers. While such models are therefore unlikely to correspond to C1–C3, they remain important for exploring less prevalent or processing-dependent defect complexes and for establishing energetic and spectroscopic bounds on possible Cr^{3+} environments.

Table S1. Mapping of experimental Cr^{3+} EPR centers to structural models used in this work.

EPR center	Key experimental characteristics	Literature interpretation	Corresponding structural models in this work
C1	Moderate axial ZFS (e.g., $D=$ 840 10^{-4} cm^{-1}); axial symmetry; observed in	Centered Cr^{3+} in a tetragonally elongated octahedron; Ti-site	Cr–Ti_ M0-Ti (isolated Cr^{3+} at Ti site); Cr–Ti_ M2d-Ti (Ti-site Cr^{3+} with distant V_O

	bulk, ceramics, and nanopowders	substitution with remote charge compensation; no nearest-neighbor V_O	
C2	Larger axial ZFS than C1; reduced symmetry; observed mainly in nanopowders	Off-centered Cr^{3+} (~0.16 Å) within TiO_6 octahedron; no oxygen vacancy in first ligand shell	Cr–Ti_ M0-Ti (after relaxation allowing off-centering); Cr–Ti_ M2d-Ti (remote V_O, relaxed)
C3	Very large axial ZFS; strongest local distortion; nanopowders	Strongly off-centered Cr^{3+} (~0.26 Å); enhanced tetragonal distortion; first-shell V_O excluded	Cr–Ti_ M0-Ti (off-centered relaxed configuration); Cr–Ti_ M2d-Ti (remote-compensation scenario)
C4	Very small ZFS; near-isotropic g-tensor; appears in ultrafine powders	Nearly regular octahedral coordination; near-cubic local environment (paraelectric-like)	Cr–Ti_ M0-Ti constrained toward cubic symmetry (high-T / weak tetragonality limit); reference undistorted Ti-site Cr^{3+}
(non-dominant / speculative)	Strong symmetry breaking; large ZFS expected	Nearest-neighbor oxygen vacancy or complex defect clusters (not dominant in EPR)	Cr–Ti_ M2b-z/xy (Ti-site Cr^{3+} + nearby V_O; Cr–Pb_ M2a-z/xy; Model3 (cation vacancies)

S2. Results of Chgnet optimization calculations on 3x3x3 supercells.

Table S2. Optimized structural and energetic parameters for representative Cr^{3+}-doped PTO models (3×3×3 supercell, fully relaxed). f_{max} is the maximum residual force after relaxation. Energies and formation energies are in eV; lattice parameters in Å; and volumes in $Å^3$.

Model-3x3x3	fmax (eV/Å)	Energy (eV)	Volume ($Å^3$)	a (Å)	b (Å)	c (Å)	Form. Energy (eV)
M0-Pb	0.0143	-1089.735	1945.11	11.3992	11.4203	14.8884	-6.575
M0-Ti	0.0180	-1081.116	1949.24	11.4194	11.4210	14.9458	-2.146
M1	0.0158	-1087.367	1940.00	11.4322	11.4322	14.8441	-7.956
M2a-z	0.0197	-1080.499	1932.34	11.4471	11.3457	14.8791	-2.27
M2a-xy	0.0181	-1080.146	1809.94	11.7051	11.7051	13.2103	-1.916
M2b-z	0.0142	-1073.195	1953.99	10.8936	11.4410	14.1877	0.846
M2b-xy	0.0194	-1071.725	1812.51	11.7236	11.6434	13.2782	2.315
M2-mix	0.0196	-1078.541	1928.51	11.3655	11.4309	14.8449	-4.061
M2d-Pb	0.0197	-1079.972	1810.31	11.6515	11.7585	13.2136	-1.742
M2d-Ti	0.0182	-1071.694	1810.02	11.6282	11.7685	13.2266	2.346
M3-VTi	0.0193	-1074.522	1954.09	11.4194	11.4194	14.9850	0.788
M3-VPb	0.0204	-1075.884	1944.27	11.2672	11.2938	14.6746	-0.574

Table S3. Magnetic and Bond Valence Properties of Cr^{3+}-Doped PTO Models (3×3×3 supercell, fully relaxed). $\langle E \rangle$ and σE are the average and standard deviation of MD energy (eV). Magnetization (M) in A/m. BVS_Cr_0 and BVS_Cr_1 denote bond valence sums; ΔBVS values indicate deviations from ideal Cr^{3+} (3.0).

Model	MD $\langle E \rangle$ (eV)	MD σE (eV)	M (A/m)	BVS Cr0	ΔBVS Cr0	BVS Cr1	ΔBVS Cr1
M0-Pb	-1083.4036	1.8170	1.430e+04	1.61	-1.39	-	-
M0-Ti	-1074.7955	1.8757	1.427e+04	3.39	0.39	-	-
M1	-1081.5341	1.7778	1.434e+04	2.89	-0.11	2.27	-0.73
M2a-z	1074.4482	1.7501	1.440e+04	1.74	-1.26	-	-
M2a-xy	1074.2754	1.7739	1.537e+04	2.04	-0.96	-	-
M2b-z	-1067.0814	1.8654	1.424e+04	2.40	-0.60	-	-
M2b-xy	1065.9313	1.7321	1.535e+04	2.91	-0.09	-	-
M2-mix	-1072.5875	1.7297	1.443e+04	2.30	-0.70	1.98	-1.02
M2d-Pb	-1073.7484	1.8631	1.537e+04	2.32	-0.68	-	-
M2d-Ti	-1065.7518	1.7932	1.537e+04	3.02	0.02	-	-
M3-VTi	-1068.5543	1.7255	1.424e+04	2.88	-0.12	-	-
M3-VPb	1069.7526	1.7709	1.431e+04	3.28	0.28	-	-

S3. Optimized Atomic Coordinates of Nearest-Neighbor Ligands Surrounding the Central Cr3+ Ion Obtained Using CHGNet

This section presents the optimized atomic coordinates of oxygen ligands in the first coordination shell around the central Cr^{3+} ion, as obtained from CHGNet-optimized structures. The coordination number is 8 for Cr^{3+} substitution at the A-site (Pb) and 6 for substitution at the B-site (Ti). Cartesian coordinates of the central Cr^{3+} 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 Cr^{3+} ion as the origin. Additionally, the local site symmetry of each Cr^{3+}ion is specified beneath the corresponding table.

M0-Pb - 2x2x2

```
◈ Central atom Cr at index 15 — (3.8945, 3.8945, 5.9309)
Atom      r (Å)     θ (°)      φ (°)      X (Å)      Y (Å)      Z (Å)
================================================================================
O         2.0227    73.1601   -90.0012    3.8945     1.9585     6.5169
O         2.0228    73.1614   179.9992    1.9585     3.8945     6.5169
O         2.0228    73.1589    0.0002     5.8305     3.8945     6.5170
O         2.0228    73.1604   90.0017     3.8945     5.8306     6.5169
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O          3.2292  119.0739  -44.9941      5.8904      1.8990      4.3617
O          3.2293  119.0739   44.9954      5.8904      5.8901      4.3617
O          3.2293  119.0727  134.9944      1.8990      5.8905      4.3617
O          3.2294  119.0729 -134.9957      1.8989      1.8986      4.3617
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◈ Local site symmetry: Low symmetry (C1 or Cs)

M0-Ti - 2x2x2

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◈ Central atom Cr at index 0 — (1.9057, 1.8936, 2.8738)
Atom        r (Å)      θ (°)      φ (°)      X (Å)      Y (Å)      Z (Å)
========================================================================
O          1.8433     1.9502   -91.0580      1.9045      1.8309      4.7161
O          2.0009   104.0181   179.8061     -0.0357      1.9002      2.3891
O          2.0011   103.4717    90.0268      1.9048      3.8396      2.4076
O          2.0013   103.9609     0.2467      3.8478      1.9020      2.3910
O          2.0018   104.4824   -89.9389      1.9077     -0.0446      2.3732
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◈ Local site symmetry: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

M1- 2x2x2

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◈ Central atom Cr at index 0 — (1.9231, 1.9231, 2.4730)
Atom        r (Å)      θ (°)      φ (°)      X (Å)      Y (Å)      Z (Å)
========================================================================
O          1.8948     4.3259  -135.0295      1.8220      1.8221      4.3624
O          2.0028    96.6810    90.2246      1.9153      3.9123      2.2400
O          2.0028    96.6802    -0.2249      3.9123      1.9153      2.2400
O          2.0081    98.4118   -89.9232      1.9258     -0.0634      2.1793
O          2.0081    98.4120   179.9235     -0.0634      1.9258      2.1793
```

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


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◈ Central atom Cr at index 15 — (3.9108, 3.9108, 6.0175)
Atom        r (Å)      θ (°)      φ (°)      X (Å)      Y (Å)      Z (Å)
========================================================================
O          2.0069    69.8421    -0.9587      5.7946      3.8793      6.7091
O          2.0070    69.8440    90.9591      3.8793      5.7946      6.7090
O          2.0307    69.6808  -178.6450      2.0070      3.8658      6.7226
O          2.0307    69.6805   -91.3549      3.8658      2.0070      6.7226
Ti         2.9798    68.4253    44.9997      5.8703      5.8702      7.1132
Ti         3.0055    67.4401   135.4621      1.9325      5.8575      7.1705
Ti         3.0055    67.4400   -45.4617      5.8576      1.9325      7.1705
O          3.0252   117.5289    44.9997      5.8078      5.8078      4.6192
Ti         3.0676    64.9448  -134.9996      1.9458      1.9458      7.3166
O          3.1464   117.7990   -45.3397      5.8672      1.9312      4.5501
O          3.1464   117.7995   135.3398      1.9312      5.8672      4.5501
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O          3.3860  119.2614 -135.0016      1.8220       1.8221       4.3624
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◈ Local site symmetry: Trigonal bipyramidal (D3h) or Square pyramidal (C4v)

M2a-z - 2x2x2

◈ Central atom Cr at index 15 — (3.9305, 3.9262, 5.8828)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0306	75.8736	-0.7705	5.8995	3.8997	6.3784
O	2.0306	75.8736	-89.2295	3.9569	1.9571	6.3784
O	2.0403	76.4393	179.8954	1.9471	3.9298	6.3612
O	2.0403	76.4392	90.1047	3.9268	5.9096	6.3612
O	3.2734	119.0339	-134.3593	1.9295	1.8799	4.2941
O	3.2734	119.0339	44.3594	5.9767	5.9272	4.2941
O	3.2881	118.3634	134.9999	1.8845	5.9721	4.3207

◈ Local site symmetry: Low symmetry (C1 or Cs)

M2a-xy - 2x2x2

◈ Central atom Cr at index 15 — (3.9159, 3.3035, 5.1606)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1140	51.5413	161.1808	2.3490	3.8375	6.4754
O	2.1140	51.5413	18.8192	5.4828	3.8375	6.4755
O	2.1390	115.0605	-144.2709	2.3430	2.1720	4.2546
O	2.1390	115.0601	-35.7291	5.4888	2.1720	4.2546
O	2.2675	48.6052	-89.9998	3.9159	1.6024	6.6600
O	3.1689	104.1225	128.9223	1.9852	5.6943	4.3874
O	3.1689	104.1223	51.0776	5.8467	5.6943	4.3874

◈ Local site symmetry: Low symmetry (C1 or Cs)

M2b-z - 2x2x2

◈ Central atom Cr at index 0 — (1.9788, 1.9544, 2.2553)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	1.9573	10.9074	180.0000	1.6085	1.9544	4.1773
O	1.9682	87.0432	0.0000	3.9444	1.9544	2.3568
O	2.0087	95.1615	-91.6470	1.9213	-0.0453	2.0746
O	2.0087	95.1614	91.6469	1.9213	3.9541	2.0746

◈ Local site symmetry: Tetrahedral (Td) or Square planar (D4h)

Model2(ii)b- 2x2x2

◈ Central atom Cr at index 0 — (1.9228, 1.9222, 2.4390)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0281	94.0299	-89.9886	1.9232	-0.1008	2.2965
O	2.0282	93.9116	179.9855	-0.1007	1.9227	2.3007
O	2.0283	93.9569	89.9924	1.9231	3.9457	2.2991
O	2.0284	94.0892	0.0175	3.9460	1.9228	2.2944

◈ Local site symmetry: Tetrahedral (Td) or Square planar (D4h)

M2-mix - 2x2x2

◈ Central atom Cr at index 0 — (1.9328, 1.9328, 2.3516)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0439	93.6964	90.3325	1.9209	3.9724	2.2198
O	2.0439	93.6964	-0.3326	3.9724	1.9209	2.2198
O	2.0455	92.9127	-89.9185	1.9357	-0.1101	2.2476
O	2.0455	92.9124	179.9182	-0.1101	1.9357	2.2476

