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Substituted Fullerenes as a Promising Capping Ligand Towards Stabilization of Exohedral Dy(III) Based Single-Ion Magnets: A Theoretical Study

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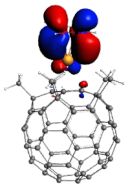
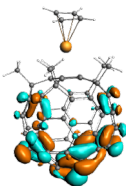
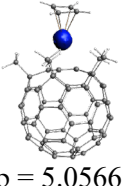
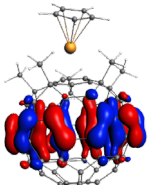
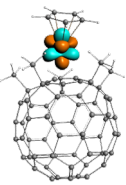
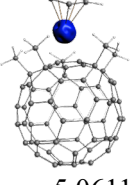
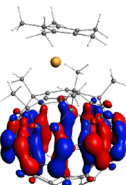
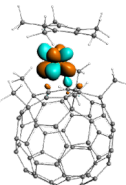
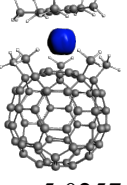
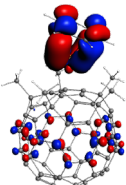
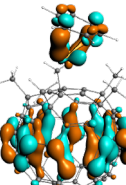
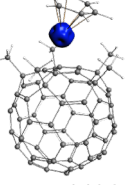
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Table S1: Selected bond parameters of the complexes studied. (X= CCH₃) Bond distances are taken from the centroid of C_mH_m rings.

| Complex | Dy- L _{cent1} (Å) | Dy- L _{cent2} (Å) | Avg. Dy-L _{cent} (Å) | ∠L _{cent1} -Dy-L _{cent2} (°) |
|---|-------------------------------|-------------------------------|-------------------------------|--|
| [Dy(η ⁵ -C ₅₅ X ₅) (C ₄ H ₄)] (1) | 2.382 | 2.325 | 2.354 | 156.9 |
| [Dy(η ⁵ -C ₅₅ X ₅) (C ₅ H ₅)] ⁺ (2) | 2.302 | 2.301 | 2.302 | 145.2 |
| [Dy (C _p) ₂] ⁺ (2a) | 2.299 | 2.297 | 2.298 | 128.9 |
| [Dy(η ⁵ -C ₅₅ X ₅) (Cp*) ₂] ⁺ (3) | 2.269 | 2.308 | 2.289 | 160.8 |
| [Dy (C ₅ (CH ₃) ₅) ₂] ⁺ (3a) | 2.268 | 2.273 | 2.270 | 148 |
| [Dy(η ⁵ -C ₅₅ X ₅) (C ₆ H ₆) ₂] ²⁺ (4) | 2.235 | 2.296 | 2.266 | 152.7 |
| [Dy(η ⁵ -C ₅₅ X ₅) (C ₈ H ₈)] (5) | 1.743 | 2.333 | 2.038 | 179.4 |
| [Dy(η ⁵ -C ₅₅ X ₅) (C ₆₀ [*])] ⁺ (6) | 2.351 | 2.351 | 2.351 | 179.7 |
| [Dy(η ⁵ -C ₅₅ B ₅) ₂] ⁺ (7) | 2.284 | 2.284 | 2.284 | 179.6 |
| [Dy(η ⁵ -C ₅₅ N ₅) ₂] ⁺ (8) | 2.390 | 2.389 | 2.389 | 179.5 |
| [Cp*DyCOT] (taken from reference 1) | 1.772 | 2.995 | 2.383 | 171.9 |

Table S2: PBE0 computed HOMO, LUMO, and spin densities of complexes **1-8**.

| Complex | HOMO | LUMO | Spin-density |
|----------|---|--|---|
| 1 |  |  |  ρ = 5.0566 |
| 2 |  |  |  ρ = 5.0611 |
| 3 |  |  |  ρ = 5.0257 |
| 4 |  |  |  ρ = 5.4438 |

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