◈ Local site symmetry: Tetrahedral (Td) or Square planar (D4h)

◈ Central atom Cr at index 15 — (3.8767, 3.8767, 6.2956)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0167	74.8652	-179.1943	1.9301	3.8494	6.8221
O	2.0167	74.8652	-90.8058	3.8494	1.9301	6.8221
O	2.0209	74.8273	0.0187	5.8271	3.8774	6.8245
O	2.0209	74.8273	89.9813	3.8774	5.8271	6.8245
O	3.2608	120.6282	-46.0500	5.8241	1.8566	4.6343
O	3.2608	120.6281	136.0503	1.8566	5.8241	4.6343
O	3.2653	119.8777	44.9996	5.8788	5.8788	4.6689

◈ Local site symmetry: Low symmetry (C1 or Cs)

M2d-Pb - 2x2x2

◈ Central atom Cr at index 15 — (3.9997, 3.9145, 5.6510)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0312	75.1178	-90.0000	3.9997	1.9515	6.1727
O	2.0313	77.2592	90.0002	3.9997	5.8958	6.0990
O	2.0437	75.2533	-0.1486	5.9761	3.9094	6.1712

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O        2.0437    75.2531 -179.8518       2.0233       3.9094       6.1712
O        3.2799   116.5475  135.9232       1.8918       5.9555       4.1851
O        3.2799   116.5474   44.0765       6.1076       5.9555       4.1851
O        3.4216   117.4787 -139.0551       1.7068       1.9252       4.0722
O        3.4216   117.4786  -40.9449       6.2926       1.9252       4.0722
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◈ Local site symmetry: Low symmetry (C1 or Cs)

M2d-Ti - 2x2x2

◈ Central atom Cr at index 0 — (1.9615, 2.0243, 2.1771)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0101	4.6815	-90.0011	1.9615	1.8602	4.1806
O	2.0493	91.8569	-174.3635	-0.0767	1.8231	2.1107
O	2.0493	91.8557	-5.6370	3.9998	1.8231	2.1108
O	2.0780	91.9821	90.0001	1.9615	4.1010	2.1053
O	2.0972	96.3358	-90.0001	1.9615	-0.0601	1.9457

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

M3-VTi - 2x2x2

◈ Central atom Cr at index 14 — (3.7900, 3.8219, 6.6679)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	1.7941	75.5154	-174.8990	2.0598	3.6674	7.1166
O	1.7945	75.7590	84.8064	3.9475	5.5541	7.1093
O	1.9063	67.9438	-2.0301	5.5557	3.7593	7.3838
O	1.9072	67.7250	-87.9530	3.8531	2.0581	7.3908
O	3.3729	124.5330	-133.0055	1.8948	1.7899	4.7558
O	3.3738	124.5201	42.9389	5.8250	5.7155	4.7560
O	3.4542	123.5856	-44.9607	5.8261	1.7885	4.7571
O	3.5349	125.0137	135.0141	1.7423	5.8685	4.6397

◈ Local site symmetry: Tetrahedral (Td) or Square planar (D4h)

M3-VPb - 2x2x2

◈ Central atom Cr at index 0 — (1.9119, 1.8332, 2.9915)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	1.6364	3.1304	-44.5451	1.9756	1.7706	4.6255
O	1.8916	108.1670	-89.8218	1.9175	0.0360	2.4018

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O          1.8951  106.1732 -179.8623     0.0918      1.8289      2.4637
O          1.8977  106.1421   90.7257     1.8888      3.6560      2.4639
```

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

M0-Pb - 3x3x3

◈ Central atom Cr at index 40 — (3.8819, 4.1656, 6.2493)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0214	66.5649	178.8197	2.0276	4.2038	7.0532
O	2.0232	72.5803	89.0071	3.9154	6.0958	6.8550
O	2.0251	66.4641	-88.7225	3.9233	2.3094	7.0580
O	2.0269	71.8615	1.1333	5.8077	4.2037	6.8803
Ti	3.0301	65.0640	133.0482	2.0063	6.1735	7.5268
Ti	3.0324	60.7836	-135.0324	2.0094	2.2952	7.7295
Ti	3.0406	68.0344	45.1777	5.8697	6.1658	7.3866
Ti	3.0411	63.8389	-43.1164	5.8744	2.3000	7.5901
O	3.2340	120.5655	-133.1895	1.9761	2.1354	4.6047
O	3.2413	124.7303	136.1715	1.9602	6.0103	4.4027
O	3.3818	121.9325	-46.2727	5.8658	2.0916	4.4606
O	3.3915	126.0790	44.0285	5.8527	6.0707	4.2520

◈ Local site symmetry: Tetrahedral (Td) or Square planar (D4h)

M0-Ti - 3x3x3

Central atom: Cr at (5.7100, 5.6867, 7.9152)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	1.8905	3.9959	-90.9443	5.7078	5.5550	9.8011
O	2.0063	104.9152	-90.0129	5.7095	3.7480	7.3988
O	2.0075	103.7662	0.2953	7.6598	5.6967	7.4375
O	2.0076	103.7801	179.7085	3.7602	5.6966	7.4370
O	2.0092	102.6987	90.0145	5.7095	7.6468	7.4735
O	3.1422	179.8788	89.7413	5.7100	5.6933	4.7730

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

M1- 3x3x3

Central atom Cr at Pb site— (5.7462, 5.7463, 7.7408)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	1.8895	3.4865	45.0109	5.8275	5.8275	9.6268
O	1.9826	104.1044	-0.8437	7.6688	5.7180	7.2577
O	1.9826	104.1059	90.8434	5.7179	7.6689	7.2576

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O          2.0307  102.2377 -178.1748      3.7627      5.6831      7.3103
O          2.0307  102.2383  -91.8260      5.6830      3.7627      7.3103
O          2.9958  178.7011   45.0195      5.7942      5.7943      4.7458
```

◈ Local site symmetry: Octahedral (Oh)

◈ Central atom Cr at Ti site — (3.7828, 3.7829, 6.5984)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0166	69.6216	-89.9280	3.7851	1.8926	7.3006
O	2.0166	69.6187	179.9295	1.8924	3.7852	7.3007
O	2.0293	69.4612	90.6060	3.7627	5.6831	7.3103
O	2.0293	69.4625	-0.6094	5.6830	3.7627	7.3103
O	3.2593	124.7043	-134.9917	1.8883	1.8879	4.7427
O	3.3422	123.9853	134.8503	1.8283	5.7476	4.7302
O	3.3426	123.9816	-44.8468	5.7479	1.8282	4.7301
O	3.3947	123.0749	44.9989	5.7942	5.7943	4.7458

◈ Local site symmetry: Tetrahedral (Td) or Square planar (D4h)

M2a-z - 3x3x3

◈ Central atom Cr at index 40 — (3.8134, 4.3531, 5.9426)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1291	121.4778	146.7778	2.2944	5.3480	4.8309
O	2.1305	121.4053	33.0697	5.3372	5.3453	4.8324
O	2.1309	51.6488	-160.2032	2.2411	3.7871	7.2648
O	2.1327	51.6920	-19.8208	5.3878	3.7857	7.2646
O	2.2105	45.5842	89.9187	3.8156	5.9320	7.4896
O	3.4765	110.3404	-128.6365	1.7781	1.8069	4.7342
O	3.4796	110.0725	-52.1502	5.8188	1.7724	4.7484

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

M2a-xy - 3x3x3

◈ Central atom Cr at index 40 — (3.8978, 3.9064, 5.9813)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0207	73.5465	-179.7798	1.9599	3.8990	6.5536
O	2.0207	73.5464	89.7799	3.9052	5.8443	6.5536
O	2.0209	74.6827	-89.0074	3.9315	1.9576	6.5151
O	2.0209	74.6826	-0.9925	5.8466	3.8727	6.5151
O	3.2098	119.7077	135.0001	1.9264	5.8778	4.3906
O	3.2148	120.1058	-135.1239	1.9270	1.9441	4.3688
O	3.2148	120.1059	45.1239	5.8601	5.8773	4.3687

◈ Local site symmetry: Low symmetry (C1 or Cs)

M2b-z - 3x3x3

◈ Central atom Cr at index 13 — (3.4163, 6.4593, 9.7732)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0206	111.8276	-179.5428	1.5406	6.4444	9.0219
O	2.0215	76.3555	0.1909	5.3806	6.4659	10.2500
O	2.0222	92.5074	-88.8056	3.4584	4.4395	9.6847
O	2.0222	95.4214	88.5335	3.4678	8.4719	9.5821
O	2.5958	162.0983	-4.0966	4.2121	6.4023	7.3030

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

Model2(ii)b- 3x3x3

◈ Central atom Cr at index 13 — (5.8146, 5.8217, 6.7179)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	1.9092	9.8245	-0.0004	6.1404	5.8217	8.5991
O	1.9449	94.2918	-179.9999	3.8751	5.8217	6.5724
O	1.9967	95.2332	86.6134	5.9320	7.8066	6.5358
O	1.9967	95.2334	-86.6135	5.9320	3.8368	6.5358
O	2.2232	178.2505	-0.0018	5.8825	5.8217	4.4957

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

M2-mix - 3x3x3

◈ Central atom Cr at Ti site — (5.5615, 5.7283, 7.8098)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	1.8710	6.9570	-91.7305	5.5547	5.5017	9.6670
O	1.9504	107.1149	90.1857	5.5555	7.5923	7.2358
O	1.9781	105.5297	-4.1388	7.4624	5.5907	7.2802
O	1.9964	107.8956	-171.1739	3.6842	5.4368	7.1963
O	3.1605	177.1435	30.6290	5.6970	5.8085	4.6533

◈ Local site symmetry: Tetrahedral (Td) or Square planar (D4h)

◈ Central atom Cr at Pb site — (3.1734, 3.8194, 5.8884)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.1246	121.7873	-122.2980	2.2085	2.2929	4.7692
O	2.1331	122.6872	123.3913	2.1854	5.3184	4.7364
O	2.1358	51.7482	-68.7633	3.7810	2.2561	7.2107
O	2.1418	52.3619	72.4736	3.6842	5.4368	7.1963
O	2.1970	45.2673	-179.2080	1.6128	3.7978	7.4346
O	3.4425	111.0254	38.2450	5.6970	5.8085	4.6533

```
O          3.4510  110.2777  -36.9600      5.7601      1.8731      4.6923
```

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

M2d-Pb - 3x3x3

◈ Central atom Cr at index 40 — (3.8841, 3.9201, 5.9618)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	2.0149	73.6375	-179.9799	1.9508	3.9194	6.5294
O	2.0153	73.6189	-0.0146	5.8176	3.9196	6.5302
O	2.0405	73.2658	-90.0096	3.8838	1.9660	6.5493
O	2.0411	73.2374	89.9771	3.8849	5.8745	6.5505
O	3.2008	119.9529	134.2347	1.9495	5.9071	4.3637
O	3.2027	119.9288	-45.7641	5.8204	1.9315	4.3639
O	3.2027	119.9283	45.7742	5.8200	5.9091	4.3639
O	3.2053	119.9097	-134.2276	1.9461	1.9292	4.3635

◈ Local site symmetry: Low symmetry (C1 or Cs)

M2d-Ti - 3x3x3

◈ Central atom Cr at index 13 — (5.8428, 5.8548, 6.7414)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	1.9320	3.3122	-99.5757	5.8242	5.7448	8.6703
O	2.0183	97.9766	-92.4759	5.7564	3.8579	6.4614
O	2.0297	96.2293	177.8515	3.8265	5.9305	6.5212
O	2.0349	95.0854	88.6872	5.8892	7.8812	6.5611
O	2.0593	94.8254	-6.1379	7.8830	5.6354	6.5682
O	2.2891	178.8083	79.2188	5.8517	5.9016	4.4528

◈ Local site symmetry: Octahedral (Oh)

M3-VTi - 3x3x3

◈ Central atom Cr at index 39 — (3.8201, 3.8199, 6.8102)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	1.8899	75.0827	96.1565	3.6242	5.6355	7.2967
O	1.8900	75.0619	-6.1528	5.6356	3.6242	7.2974
O	1.9535	72.5017	-91.6617	3.7660	1.9575	7.3976
O	1.9536	72.5038	-178.3443	1.9576	3.7661	7.3976
Ti	3.0249	66.8589	135.9169	1.8220	5.7550	7.9990
Ti	3.0250	66.8523	-45.9154	5.7552	1.8219	7.9994
Ti	3.0560	66.5216	-135.0034	1.8379	1.8380	8.0278
O	3.4811	126.7242	44.9991	5.7931	5.7928	4.7286
O	3.4873	126.8886	-135.0003	1.8478	1.8477	4.7169

```
O          3.5426  126.3937  -46.5156       5.7824       1.7509       4.7083
O          3.5455  126.3610  136.5055       1.7488       5.7851       4.7082
```

◈ Local site symmetry: Tetrahedral (Td) or Square planar (D4h)

M3-VPb - 3x3x3

◈ Central atom Cr at index 13 — (4.5605, 4.3741, 9.4463)

Atom	r (Å)	θ (°)	φ (°)	X (Å)	Y (Å)	Z (Å)
O	1.8585	6.9047	-124.7945	4.4330	4.1906	11.2914
O	1.9545	105.8449	174.9790	2.6874	4.5387	8.9127
O	1.9584	107.3378	-85.6366	4.7027	2.5101	8.8627
O	2.0090	98.9410	2.3099	6.5434	4.4541	9.1341
O	2.0092	97.3934	87.6459	4.6423	6.3649	9.1878
O	3.2385	165.7487	44.8030	5.1261	4.9359	6.3075

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

S4. Outputs of the Superposition Model (SPM)–based ZFS calculations obtained using the Python workflow

M0-Pb

```
Nearest ligands:
Atom   R (Å)   Theta (deg)   Phi (deg)
   O 2.02143      66.56488   178.81968
   O 2.02325      72.58025    89.00713
   O 2.02510      66.46406   -88.72254
   O 2.02688      71.86153     1.13335
   O 3.23397     120.56554  -133.18955
   O 3.24125     124.73030   136.17147
   O 3.38180     121.93254   -46.27275
   O 3.39155     126.07895    44.02852

Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.668153 Å
B(2):  23400
B(4):  0
B(6):  0
t(2):  0.36
t(4):  0
t(6):  0

Initial ZFS (calc):
  B(2,0): -36173.284391
  B(4,0): 0.000000
  B(6,0): 0.000000
```

```
Enter experimental ZFS parameters (same units as your model outputs):
B(2,0):  850
B(4,0):  0
B(6,0):  0
Max % variation for MODEL parameters (e.g. 5):  5
Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `ftol` termination condition is satisfied.
Fit error (RMS over targets): 2.077103e+04

B(2,0):  calc = -19921.031956 | exp =  850.000000 | Δ = -2.077103e+04
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.668153 Å
R0 (fitted)  = 2.534745 Å
ΔR0 (%)      = -5.000
B(2) initial = 2.340000e+04 | fitted = 2.223000e+04 | Δ% = -5.000
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.342000 | Δ% = -5.000
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
```

[Structural parameters: ligand shell]

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)
Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)			
1	2.0214	2.0619	0.0404	2.0000	66.5649	62.9649
-3.6	178.8197	181.6547	2.8351			
2	2.0232	2.0637	0.0405	2.0000	72.5803	68.9803
-3.6	89.0071	88.1008	-0.9063			
3	2.0251	2.0656	0.0405	2.0000	66.4641	62.8641
-3.6	-88.7225	-92.3223	-3.5998			
4	2.0269	2.0674	0.0405	2.0000	71.8615	68.2615
-3.6	1.1333	1.1333	0.0000			
5	3.2340	3.2986	0.0647	1.9995	120.5655	124.1655
3.6	-133.1895	-133.1895	0.0000			
6	3.2413	3.1764	-0.0648	-1.9999	124.7303	128.3303
3.6	136.1715	136.1715	0.0000			
7	3.3818	3.3144	-0.0674	-1.9940	121.9325	125.5325
3.6	-46.2727	-46.2727	0.0000			
8	3.3915	3.3237	-0.0678	-2.0000	126.0790	129.6790
3.6	44.0285	44.0285	0.0000			

```
Nearest ligands:
Atom   R (Å)   Theta (deg)   Phi (deg)
   O 1.89047       3.99588   -90.94430
   O 2.00633     104.91519   -90.01287
   O 2.00751     103.76618     0.29532
   O 2.00761     103.78011   179.70847
   O 2.00925     102.69869    90.01449
   O 3.14222     179.87878    89.74127


Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.177233 Å
B(2):  23400
B(4):  0
B(6):  0
t(2):  0.36
t(4):  0
t(6):  0


Initial ZFS (calc):
  B(2,0): 4997.323625
  B(4,0): 0.000000
  B(6,0): 0.000000


        Enter experimental ZFS parameters (same units as your model outputs):
                               B(2,0):  850
                               B(4,0):  0
                               B(6,0):  0
                Max % variation for MODEL parameters (e.g. 5):  5
              Max % variation for STRUCTURAL parameters (e.g. 2):  2


=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 0.000000e+00

B(2,0):  calc =  850.000000 | exp =  850.000000 | Δ =  0.000000e+00
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00


=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.177233 Å
R0 (fitted)  = 2.098930 Å
ΔR0 (%)      = -3.596
B(2) initial = 2.340000e+04 | fitted = 2.231291e+04 | Δ% = -4.646
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.377871 | Δ% = 4.964
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)


[Structural parameters: ligand shell]
```

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	1.8905	1.9283	0.0378	2.0000	3.9959	6.3571	2.3613	-90.9443	-90.9443	0.0
2	2.0063	1.9663	-0.0400	-1.9959	104.9152	101.9943	-2.9209	-90.0129	-90.0129	0.0
3	2.0075	1.9674	-0.0401	-1.9967	103.7662	100.9146	-2.8516	0.2953	0.2953	0.0
4	2.0076	1.9675	-0.0401	-1.9967	103.7801	100.9277	-2.8524	179.7085	179.7085	0.0
5	2.0092	1.9691	-0.0401	-1.9972	102.6987	99.9182	-2.7805	90.0145	90.0145	0.0
6	3.1422	3.2051	0.0628	2.0000	179.8788	178.8042	-1.0746	89.7413	89.7413	0.0

Enter experimental ZFS parameters (same units as your model outputs):
B(2,0): 1600
B(4,0): 0
B(6,0): 0
Max % variation for MODEL parameters (e.g. 5): 5
Max % variation for STRUCTURAL parameters (e.g. 2): 2

=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 7.275958e-12

B(2,0): calc = 1600.000000 | exp = 1600.000000 | Δ = 7.275958e-12
B(4,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00
B(6,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.177233 Å
R0 (fitted) = 2.102799 Å
ΔR0 (%)   = -3.419
B(2) initial = 2.340000e+04 | fitted = 2.225749e+04 | Δ% = -4.883
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.377525 | Δ% = 4.868
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	1.8905	1.9283	0.0378	2.0000	3.9959	5.0355	1.0396	-90.9443	-90.9443	0.0
2	2.0063	1.9666	-0.0397	-1.9799	104.9152	102.5889	-2.3263	-90.0129	-90.0129	0.0
3	2.0075	1.9677	-0.0398	-1.9833	103.7662	101.5473	-2.2188	0.2953	0.2953	0.0
4	2.0076	1.9678	-0.0398	-1.9832	103.7801	101.5600	-2.2202	179.7085	179.7085	0.0

```
     5          2.0092       1.9693 -0.0399 -1.9858        102.6987           100.5885
-2.1102           90.0145          90.0145       0.0
     6          3.1422       3.2051  0.0628  2.0000        179.8788           179.8489
-0.0299           89.7413          89.7413       0.0


              Enter experimental ZFS parameters (same units as your model outputs):
                                    B(2,0):  3090
                                     B(4,0):  0
                                     B(6,0):  0
                      Max % variation for MODEL parameters (e.g. 5):  5
                  Max % variation for STRUCTURAL parameters (e.g. 2):  2


=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 5.456968e-12

B(2,0):  calc =  3090.000000 | exp =  3090.000000 | Δ = -5.456968e-12
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.177233 Å
R0 (fitted)  = 2.135033 Å
ΔR0 (%)      = -1.938
B(2) initial = 2.340000e+04 | fitted = 2.244510e+04 | Δ% = -4.081
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.371258 | Δ% = 3.127
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)


[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
     1          1.8905       1.9283  0.0378  1.9999          3.9959             4.3241
0.3283          -90.9443         -90.9443       0.0
     2          2.0063       1.9775 -0.0288 -1.4374        104.9152           103.8911
-1.0241          -90.0129         -90.0129       0.0
     3          2.0075       1.9780 -0.0295 -1.4678        103.7662           102.8080
-0.9582           0.2953           0.2953       0.0
     4          2.0076       1.9782 -0.0295 -1.4675        103.7801           102.8211
-0.9590          179.7085         179.7085       0.0
     5          2.0092       1.9792 -0.0300 -1.4931        102.6987           101.8039
-0.8948           90.0145          90.0145       0.0
     6          3.1422       3.2040  0.0618  1.9660        179.8788           179.8703
-0.0085           89.7413          89.7413       0.0


              Enter experimental ZFS parameters (same units as your model outputs):
                                    B(2,0):  10
                                     B(4,0):  0
```

```
                          B(6,0):  0
          Max % variation for MODEL parameters (e.g. 5):  5
          Max % variation for STRUCTURAL parameters (e.g. 2):  2


=== BEST FIT RESULTS ===
Success: True
Message: `xtol` termination condition is satisfied.
Fit error (RMS over targets): 1.818989e-11

B(2,0):  calc =  10.000000 | exp =  10.000000 | Δ = -1.818989e-11
B(4,0):  calc =   0.000000 | exp =   0.000000 | Δ =  0.000000e+00
B(6,0):  calc =   0.000000 | exp =   0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.177233 Å
R0 (fitted)  = 2.083336 Å
ΔR0 (%)      = -4.313
B(2) initial = 2.340000e+04 | fitted = 2.224525e+04 | Δ% = -4.935
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.378000 | Δ% = 5.000
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)


[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
    1        1.8905         1.9283  0.0378     2.0          3.9959           7.5880
3.5922      -90.9443        -90.9443       0.0
    2        2.0063         1.9662 -0.0401    -2.0        104.9152         101.3154
-3.5998     -90.0129        -90.0129       0.0
    3        2.0075         1.9674 -0.0402    -2.0        103.7662         100.1667
-3.5995       0.2953          0.2953       0.0
    4        2.0076         1.9675 -0.0402    -2.0        103.7801         100.1807
-3.5995     179.7085        179.7085       0.0
    5        2.0092         1.9691 -0.0402    -2.0        102.6987          99.0999
-3.5988      90.0145         90.0145       0.0
    6        3.1422         3.2051  0.0628     2.0        179.8788         178.1626
-1.7162      89.7413         89.7413       0.0


                              M1_Cr1


Nearest ligands:
  Atom      R      Theta       Phi
0    O  1.8895     3.4865    45.0109
1    O  1.9826   104.1044    -0.8437
2    O  1.9826   104.1059    90.8434
3    O  2.0307   102.2377  -178.1748
4    O  2.0307   102.2383   -91.8260
5    O  2.9958   178.7011    45.0195


Using initial R0 = <R> = 2.151983 Å
```

```
B(2):  23400
B(4):  0
B(6):  0
t(2):  0.36
t(4):  0
t(6):  0

                              Initial ZFS (calc):
                              B(2,0): 4662.628289
                               B(4,0): 0.000000
                               B(6,0): 0.000000


Enter experimental ZFS parameters (same units as your model outputs):
B(2,0):  850
B(4,0):  0
B(6,0):  0


=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS): 2.182787e-11
B(2,0): calc=850.000000, exp=850.000000
B(4,0): calc=0.000000, exp=0.000000
B(6,0): calc=0.000000, exp=0.000000


=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.151983 Å
R0 (fitted)  = 2.079479 Å
ΔR0 (%)      = -3.369
B(2) initial = 2.340000e+04 | fitted = 2.235352e+04 | Δ% = -4.472
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.377608 | Δ% = 4.891
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)


[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
     1          1.8895         1.9273  0.0378  2.0000           3.4865          5.6139
2.1275         45.0109         45.0109        0.0
     2          1.9826         1.9431 -0.0395 -1.9912         104.1044        101.3679
-2.7366         -0.8437         -0.8437        0.0
     3          1.9826         1.9431 -0.0395 -1.9912         104.1059        101.3693
-2.7367         90.8434         90.8434        0.0
     4          2.0307         1.9903 -0.0405 -1.9929         102.2377         99.6334
-2.6043       -178.1748       -178.1748        0.0
     5          2.0307         1.9903 -0.0405 -1.9929         102.2383         99.6340
-2.6043        -91.8260        -91.8260        0.0
     6          2.9958         3.0557  0.0599  2.0000         178.7011        177.0617
-1.6394         45.0195         45.0195        0.0
```

```
              Enter experimental ZFS parameters (same units as your model outputs):
                                    B(2,0):  1600
                                     B(4,0):  0
                                     B(6,0):  0


        === BEST FIT RESULTS ===
        Success: True
        Message: `gtol` termination condition is satisfied.
        Fit error (RMS): 3.637979e-12
        B(2,0): calc=1600.000000, exp=1600.000000
        B(4,0): calc=0.000000, exp=0.000000
        B(6,0): calc=0.000000, exp=0.000000

        === FINAL FITTED PARAMETERS ===

        [Model / SPM parameters]
        R0 (initial) = 2.151983 Å
        R0 (fitted)  = 2.083897 Å
        ΔR0 (%)      = -3.164
        B(2) initial = 2.340000e+04 | fitted = 2.227612e+04 | Δ% = -4.803
        B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
        B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
        t(2) initial = 0.360000 | fitted = 0.377021 | Δ% = 4.728
        t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
        t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)


        [Structural parameters: ligand shell]
         Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
        Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
            1         1.8895        1.9273  0.0378  2.0000          3.4865          4.3265
        0.8401       45.0109         45.0109       0.0
            2         1.9826        1.9435 -0.0391 -1.9715        104.1044        101.9714
        -2.1330       -0.8437         -0.8437       0.0
            3         1.9826        1.9435 -0.0391 -1.9715        104.1059        101.9728
        -2.1331       90.8434         90.8434       0.0
            4         2.0307        1.9906 -0.0401 -1.9768        102.2377        100.3032
        -1.9345      -178.1748        -178.1748      0.0
            5         2.0307        1.9906 -0.0401 -1.9768        102.2383        100.3037
        -1.9346      -91.8260         -91.8260      0.0
            6         2.9958        3.0557  0.0599  2.0000        178.7011        178.4186
        -0.2825       45.0195         45.0195       0.0


              Enter experimental ZFS parameters (same units as your model outputs):
                                    B(2,0):  3090
                                     B(4,0):  0
                                     B(6,0):  0


        === BEST FIT RESULTS ===
        Success: True
        Message: `gtol` termination condition is satisfied.
        Fit error (RMS): 3.637979e-12
        B(2,0): calc=3090.000000, exp=3090.000000
        B(4,0): calc=0.000000, exp=0.000000
        B(6,0): calc=0.000000, exp=0.000000
```

```
=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.151983 Å
R0 (fitted)  = 2.118086 Å
ΔR0 (%)      = -1.575
B(2) initial = 2.340000e+04 | fitted = 2.256542e+04 | Δ% = -3.567
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.368924 | Δ% = 2.479
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
     1          1.8895        1.9269  0.0373  1.9758          3.4865          3.7214
0.2349        45.0109        45.0109      0.0
     2          1.9826        1.9570 -0.0255 -1.2872        104.1044        103.2826
-0.8218       -0.8437        -0.8437      0.0
     3          1.9826        1.9571 -0.0255 -1.2872        104.1059        103.2840
-0.8219       90.8434        90.8434      0.0
     4          2.0307        2.0038 -0.0269 -1.3244        102.2377        101.5165
-0.7212      -178.1748      -178.1748      0.0
     5          2.0307        2.0038 -0.0269 -1.3244        102.2383        101.5170
-0.7212       -91.8260       -91.8260      0.0
     6          2.9958        3.0526  0.0569  1.8979        178.7011        178.6260
-0.0751       45.0195        45.0195      0.0


         Enter experimental ZFS parameters (same units as your model outputs):
                           B(2,0):  10
                           B(4,0):  0
                           B(6,0):  0


=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS): 3.637979e-12
B(2,0): calc=10.000000, exp=10.000000
B(4,0): calc=0.000000, exp=0.000000
B(6,0): calc=0.000000, exp=0.000000


=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.151983 Å
R0 (fitted)  = 2.067347 Å
ΔR0 (%)      = -3.933
B(2) initial = 2.340000e+04 | fitted = 2.227360e+04 | Δ% = -4.814
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.378000 | Δ% = 5.000
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
```

t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	1.8895	1.9273	0.0378	2.0	3.4865	6.6579	3.1714	45.0109	45.0109	0.0
2	1.9826	1.9429	-0.0397	-2.0	104.1044	100.5847	-3.5197	-0.8437	-0.8437	0.0
3	1.9826	1.9429	-0.0397	-2.0	104.1059	100.5862	-3.5197	90.8434	90.8434	0.0
4	2.0307	1.9901	-0.0406	-2.0	102.2377	98.7768	-3.4609	-178.1748	-178.1748	0.0
5	2.0307	1.9901	-0.0406	-2.0	102.2383	98.7773	-3.4609	-91.8260	-91.8260	0.0
6	2.9958	3.0557	0.0599	2.0	178.7011	176.5566	-2.1445	45.0195	45.0195	0.0

M1_Cr2

Nearest ligands:

Atom	R (Å)	Theta (deg)	Phi (deg)
O	1.88954	3.48648	45.01093
O	1.98255	104.10441	-0.84366
O	1.98257	104.10594	90.84336
O	2.03073	102.23773	-178.17482
O	2.03073	102.23828	-91.82597
O	2.99577	178.70110	45.01946
O	4.18880	63.56495	-0.98903
O	4.18897	63.56665	90.99094

Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.661209 Å
B(2): 23400
B(4): 0
B(6): 0
t(2): 0.36
t(4): 0
t(6): 0

Initial ZFS (calc):
  B(2,0): -3025.292463
  B(4,0): 0.000000
  B(6,0): 0.000000

Enter experimental ZFS parameters (same units as your model outputs):
B(2,0): 850
B(4,0): 0
B(6,0): 0
Max % variation for MODEL parameters (e.g. 5): 5
Max % variation for STRUCTURAL parameters (e.g. 2): 2

=== BEST FIT RESULTS ===
Success: True

```
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 1.818989e-12

B(2,0):  calc =  850.000000 | exp =  850.000000 | Δ =  1.818989e-12
B(4,0):  calc =    0.000000 | exp =    0.000000 | Δ =  0.000000e+00
B(6,0):  calc =    0.000000 | exp =    0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.661209 Å
R0 (fitted)  = 2.638158 Å
ΔR0 (%)      = -0.866
B(2) initial = 2.340000e+04 | fitted = 2.290190e+04 | Δ% = -2.129
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.357033 | Δ% = -0.824
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
    1         1.8895        1.8517 -0.0378 -2.0000         3.4865          3.0813
-0.4052      45.0109         45.0109        0.0
    2         1.9826        2.0161  0.0336  1.6930       104.1044        105.5577
1.4533       -0.8437         -0.8437        0.0
    3         1.9826        2.0161  0.0336  1.6930       104.1059        105.5593
1.4534       90.8434         90.8434        0.0
    4         2.0307        2.0658  0.0351  1.7268       102.2377        103.5334
1.2956     -178.1748       -178.1748        0.0
    5         2.0307        2.0658  0.0351  1.7268       102.2383        103.5340
1.2957      -91.8260        -91.8260        0.0
    6         2.9958        2.9359 -0.0599 -1.9979       178.7011        178.8341
0.1330       45.0195         45.0195        0.0
    7         4.1888        4.2255  0.0367  0.8758        63.5650         61.8120
-1.7530       -0.9890         -0.9890        0.0
    8         4.1890        4.2257  0.0367  0.8759        63.5666         61.8138
-1.7529       90.9909         90.9909        0.0


            Enter experimental ZFS parameters (same units as your model outputs):
                              B(2,0):  1600
                               B(4,0):  0
                               B(6,0):  0
                 Max % variation for MODEL parameters (e.g. 5):  5
             Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 1.273293e-11

B(2,0):  calc =  1600.000000 | exp =  1600.000000 | Δ = -1.273293e-11
B(4,0):  calc =     0.000000 | exp =     0.000000 | Δ =  0.000000e+00
```

```
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.661209 Å
R0 (fitted)  = 2.621784 Å
ΔR0 (%)      = -1.481
B(2) initial = 2.340000e+04 | fitted = 2.316053e+04 | Δ% = -1.023
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.352729 | Δ% = -2.020
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
```

[Structural parameters: ligand shell]

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	1.8895	1.8518	-0.0378	-1.9991	3.4865	2.1451	-1.3414	45.0109	45.0109	-0.0
2	1.9826	2.0117	0.0291	1.4703	104.1044	105.9264	1.8220	-0.8437	-0.8437	0.0
3	1.9826	2.0117	0.0291	1.4703	104.1059	105.9280	1.8221	90.8434	90.8434	0.0
4	2.0307	2.0612	0.0305	1.5006	102.2377	103.9962	1.7585	-178.1748	-178.1748	0.0
5	2.0307	2.0612	0.0305	1.5005	102.2383	103.9968	1.7585	-91.8260	-91.8260	0.0
6	2.9958	2.9374	-0.0584	-1.9496	178.7011	179.9437	1.2426	45.0195	45.0195	0.0
7	4.1888	4.2306	0.0418	0.9983	63.5650	61.6228	-1.9421	-0.9890	-0.9890	0.0
8	4.1890	4.2308	0.0418	0.9983	63.5666	61.6245	-1.9421	90.9909	90.9909	0.0

```
        Enter experimental ZFS parameters (same units as your model outputs):
                              B(2,0):  3090
                               B(4,0):  0
                               B(6,0):  0
               Max % variation for MODEL parameters (e.g. 5):  5
            Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 9.094947e-12

B(2,0):  calc =  3090.000000 | exp =  3090.000000 | Δ = -9.094947e-12
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
```

```
R0 (initial) = 2.661209 Å
R0 (fitted)  = 2.654419 Å
ΔR0 (%)      = -0.255
B(2) initial = 2.340000e+04 | fitted = 2.382520e+04 | Δ% = 1.817
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.352108 | Δ% = -2.192
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)


[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
     1         1.8895       1.8517  -0.0378  -2.0000        3.4865         2.3195
-1.1669       45.0109        45.0109       0.0
     2         1.9826       2.0191   0.0366   1.8442      104.1044       106.5231
2.4187        -0.8437        -0.8437       0.0
     3         1.9826       2.0191   0.0366   1.8441      104.1059       106.5247
2.4188        90.8434        90.8434       0.0
     4         2.0307       2.0686   0.0379   1.8650      102.2377       104.5368
2.2990      -178.1748      -178.1748       0.0
     5         2.0307       2.0686   0.0379   1.8650      102.2383       104.5373
2.2991       -91.8260       -91.8260       0.0
     6         2.9958       2.9359  -0.0599  -1.9996      178.7011       179.2461
0.5450        45.0195        45.0195       0.0
     7         4.1888       4.2432   0.0544   1.2990       63.5650        60.9538
-2.6112        -0.9890        -0.9890       0.0
     8         4.1890       4.2434   0.0544   1.2991       63.5666        60.9555
-2.6111        90.9909        90.9909       0.0


          Enter experimental ZFS parameters (same units as your model outputs):
                              B(2,0):  10
                              B(4,0):   0
                              B(6,0):   0
                 Max % variation for MODEL parameters (e.g. 5):   5
               Max % variation for STRUCTURAL parameters (e.g. 2):   2


=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 4.547474e-12

B(2,0):  calc =  10.000000 | exp =  10.000000 | Δ = -4.547474e-12
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.661209 Å
R0 (fitted)  = 2.637406 Å
ΔR0 (%)      = -0.894
B(2) initial = 2.340000e+04 | fitted = 2.286795e+04 | Δ% = -2.274
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
```

```
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.357490 | Δ% = -0.697
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
```

[Structural parameters: ligand shell]

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	1.8895	1.8517	-0.0378	-2.0000	3.4865	3.1912	-0.2953	45.0109	45.0109	0.0
2	1.9826	2.0117	0.0291	1.4700	104.1044	105.1899	1.0855	-0.8437	-0.8437	0.0
3	1.9826	2.0117	0.0291	1.4700	104.1059	105.1916	1.0856	90.8434	90.8434	0.0
4	2.0307	2.0614	0.0307	1.5103	102.2377	103.1963	0.9586	-178.1748	-178.1748	0.0
5	2.0307	2.0614	0.0307	1.5103	102.2383	103.1969	0.9586	-91.8260	-91.8260	0.0
6	2.9958	2.9364	-0.0593	-1.9811	178.7011	178.7967	0.0956	45.0195	45.0195	0.0
7	4.1888	4.2175	0.0287	0.6844	63.5650	62.2244	-1.3405	-0.9890	-0.9890	0.0
8	4.1890	4.2176	0.0287	0.6845	63.5666	62.2262	-1.3405	90.9909	90.9909	0.0

<center>M2a-z</center>

```
Nearest ligands:
Atom    R (Å)    Theta (deg)   Phi (deg)
  O 2.12911    121.47777   146.77779
  O 2.13050    121.40530    33.06969
  O 2.13086     51.64883 -160.20316
  O 2.13268     51.69197  -19.82075
  O 2.21049     45.58418   89.91874
  O 3.47646    110.34042 -128.63654
  O 3.47958    110.07246  -52.15018

Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.527098 Å
B(2):  23400
B(4):  0
B(6):  0
t(2):  0.36
t(4):  0
t(6):  0

Initial ZFS (calc):
  B(2,0): -8372.855801
  B(4,0): 0.000000
  B(6,0): 0.000000

        Enter experimental ZFS parameters (same units as your model outputs):
                        B(2,0):  850
                        B(4,0):  0
```

```
                           B(6,0):  0
           Max % variation for MODEL parameters (e.g. 5):  5
         Max % variation for STRUCTURAL parameters (e.g. 2):  2


=== BEST FIT RESULTS ===
Success: True
Message: `xtol` termination condition is satisfied.
Fit error (RMS over targets): 2.637535e-11

B(2,0):  calc =  850.000000 | exp =  850.000000 | Δ = -2.637535e-11
B(4,0):  calc =   0.000000 | exp =   0.000000 | Δ =  0.000000e+00
B(6,0):  calc =   0.000000 | exp =   0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.527098 Å
R0 (fitted)  = 2.465039 Å
ΔR0 (%)      = -2.456
B(2) initial = 2.340000e+04 | fitted = 2.261448e+04 | Δ% = -3.357
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.371728 | Δ% = 3.258
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)


[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)   ΔR (Å)   ΔR (%)   θ_initial (deg)  θ_fitted (deg)
Δθ (deg)   φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
    1        2.1291        2.1463  0.0172  0.8085       121.4778         123.8772
2.3994       146.7778        146.7778        0.0
    2        2.1305        2.1479  0.0174  0.8158       121.4053         123.8034
2.3981        33.0697         33.0697        0.0
    3        2.1309        2.1098 -0.0211 -0.9900        51.6488          49.1733
-2.4755      -160.2032       -160.2032        0.0
    4        2.1327        2.1117 -0.0210 -0.9852        51.6920          49.2171
-2.4749       -19.8208        -19.8208        0.0
    5        2.2105        2.1791 -0.0314 -1.4218        45.5842          43.1062
-2.4780        89.9187         89.9187        0.0
    6        3.4765        3.5235  0.0471  1.3543       110.3404         112.3382
1.9978      -128.6365       -128.6365        0.0
    7        3.4796        3.5270  0.0474  1.3628       110.0725         112.0620
1.9896       -52.1502        -52.1502        0.0


        Enter experimental ZFS parameters (same units as your model outputs):
                         B(2,0):  1600
                          B(4,0):  0
                          B(6,0):  0
           Max % variation for MODEL parameters (e.g. 5):  5
         Max % variation for STRUCTURAL parameters (e.g. 2):  2


=== BEST FIT RESULTS ===
Success: True
Message: `xtol` termination condition is satisfied.
```

```
Fit error (RMS over targets): 9.094947e-12

B(2,0):  calc =  1600.000000 | exp =  1600.000000 | Δ =  9.094947e-12
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.527098 Å
R0 (fitted)  = 2.465896 Å
ΔR0 (%)      = -2.422
B(2) initial = 2.340000e+04 | fitted = 2.265760e+04 | Δ% = -3.173
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.372748 | Δ% = 3.541
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
    1        2.1291       2.1459  0.0168  0.7891      121.4778        124.0837
2.6060     146.7778       146.7778     0.0
    2        2.1305       2.1475  0.0170  0.7989      121.4053        124.0098
2.6045      33.0697        33.0697     0.0
    3        2.1309       2.1087 -0.0221 -1.0385       51.6488         48.9590
-2.6898    -160.2032      -160.2032     0.0
    4        2.1327       2.1107 -0.0220 -1.0324       51.6920         49.0028
-2.6891     -19.8208       -19.8208     0.0
    5        2.2105       2.1762 -0.0343 -1.5502       45.5842         42.8919
-2.6923      89.9187        89.9187     0.0
    6        3.4765       3.5276  0.0511  1.4711      110.3404        112.4691
2.1286    -128.6365      -128.6365     0.0
    7        3.4796       3.5311  0.0515  1.4806      110.0725        112.1908
2.1184     -52.1502       -52.1502     0.0


       Enter experimental ZFS parameters (same units as your model outputs):
                           B(2,0):  3090
                            B(4,0):  0
                            B(6,0):  0
             Max % variation for MODEL parameters (e.g. 5):  5
           Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 2.000888e-11

B(2,0):  calc =  3090.000000 | exp =  3090.000000 | Δ = -2.000888e-11
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===
```

```
[Model / SPM parameters]
R0 (initial) = 2.527098 Å
R0 (fitted)  = 2.485109 Å
ΔR0 (%)      = -1.662
B(2) initial = 2.340000e+04 | fitted = 2.319980e+04 | Δ% = -0.856
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.374719 | Δ% = 4.089
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
     1        2.1291        2.1460  0.0169  0.7945       121.4778       124.4638
2.9860       146.7778       146.7778      0.0
     2        2.1305        2.1477  0.0172  0.8084       121.4053       124.3898
2.9845        33.0697        33.0697      0.0
     3        2.1309        2.1048 -0.0261 -1.2234        51.6488        48.5806
-3.0683      -160.2032      -160.2032      0.0
     4        2.1327        2.1067 -0.0259 -1.2163        51.6920        48.6243
-3.0676       -19.8208       -19.8208      0.0
     5        2.2105        2.1713 -0.0392 -1.7728        45.5842        42.5150
-3.0692        89.9187        89.9187      0.0
     6        3.4765        3.5348  0.0583  1.6769       110.3404       112.7844
2.4440      -128.6365      -128.6365      0.0
     7        3.4796        3.5383  0.0587  1.6865       110.0725       112.5039
2.4314       -52.1502       -52.1502      0.0


              Enter experimental ZFS parameters (same units as your model outputs):
                                   B(2,0):  10
                                   B(4,0):   0
                                   B(6,0):   0
                    Max % variation for MODEL parameters (e.g. 5):  5
                  Max % variation for STRUCTURAL parameters (e.g. 2):  2


=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 1.000444e-11

B(2,0):  calc =  10.000000 | exp =  10.000000 | Δ = -1.000444e-11
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.527098 Å
R0 (fitted)  = 2.467625 Å
ΔR0 (%)      = -2.353
B(2) initial = 2.340000e+04 | fitted = 2.265198e+04 | Δ% = -3.197
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
```

```
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.370615 | Δ% = 2.949
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
```

[Structural parameters: ligand shell]

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	2.1291	2.1477	0.0186	0.8746	121.4778	123.6393	2.1616	146.7778	146.7778	0.0
2	2.1305	2.1492	0.0187	0.8775	121.4053	123.5659	2.1606	33.0697	33.0697	0.0
3	2.1309	2.1094	-0.0215	-1.0090	51.6488	49.4270	-2.2218	-160.2032	-160.2032	0.0
4	2.1327	2.1112	-0.0215	-1.0073	51.6920	49.4706	-2.2213	-19.8208	-19.8208	0.0
5	2.2105	2.1824	-0.0281	-1.2716	45.5842	43.3609	-2.2233	89.9187	89.9187	0.0
6	3.4765	3.5187	0.0422	1.2145	110.3404	112.2271	1.8867	-128.6365	-128.6365	0.0
7	3.4796	3.5221	0.0425	1.2213	110.0725	111.9543	1.8819	-52.1502	-52.1502	0.0

M2a-xy

Nearest ligands:

Atom	R (Å)	Theta (deg)	Phi (deg)
O	2.02066	73.54650	-179.77980
O	2.02066	73.54638	89.77992
O	2.02088	74.68266	-89.00742
O	2.02088	74.68265	-0.99250
O	3.20979	119.70769	135.00007
O	3.21481	120.10584	-135.12390
O	3.21482	120.10591	45.12386

```
Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.531788 Å
B(2):  23400
B(4):  0
B(6):  0
t(2):  0.36
t(4):  0
t(6):  0

Initial ZFS (calc):
  B(2,0): -47428.192218
  B(4,0): 0.000000
  B(6,0): 0.000000

Enter experimental ZFS parameters (same units as your model outputs):
B(2,0):  850
B(4,0):  0
B(6,0):  0
Max % variation for MODEL parameters (e.g. 5):  5
```

```
Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `ftol` termination condition is satisfied.
Fit error (RMS over targets): 3.454043e+04

B(2,0):  calc = -33690.433268 | exp =  850.000000 | Δ = -3.454043e+04
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.531788 Å
R0 (fitted)  = 2.405199 Å
ΔR0 (%)      = -5.000
B(2) initial = 2.340000e+04 | fitted = 2.223000e+04 | Δ% = -5.000
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.342000 | Δ% = -5.000
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
    1        2.0207        2.0611  0.0404  2.0000      73.5465          69.9465
-3.6      -179.7798      -176.6589    3.1209
    2        2.0207        2.0611  0.0404  2.0000      73.5464          69.9464
-3.6        89.7799        90.5001    0.7202
    3        2.0209        2.0613  0.0404  2.0000      74.6827          71.0827
-3.6       -89.0074       -92.3438   -3.3364
    4        2.0209        2.0613  0.0404  2.0000      74.6826          71.0826
-3.6        -0.9925        -0.9925    0.0000
    5        3.2098        3.2740  0.0642  1.9999     119.7077         123.3077
3.6       135.0001       135.0001    0.0000
    6        3.2148        3.2791  0.0643  1.9999     120.1058         123.7058
3.6      -135.1239      -135.1239    0.0000
    7        3.2148        3.2791  0.0643  1.9999     120.1059         123.7059
3.6        45.1239        45.1239    0.0000
```

M2b-z

```
Nearest ligands:
Atom   R (Å)   Theta (deg)  Phi (deg)
   O 2.02061    111.82760 -179.54280
   O 2.02145     76.35553    0.19090
   O 2.02222     92.50738  -88.80560
   O 2.02224     95.42141   88.53347
   O 2.59585    162.09828   -4.09658

Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.136473 Å
```

```
B(2):  23400
B(4):  0
B(6):  0
t(2):  0.36
t(4):  0
t(6):  0

Initial ZFS (calc):
  B(2,0): -21685.082523
  B(4,0): 0.000000
  B(6,0): 0.000000

Enter experimental ZFS parameters (same units as your model outputs):
B(2,0):  850
B(4,0):  0
B(6,0):  0
Max % variation for MODEL parameters (e.g. 5):  5
Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `ftol` termination condition is satisfied.
Fit error (RMS over targets): 1.615503e+04

B(2,0):  calc = -15305.027845 | exp =  850.000000 | Δ = -1.615503e+04
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.136473 Å
R0 (fitted)  = 2.029649 Å
ΔR0 (%)      = -5.000
B(2) initial = 2.340000e+04 | fitted = 2.223000e+04 | Δ% = -5.000
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.342000 | Δ% = -5.000
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
     1        2.0206         2.0610  0.0404     2.0        111.8276        115.4276
3.6        -179.5428       -179.5428       0.0
     2        2.0215         2.0619  0.0404     2.0         76.3555         72.7555
-3.6          0.1909          0.1909       0.0
     3        2.0222         2.0627  0.0404     2.0         92.5074         96.1074
3.6        -88.8056        -88.8056       0.0
     4        2.0222         2.0627  0.0404     2.0         95.4214         99.0214
3.6        88.5335         88.5335       0.0
     5        2.5958         2.5439 -0.0519    -2.0        162.0983        165.6983
3.6         -4.0966         -4.0966       0.0
```

Nearest ligands:
```
Atom   R (Å)   Theta (deg)  Phi (deg)
  O 1.90917      9.82448    -0.00039
  O 1.94494     94.29177  -179.99993
  O 1.99666     95.23315    86.61341
  O 1.99667     95.23338   -86.61348
  O 2.22323    178.25050    -0.00182
```

Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.014134 Å
B(2): 23400
B(4): 0
B(6): 0
t(2): 0.36
t(4): 0
t(6): 0

Initial ZFS (calc):
  B(2,0): 10827.658360
  B(4,0): 0.000000
  B(6,0): 0.000000

Enter experimental ZFS parameters (same units as your model outputs):
B(2,0): 850
B(4,0): 0
B(6,0): 0
Max % variation for MODEL parameters (e.g. 5): 5
Max % variation for STRUCTURAL parameters (e.g. 2): 2

=== BEST FIT RESULTS ===
Success: True
Message: `ftol` termination condition is satisfied.
Fit error (RMS over targets): 6.907666e+03

```
B(2,0):  calc =  7757.665795 | exp =  850.000000 | Δ =  6.907666e+03
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
```

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.014134 Å
R0 (fitted) = 1.913428 Å
ΔR0 (%)   = -5.000
B(2) initial = 2.340000e+04 | fitted = 2.223000e+04 | Δ% = -5.000
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.378000 | Δ% = 5.000
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	1.9092	1.9474	0.0382	2.0	9.8245	13.4245	3.6	-0.0004	-0.0004	0.0
2	1.9449	1.9060	-0.0389	-2.0	94.2918	90.6918	-3.6	-179.9999	-179.9999	0.0
3	1.9967	1.9567	-0.0399	-2.0	95.2332	91.6332	-3.6	86.6134	86.6134	0.0
4	1.9967	1.9567	-0.0399	-2.0	95.2334	91.6334	-3.6	-86.6135	-86.6135	0.0
5	2.2232	2.2677	0.0445	2.0	178.2505	174.6505	-3.6	-0.0018	-0.0018	0.0

$$\underline{M2\text{-mix \_Cr1}}$$

Nearest ligands:

	Atom	R	Theta	Phi
0	O	2.1246	121.7873	-122.2980
1	O	2.1331	122.6872	123.3913
2	O	2.1358	51.7482	-68.7633
3	O	2.1418	52.3619	72.4736
4	O	2.1970	45.2673	-179.2080

Using initial R0 = <R> = 2.146463 Å
B(2): 23400
B(4): 0
B(6): 0
t(2): 0.36
t(4): 0
t(6): 0

Initial ZFS (calc):
  B(2,0): 5352.936086
  B(4,0): 0.000000
  B(6,0): 0.000000

        Enter experimental ZFS parameters (same units as your model outputs):
                                B(2,0): 850
                                B(4,0): 0
                                B(6,0): 0

=== BEST FIT RESULTS ===
Success: True
Message: `xtol` termination condition is satisfied.
Fit error (RMS): 1.682565e-11
B(2,0): calc=850.000000, exp=850.000000
B(4,0): calc=0.000000, exp=0.000000
B(6,0): calc=0.000000, exp=0.000000

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.146463 Å
R0 (fitted) = 2.112476 Å

```
ΔR0 (%)      = -1.583
B(2) initial = 2.340000e+04 | fitted = 2.249162e+04 | Δ% = -3.882
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.360273 | Δ% = 0.076
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
    1        2.1246        2.1170 -0.0076 -0.3578      121.7873        120.3205
-1.4668     -122.2980       -122.2980      0.0
    2        2.1331        2.1271 -0.0060 -0.2813      122.6872        121.2026
-1.4845      123.3913        123.3913      0.0
    3        2.1358        2.1409  0.0052  0.2423       51.7482         53.3232
1.5750      -68.7633        -68.7633      0.0
    4        2.1418        2.1458  0.0039  0.1839       52.3619         53.9280
1.5661       72.4736         72.4736      0.0
    5        2.1970        2.2146  0.0176  0.7997       45.2673         46.8703
1.6029     -179.2080       -179.2080      0.0

            Enter experimental ZFS parameters (same units as your model outputs):
                              B(2,0):  1600
                               B(4,0):  0
                               B(6,0):  0

=== BEST FIT RESULTS ===
Success: True
Message: `xtol` termination condition is satisfied.
Fit error (RMS): 6.366463e-12
B(2,0): calc=1600.000000, exp=1600.000000
B(4,0): calc=0.000000, exp=0.000000
B(6,0): calc=0.000000, exp=0.000000

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.146463 Å
R0 (fitted)  = 2.116718 Å
ΔR0 (%)      = -1.386
B(2) initial = 2.340000e+04 | fitted = 2.258693e+04 | Δ% = -3.475
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.360209 | Δ% = 0.058
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
    1        2.1246        2.1186 -0.0059 -0.2790      121.7873        120.5797
-1.2076     -122.2980       -122.2980      0.0
    2        2.1331        2.1285 -0.0046 -0.2164      122.6872        121.4645
-1.2227      123.3913        123.3913      0.0
```

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
3	2.1358	2.1401	0.0043	0.2034	51.7482	53.0485	1.3003	-68.7633	-68.7633	0.0
4	2.1418	2.1452	0.0034	0.1564	52.3619	53.6545	1.2926	72.4736	72.4736	0.0
5	2.1970	2.2116	0.0146	0.6653	45.2673	46.5909	1.3236	-179.2080	-179.2080	0.0

Enter experimental ZFS parameters (same units as your model outputs):
B(2,0): 3090
B(4,0): 0
B(6,0): 0

=== BEST FIT RESULTS ===
Success: True
Message: `xtol` termination condition is satisfied.
Fit error (RMS): 5.456968e-12
B(2,0): calc=3090.000000, exp=3090.000000
B(4,0): calc=0.000000, exp=0.000000
B(6,0): calc=0.000000, exp=0.000000

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.146463 Å
R0 (fitted) = 2.127249 Å
ΔR0 (%)   = -0.895
B(2) initial = 2.340000e+04 | fitted = 2.284612e+04 | Δ% = -2.367
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.360108 | Δ% = 0.030
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	2.1246	2.1214	-0.0032	-0.1501	121.7873	121.0780	-0.7093	-122.2980	-122.2980	0.0
2	2.1331	2.1307	-0.0024	-0.1138	122.6872	121.9685	-0.7187	123.3913	123.3913	0.0
3	2.1358	2.1384	0.0026	0.1231	51.7482	52.5150	0.7669	-68.7633	-68.7633	0.0
4	2.1418	2.1439	0.0021	0.0964	52.3619	53.1240	0.7621	72.4736	72.4736	0.0
5	2.1970	2.2058	0.0087	0.3979	45.2673	46.0480	0.7807	-179.2080	-179.2080	0.0

Enter experimental ZFS parameters (same units as your model outputs):
B(2,0): 10
B(4,0): 0
B(6,0): 0

=== BEST FIT RESULTS ===

```
Success: True
Message: `xtol` termination condition is satisfied.
Fit error (RMS): 1.455192e-11
B(2,0): calc=10.000000, exp=10.000000
B(4,0): calc=0.000000, exp=0.000000
B(6,0): calc=0.000000, exp=0.000000

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.146463 Å
R0 (fitted)  = 2.108816 Å
ΔR0 (%)      = -1.754
B(2) initial = 2.340000e+04 | fitted = 2.240779e+04 | Δ% = -4.240
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.360355 | Δ% = 0.099
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
```

[Structural parameters: ligand shell]

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	2.1246	2.1148	-0.0098	-0.4606	121.7873	120.0240	-1.7633	-122.2980	-122.2980	0.0
2	2.1331	2.1253	-0.0079	-0.3682	122.6872	120.9038	-1.7834	123.3913	123.3913	0.0
3	2.1358	2.1418	0.0061	0.2839	51.7482	53.6342	1.8860	-68.7633	-68.7633	0.0
4	2.1418	2.1464	0.0045	0.2113	52.3619	54.2379	1.8760	72.4736	72.4736	0.0
5	2.1970	2.2179	0.0209	0.9497	45.2673	47.1860	1.9187	-179.2080	-179.2080	0.0

M2-mix_Cr2

```
Nearest ligands:
Atom   R (Å)    Theta (deg)   Phi (deg)
  O 1.87098      6.95701    -91.73051
  O 1.95038    107.11487     90.18573
  O 1.97805    105.52968     -4.13878
  O 1.99641    107.89564   -171.17388
  O 3.16045    177.14354     30.62903
  O 3.94783     98.72912   -117.14923
  O 4.05411     97.15783    -63.50600
  O 4.12339     64.54116     89.77732

Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.885200 Å
B(2):  23400
B(4):  0
B(6):  0
t(2):  0.36
t(4):  0
```

```
t(6):  0

                          Initial ZFS (calc):
                          B(2,0): -4942.710870
                           B(4,0): 0.000000
                           B(6,0): 0.000000

        Enter experimental ZFS parameters (same units as your model outputs):
                           B(2,0):  850
                            B(4,0):  0
                            B(6,0):  0
              Max % variation for MODEL parameters (e.g. 5):  5
           Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `xtol` termination condition is satisfied.
Fit error (RMS over targets): 9.094947e-12

B(2,0):  calc =  850.000000 | exp =  850.000000 | Δ =  9.094947e-12
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.885200 Å
R0 (fitted)  = 2.824100 Å
ΔR0 (%)       = -2.118
B(2) initial = 2.340000e+04 | fitted = 2.283091e+04 | Δ% = -2.432
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.375416 | Δ% = 4.282
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
     1          1.8710       1.8336 -0.0374 -2.0000           6.9570          5.3062
-1.6508        -91.7305         -91.7305        0.0
     2          1.9504       1.9850  0.0346  1.7764         107.1149        109.6021
2.4872         90.1857          90.1857         0.0
     3          1.9781       2.0138  0.0357  1.8060         105.5297        107.9407
2.4111         -4.1388          -4.1388         0.0
     4          1.9964       2.0314  0.0350  1.7544         107.8956        110.4072
2.5115        -171.1739        -171.1739        0.0
     5          3.1605       3.0973 -0.0632 -1.9992         177.1435        178.1243
0.9808         30.6290          30.6290         0.0
     6          3.9478       4.0183  0.0705  1.7860          98.7291        100.5110
1.7819        -117.1492        -117.1492        0.0
     7          4.0541       4.1269  0.0728  1.7951          97.1578         98.7986
1.6408         -63.5060         -63.5060        0.0
     8          4.1234       4.1783  0.0550  1.3328          64.5412         62.0448
-2.4963         89.7773          89.7773         0.0
```

Enter experimental ZFS parameters (same units as your model outputs):
                        B(2,0): 1600
                        B(4,0): 0
                        B(6,0): 0
              Max % variation for MODEL parameters (e.g. 5): 5
           Max % variation for STRUCTURAL parameters (e.g. 2): 2

=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 1.818989e-12

B(2,0): calc = 1600.000000 | exp = 1600.000000 | Δ = -1.818989e-12
B(4,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00
B(6,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.885200 Å
R0 (fitted) = 2.840155 Å
ΔR0 (%)   = -1.561
B(2) initial = 2.340000e+04 | fitted = 2.319583e+04 | Δ% = -0.873
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.376871 | Δ% = 4.686
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand R_initial (Å) R_fitted (Å) ΔR (Å) ΔR (%) θ_initial (deg) θ_fitted (deg)
Δθ (deg) φ_initial (deg) φ_fitted (deg) Δφ (deg)

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)
1	1.8710	1.8336	-0.0374	-2.0000	6.9570	5.1518
2	1.9504	1.9875	0.0372	1.9054	107.1149	109.9553
3	1.9781	2.0161	0.0381	1.9239	105.5297	108.2894
4	1.9964	2.0342	0.0377	1.8908	107.8956	110.7610
5	3.1605	3.0972	-0.0632	-2.0000	177.1435	178.0917
6	3.9478	4.0234	0.0756	1.9139	98.7291	100.7250
7	4.0541	4.1319	0.0778	1.9196	97.1578	98.9687
8	4.1234	4.1855	0.0621	1.5071	64.5412	61.6965

Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
-1.8052	-91.7305	-91.7305	0.0
2.8405	90.1857	90.1857	0.0
2.7597	-4.1388	-4.1388	-0.0
2.8653	-171.1739	-171.1739	0.0
0.9482	30.6290	30.6290	0.0
1.9958	-117.1492	-117.1492	0.0
1.8108	-63.5060	-63.5060	0.0
-2.8447	89.7773	89.7773	0.0

Enter experimental ZFS parameters (same units as your model outputs):
                        B(2,0): 3090
                        B(4,0): 0
                        B(6,0): 0

```
                  Max % variation for MODEL parameters (e.g. 5):  5
               Max % variation for STRUCTURAL parameters (e.g. 2):  2


=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 1.455192e-11

B(2,0):  calc =  3090.000000 | exp =  3090.000000 | Δ = -1.455192e-11
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.885200 Å
R0 (fitted)  = 2.930422 Å
ΔR0 (%)      = 1.567
B(2) initial = 2.340000e+04 | fitted = 2.434840e+04 | Δ% = 4.053
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.377938 | Δ% = 4.983
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)


[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
    1         1.8710        1.8336  -0.0374 -2.0000        6.9570          4.6777
-2.2793      -91.7305        -91.7305       0.0
    2         1.9504        1.9893   0.0389  1.9944      107.1149        110.5114
3.3965       90.1857         90.1857        0.0
    3         1.9781        2.0175   0.0395  1.9966      105.5297        108.8781
3.3485        -4.1388         -4.1388        0.0
    4         1.9964        2.0362   0.0398  1.9924      107.8956        111.3057
3.4100      -171.1739       -171.1739       0.0
    5         3.1605        3.0972  -0.0632 -2.0000      177.1435        178.2599
1.1164        30.6290         30.6290        0.0
    6         3.9478        4.0266   0.0788  1.9960       98.7291        101.3668
2.6376      -117.1492       -117.1492       0.0
    7         4.0541        4.1351   0.0809  1.9966       97.1578         99.5716
2.4138       -63.5060        -63.5060        0.0
    8         4.1234        4.1978   0.0745  1.8057       64.5412         61.1497
-3.3915        89.7773         89.7773        0.0


            Enter experimental ZFS parameters (same units as your model outputs):
                               B(2,0):  10
                               B(4,0):   0
                               B(6,0):   0
                  Max % variation for MODEL parameters (e.g. 5):  5
               Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
```

```
Message: `xtol` termination condition is satisfied.
Fit error (RMS over targets): 2.182787e-11

B(2,0):  calc =  10.000000 | exp =  10.000000 | Δ =  2.182787e-11
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.885200 Å
R0 (fitted)  = 2.823565 Å
ΔR0 (%)      = -2.136
B(2) initial = 2.340000e+04 | fitted = 2.276975e+04 | Δ% = -2.693
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.372856 | Δ% = 3.571
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
    1         1.8710       1.8336 -0.0374 -2.0000        6.9570          5.4334
-1.5236      -91.7305        -91.7305       0.0
    2         1.9504       1.9802  0.0298  1.5295      107.1149        109.1744
2.0595        90.1857         90.1857      -0.0
    3         1.9781       2.0090  0.0310  1.5655      105.5297        107.5323
2.0026        -4.1388         -4.1388       0.0
    4         1.9964       2.0264  0.0300  1.5036      107.8956        109.9739
2.0782      -171.1739       -171.1739       0.0
    5         3.1605       3.0979 -0.0625 -1.9785      177.1435        178.3263
1.1827        30.6290         30.6290       0.0
    6         3.9478       4.0084  0.0606  1.5352       98.7291        100.3376
1.6085      -117.1492       -117.1492       0.0
    7         4.0541       4.1168  0.0627  1.5461       97.1578         98.6927
1.5349       -63.5060        -63.5060       0.0
    8         4.1234       4.1695  0.0461  1.1179       64.5412         62.4714
-2.0697        89.7773         89.7773       0.0
```

<u>M2d-Pb</u>

```
Nearest ligands:
Atom   R (Å)   Theta (deg)  Phi (deg)
   O 2.01487      73.63746 -179.97988
   O 2.01527      73.61886   -0.01464
   O 2.04053      73.26583  -90.00963
   O 2.04110      73.23742   89.97714
   O 3.20077     119.95290  134.23474
   O 3.20268     119.92881  -45.76414
   O 3.20268     119.92828   45.77417
   O 3.20529     119.90973 -134.22757

Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.615397 Å
B(2):  23400
```

```
B(4):  0
B(6):  0
t(2):  0.36
t(4):  0
t(6):  0

Initial ZFS (calc):
  B(2,0): -49803.555180
  B(4,0): 0.000000
  B(6,0): 0.000000

Enter experimental ZFS parameters (same units as your model outputs):
B(2,0):  850
B(4,0):  0
B(6,0):  0
Max % variation for MODEL parameters (e.g. 5):  5
Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `ftol` termination condition is satisfied.
Fit error (RMS over targets): 3.474564e+04

B(2,0):  calc = -33895.637923 | exp =  850.000000 | Δ = -3.474564e+04
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.615397 Å
R0 (fitted)  = 2.484628 Å
ΔR0 (%)      = -5.000
B(2) initial = 2.340000e+04 | fitted = 2.223000e+04 | Δ% = -5.000
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.342000 | Δ% = -5.000
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
     1          2.0149        2.0552  0.0403  2.0000         73.6375          70.0375
-3.6        -179.9799       -177.4785    2.5014
     2          2.0153        2.0556  0.0403  2.0000         73.6189          70.0189
-3.6          -0.0146         -2.3661   -2.3514
     3          2.0405        2.0813  0.0408  2.0000         73.2658          69.6658
-3.6         -90.0096        -86.5051    3.5045
     4          2.0411        2.0819  0.0408  2.0000         73.2374          69.6374
-3.6          89.9771         89.9771    0.0000
     5          3.2008        3.2648  0.0640  1.9999        119.9529         123.5529
3.6         134.2347        134.2347    0.0000
     6          3.2027        3.2667  0.0641  1.9999        119.9288         123.5288
3.6         -45.7641        -45.7641    0.0000
```

7	3.2027	3.2667	0.0641	1.9999	119.9283	123.5283
3.6	45.7742	45.7742	0.0000			
8	3.2053	3.2694	0.0641	1.9999	119.9097	123.5097
3.6	-134.2276	-134.2276	0.0000			

M2d-Ti

Nearest ligands:
```
Atom   R (Å)   Theta (deg)  Phi (deg)
   O 1.93204     3.31223   -99.57568
   O 2.01828    97.97656   -92.47591
   O 2.02968    96.22925   177.85151
   O 2.03491    95.08545    88.68722
   O 2.05926    94.82544    -6.13795
   O 2.28913   178.80831    79.21882
```

Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.060551 Å
```
B(2):  23400
B(4):  0
B(6):  0
t(2):  0.36
t(4):  0
t(6):  0
```

Initial ZFS (calc):
```
  B(2,0): 959.737074
  B(4,0): 0.000000
  B(6,0): 0.000000
```

        Enter experimental ZFS parameters (same units as your model outputs):
                              B(2,0): 850
                              B(4,0): 0
                              B(6,0): 0
                Max % variation for MODEL parameters (e.g. 5): 5
              Max % variation for STRUCTURAL parameters (e.g. 2): 2

=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 7.275958e-12

B(2,0): calc = 850.000000 | exp = 850.000000 | Δ = 7.275958e-12
B(4,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00
B(6,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.060551 Å
R0 (fitted) = 2.059791 Å
ΔR0 (%)   = -0.037
B(2) initial = 2.340000e+04 | fitted = 2.337605e+04 | Δ% = -0.102
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)

```
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.360198 | Δ% = 0.055
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
    1        1.9320        1.9391   0.0070  0.3636         3.3122           3.3325
0.0203       -99.5757        -99.5757        0.0
    2        2.0183        2.0148  -0.0035 -0.1715        97.9766          97.9291
-0.0475       -92.4759        -92.4759        0.0
    3        2.0297        2.0261  -0.0036 -0.1751        96.2293          96.1921
-0.0372       177.8515        177.8515        0.0
    4        2.0349        2.0313  -0.0036 -0.1771        95.0854          95.0550
-0.0304        88.6872         88.6872        0.0
    5        2.0593        2.0556  -0.0036 -0.1768        94.8254          94.7967
-0.0288        -6.1379         -6.1379        0.0
    6        2.2891        2.2970   0.0079  0.3440       178.8083         178.8014
-0.0069        79.2188         79.2188        0.0


          Enter experimental ZFS parameters (same units as your model outputs):
                              B(2,0):  1600
                               B(4,0):  0
                               B(6,0):  0
                 Max % variation for MODEL parameters (e.g. 5):  5
                Max % variation for STRUCTURAL parameters (e.g. 2):  2


=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 3.637979e-12

B(2,0):  calc =  1600.000000 | exp =  1600.000000 | Δ =  3.637979e-12
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.060551 Å
R0 (fitted)  = 2.067719 Å
ΔR0 (%)      = 0.348
B(2) initial = 2.340000e+04 | fitted = 2.361657e+04 | Δ% = 0.926
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.359100 | Δ% = -0.250
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
```

```
       1          1.9320        1.8984 -0.0337 -1.7422        3.3122          3.1616
-0.1506        -99.5757        -99.5757       0.0
       2          2.0183        2.0395  0.0213  1.0537       97.9766         98.3317
 0.3551        -92.4759        -92.4759       0.0
       3          2.0297        2.0514  0.0218  1.0718       96.2293         96.5095
 0.2802        177.8515        177.8515       0.0
       4          2.0349        2.0569  0.0220  1.0813       95.0854         95.3157
 0.2303         88.6872         88.6872       0.0
       5          2.0593        2.0815  0.0222  1.0798       94.8254         95.0434
 0.2179         -6.1379         -6.1379       0.0
       6          2.2891        2.2503 -0.0388 -1.6946      178.8083        178.8599
 0.0516         79.2188         79.2188       0.0
```

Enter experimental ZFS parameters (same units as your model outputs):
                     B(2,0): 3090
                      B(4,0): 0
                      B(6,0): 0
         Max % variation for MODEL parameters (e.g. 5): 5
         Max % variation for STRUCTURAL parameters (e.g. 2): 2

=== BEST FIT RESULTS ===
Success: True
Message: `xtol` termination condition is satisfied.
Fit error (RMS over targets): 1.091394e-11

B(2,0): calc = 3090.000000 | exp = 3090.000000 | Δ = 1.091394e-11
B(4,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00
B(6,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.060551 Å
R0 (fitted) = 2.125527 Å
ΔR0 (%)   = 3.153
B(2) initial = 2.340000e+04 | fitted = 2.441687e+04 | Δ% = 4.346
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.353578 | Δ% = -1.784
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
```
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
       1          1.9320        1.8934 -0.0386 -2.0000        3.3122          1.7261
-1.5861        -99.5757        -99.5757       0.0
       2          2.0183        2.0566  0.0383  1.8991       97.9766        100.1542
 2.1776        -92.4759        -92.4759       0.0
       3          2.0297        2.0684  0.0387  1.9082       96.2293         98.2884
 2.0591        177.8515        177.8515       0.0
       4          2.0349        2.0738  0.0389  1.9129       95.0854         97.0579
 1.9725         88.6872         88.6872       0.0
```

```
        5           2.0593        2.0987  0.0394   1.9127              94.8254              96.7748
1.9494              -6.1379          -6.1379         0.0
        6           2.2891        2.2433 -0.0458  -2.0000             178.8083             180.0486
1.2403              79.2188          79.2188         0.0


            Enter experimental ZFS parameters (same units as your model outputs):
                                   B(2,0):  10
                                   B(4,0):  0
                                   B(6,0):  0
                   Max % variation for MODEL parameters (e.g. 5):  5
                 Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 3.637979e-12

B(2,0):  calc =  10.000000 | exp =  10.000000 | Δ =  3.637979e-12
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.060551 Å
R0 (fitted)  = 2.054253 Å
ΔR0 (%)      = -0.306
B(2) initial = 2.340000e+04 | fitted = 2.320816e+04 | Δ% = -0.820
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.365167 | Δ% = 1.435
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)  ΔR (Å)  ΔR (%)  θ_initial (deg)  θ_fitted (deg)
Δθ (deg)  φ_initial (deg)  φ_fitted (deg)  Δφ (deg)
        1           1.9320        1.9707  0.0386   1.9999               3.3122               3.6598
0.3476              -99.5757         -99.5757        0.0
        2           2.0183        1.9836 -0.0347  -1.7192              97.9766              97.2458
-0.7308             -92.4759         -92.4759        0.0
        3           2.0297        1.9945 -0.0352  -1.7338              96.2293              95.6470
-0.5822             177.8515         177.8515        0.0
        4           2.0349        1.9995 -0.0354  -1.7413              95.0854              94.6040
-0.4815              88.6872          88.6872        0.0
        5           2.0593        2.0234 -0.0358  -1.7398              94.8254              94.3690
-0.4565              -6.1379          -6.1379         0.0
        6           2.2891        2.3349  0.0457   1.9979             178.8083             178.6877
-0.1206             79.2188          79.2188         0.0


                                      M3-VTi
Nearest ligands:
Atom   R (Å)   Theta (deg)   Phi (deg)
```

```
      O 1.88986      75.08268    96.15653
      O 1.88996      75.06192    -6.15277
      O 1.95355      72.50169   -91.66171
      O 1.95360      72.50378  -178.34435
      O 3.48112     126.72418    44.99908
      O 3.48730     126.88864  -135.00033
      O 3.54257     126.39367   -46.51559
      O 3.54547     126.36099   136.50549
```

Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.717928 Å
B(2): 23400
B(4): 0
B(6): 0
t(2): 0.36
t(4): 0
t(6): 0

Initial ZFS (calc):
  B(2,0): -37747.770343
  B(4,0): 0.000000
  B(6,0): 0.000000

Enter experimental ZFS parameters (same units as your model outputs):
B(2,0): 850
B(4,0): 0
B(6,0): 0
Max % variation for MODEL parameters (e.g. 5): 5
Max % variation for STRUCTURAL parameters (e.g. 2): 2

=== BEST FIT RESULTS ===
Success: True
Message: `ftol` termination condition is satisfied.
Fit error (RMS over targets): 2.277236e+04

B(2,0): calc = -21922.357676 | exp = 850.000000 | Δ = -2.277236e+04
B(4,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00
B(6,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.717928 Å
R0 (fitted) = 2.582031 Å
ΔR0 (%)   = -5.000
B(2) initial = 2.340000e+04 | fitted = 2.223000e+04 | Δ% = -5.000
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.342000 | Δ% = -5.000
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand R_initial (Å) R_fitted (Å) ΔR (Å) ΔR (%) θ_initial (deg) θ_fitted (deg)
Δθ (deg) φ_initial (deg) φ_fitted (deg) Δφ (deg)

	1	1.8899	1.9277	0.0378	2.0	75.0827	71.4827
-3.6		96.1565	99.4622	3.3056			
	2	1.8900	1.9278	0.0378	2.0	75.0619	71.4619
-3.6		-6.1528	-5.1086	1.0442			
	3	1.9535	1.9926	0.0391	2.0	72.5017	68.9017
-3.6		-91.6617	-95.1628	-3.5011			
	4	1.9536	1.9927	0.0391	2.0	72.5038	68.9038
-3.6		-178.3443	-178.3443	0.0000			
	5	3.4811	3.4115	-0.0696	-2.0	126.7242	130.3242
3.6		44.9991	44.9991	0.0000			
	6	3.4873	3.4176	-0.0697	-2.0	126.8886	130.4886
3.6		-135.0003	-135.0003	0.0000			
	7	3.5426	3.4717	-0.0709	-2.0	126.3937	129.9937
3.6		-46.5156	-46.5156	0.0000			
	8	3.5455	3.4746	-0.0709	-2.0	126.3610	129.9610
3.6		136.5055	136.5055	0.0000			

M3-VPb

Nearest ligands:

Atom	R (Å)	Theta (deg)	Phi (deg)
O	1.85853	6.90474	-124.79451
O	1.95454	105.84494	174.97902
O	1.95843	107.33782	-85.63663
O	2.00897	98.94104	2.30992
O	2.00917	97.39338	87.64594
O	3.23851	165.74874	44.80300

Initial model parameters (enter your starting guesses)
Using initial R0 = <R> = 2.171357 Å
B(2): 23400
B(4): 0
B(6): 0
t(2): 0.36
t(4): 0
t(6): 0

Initial ZFS (calc):
  B(2,0): 1697.118996
  B(4,0): 0.000000
  B(6,0): 0.000000

          Enter experimental ZFS parameters (same units as your model outputs):
                              B(2,0): 850
                               B(4,0): 0
                               B(6,0): 0
               Max % variation for MODEL parameters (e.g. 5): 5
            Max % variation for STRUCTURAL parameters (e.g. 2): 2

=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 3.637979e-12

B(2,0): calc = 850.000000 | exp = 850.000000 | Δ = 3.637979e-12

```
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.171357 Å
R0 (fitted)  = 2.165448 Å
ΔR0 (%)      = -0.272
B(2) initial = 2.340000e+04 | fitted = 2.322619e+04 | Δ% = -0.743
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.364601 | Δ% = 1.278
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
```

[Structural parameters: ligand shell]

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	1.8585	1.8852	0.0267	1.4349	6.9047	7.1059	0.2012	-124.7945	-124.7945	0.0
2	1.9545	1.9420	-0.0125	-0.6410	105.8449	105.4201	-0.4248	174.9790	174.9790	0.0
3	1.9584	1.9465	-0.0119	-0.6083	107.3378	106.8790	-0.4588	-85.6366	-85.6366	0.0
4	2.0090	1.9940	-0.0150	-0.7461	98.9410	98.6926	-0.2485	2.3099	2.3099	0.0
5	2.0092	1.9939	-0.0153	-0.7625	97.3934	97.1864	-0.2070	87.6459	87.6459	0.0
6	3.2385	3.2757	0.0372	1.1498	165.7487	165.4225	-0.3262	44.8030	44.8030	0.0

```
        Enter experimental ZFS parameters (same units as your model outputs):
                              B(2,0):  1600
                              B(4,0):  0
                              B(6,0):  0
              Max % variation for MODEL parameters (e.g. 5):  5
            Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 7.275958e-12

B(2,0):  calc =  1600.000000 | exp =  1600.000000 | Δ = -7.275958e-12
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.171357 Å
R0 (fitted)  = 2.170650 Å
ΔR0 (%)      = -0.033
```

```
B(2) initial = 2.340000e+04 | fitted = 2.337883e+04 | Δ% = -0.090
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.360503 | Δ% = 0.140
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
 Ligand  R_initial (Å)  R_fitted (Å)   ΔR (Å)   ΔR (%)   θ_initial (deg)   θ_fitted (deg)
Δθ (deg)   ϕ_initial (deg)   ϕ_fitted (deg)   Δϕ (deg)
      1         1.8585         1.8620   0.0035   0.1857            6.9047           6.9262
0.0214        -124.7945       -124.7945          0.0
      2         1.9545         1.9531  -0.0014  -0.0725          105.8449         105.7987
-0.0463         174.9790        174.9790          0.0
      3         1.9584         1.9571  -0.0013  -0.0685          107.3378         107.2877
-0.0501         -85.6366        -85.6366          0.0
      4         2.0090         2.0072  -0.0017  -0.0858           98.9410          98.9142
-0.0268          2.3099          2.3099          0.0
      5         2.0092         2.0074  -0.0018  -0.0879           97.3934          97.3711
-0.0223         87.6459         87.6459          0.0
      6         3.2385         3.2431   0.0046   0.1414          165.7487         165.7137
-0.0351         44.8030         44.8030          0.0


           Enter experimental ZFS parameters (same units as your model outputs):
                               B(2,0):  3090
                                B(4,0):  0
                                B(6,0):  0
                Max % variation for MODEL parameters (e.g. 5):  5
              Max % variation for STRUCTURAL parameters (e.g. 2):  2

=== BEST FIT RESULTS ===
Success: True
Message: `gtol` termination condition is satisfied.
Fit error (RMS over targets): 7.275958e-12

B(2,0):  calc =  3090.000000 | exp =  3090.000000 | Δ = -7.275958e-12
B(4,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00
B(6,0):  calc =  0.000000 | exp =  0.000000 | Δ =  0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.171357 Å
R0 (fitted)  = 2.184961 Å
ΔR0 (%)      = 0.627
B(2) initial = 2.340000e+04 | fitted = 2.378184e+04 | Δ% = 1.632
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.353099 | Δ% = -1.917
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]
```

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	1.8585	1.8230	-0.0355	-1.9091	6.9047	6.5681	-0.3366	-124.7945	-124.7945	0.0
2	1.9545	1.9739	0.0194	0.9920	105.8449	106.5643	0.7193	174.9790	174.9790	0.0
3	1.9584	1.9769	0.0185	0.9444	107.3378	108.1124	0.7746	-85.6366	-85.6366	0.0
4	2.0090	2.0319	0.0229	1.1409	98.9410	99.3680	0.4270	2.3099	2.3099	0.0
5	2.0092	2.0325	0.0234	1.1634	97.3934	97.7503	0.3569	87.6459	87.6459	0.0
6	3.2385	3.1851	-0.0534	-1.6492	165.7487	166.2929	0.5441	44.8030	44.8030	0.0

Enter experimental ZFS parameters (same units as your model outputs):
                          B(2,0): 10
                          B(4,0):   0
                          B(6,0):   0
          Max % variation for MODEL parameters (e.g. 5): 5
       Max % variation for STRUCTURAL parameters (e.g. 2): 2

=== BEST FIT RESULTS ===
Success: True
Message: `xtol` termination condition is satisfied.
Fit error (RMS over targets): 1.455192e-11

B(2,0): calc = 10.000000 | exp = 10.000000 | Δ = 1.455192e-11
B(4,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00
B(6,0): calc = 0.000000 | exp = 0.000000 | Δ = 0.000000e+00

=== FINAL FITTED PARAMETERS ===

[Model / SPM parameters]
R0 (initial) = 2.171357 Å
R0 (fitted) = 2.161184 Å
ΔR0 (%)   = -0.469
B(2) initial = 2.340000e+04 | fitted = 2.310657e+04 | Δ% = -1.254
B(4) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
B(6) initial = 0.000000e+00 | fitted = 0.000000e+00 | Δ% = n/a (initial≈0)
t(2) initial = 0.360000 | fitted = 0.369838 | Δ% = 2.733
t(4) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)
t(6) initial = 0.000000 | fitted = 0.000000 | Δ% = n/a (initial≈0)

[Structural parameters: ligand shell]

Ligand	R_initial (Å)	R_fitted (Å)	ΔR (Å)	ΔR (%)	θ_initial (deg)	θ_fitted (deg)	Δθ (deg)	φ_initial (deg)	φ_fitted (deg)	Δφ (deg)
1	1.8585	1.8957	0.0371	1.9989	6.9047	7.3718	0.4671	-124.7945	-124.7945	0.0
2	1.9545	1.9295	-0.0250	-1.2795	105.8449	104.9089	-0.9360	174.9790	174.9790	0.0
3	1.9584	1.9344	-0.0241	-1.2289	107.3378	106.3316	-1.0063	-85.6366	-85.6366	0.0

```
    4          2.0090       1.9802 -0.0288 -1.4314         98.9410           98.3803
-0.5607           2.3099          2.3099      0.0
    5          2.0092       1.9800 -0.0292 -1.4537         97.3934           96.9236
-0.4698          87.6459         87.6459      0.0
    6          3.2385       3.2987  0.0602  1.8579        165.7487          165.0080
-0.7407          44.8030         44.8030      0.0
```

Table S4. The numerical basis for the weighted plausibility matrix (Figure 3) discussed in the main text.

Model	$|\Delta D|$	Max ΔR (%)	Max $\Delta\theta$ (°)	Ef (eV)	BVS(Cr)
	C1 ($|D|$=850×10^{-4} cm^{-1})				
M0-Ti	4987.3	2.000	3.600	-1.4	2.93
M1-Cr1	4652.6	2.000	3.520	-7.3	2.95
M1-Cr2	3035.3	2.000	1.341	-7.3	2.23
M2-mix-Cr1	5342.9	0.950	0.950	-4.3	2.06
M2-mix-Cr2	4952.7	2.000	2.000	-4.3	2.25
M2d-Ti	949.7	1.999	0.731	2.4	2.84
M3-VPb	1687.1	1.999	1.006	1.3	4.60
M2a-z	8382.9	1.272	2.223	-1.3	1.86
	C1 ($|D|$=1600×10^{-4} cm^{-1})				
M0-Ti	3397.3	2.000	2.326	-1.4	2.93
M1-Cr1	3062.6	2.000	2.133	-7.3	2.95
M1-Cr2	4625.3	1.999	1.942	-7.3	2.23
M2-mix-Cr1	3752.9	0.665	1.324	-4.3	2.06
M2-mix-Cr2	6542.7	2.000	2.865	-4.3	2.25
M2d-Ti	640.3	1.724	0.355	2.4	2.84
M3-VPb	97.1	0.186	0.050	1.3	4.60
M2a-z	9972.9	1.550	2.692	-1.3	1.86
	C1 ($|D|$=3090×10^{-4} cm^{-1})				
M0-Ti	1907.3	1.999	1.024	-1.4	2.93
M1-Cr1	1572.6	1.976	0.822	-7.3	2.95
M1-Cr2	6115.3	2.000	2.611	-7.3	2.23
M2-mix-Cr1	2262.9	0.398	0.781	-4.3	2.06
M2-mix-Cr2	8032.7	2.000	3.410	-4.3	2.25
M2d-Ti	2130.3	2.000	2.178	2.4	2.84
M3-VPb	1392.9	1.910	0.775	1.3	4.60
M2a-z	11462.9	1.773	3.069	-1.3	1.86
	C1 ($|D|$=10×10^{-4} cm^{-1})				
M0-Ti	4987.3	2.000	3.600	-1.4	2.93
M1-Cr1	4652.6	2.000	3.520	-7.3	2.95
M1-Cr2	3035.3	2.000	1.341	-7.3	2.23
M2-mix-Cr1	5342.9	0.950	1.919	-4.3	2.06
M2-mix-Cr2	4952.7	2.000	2.078	-4.3	2.25
M2d-Ti	949.7	1.999	0.731	2.4	2.84
M3-VPb	1687.1	1.999	1.006	1.3	4.60
M2a-z	8382.9	1.272	2.223	-1.3	1.86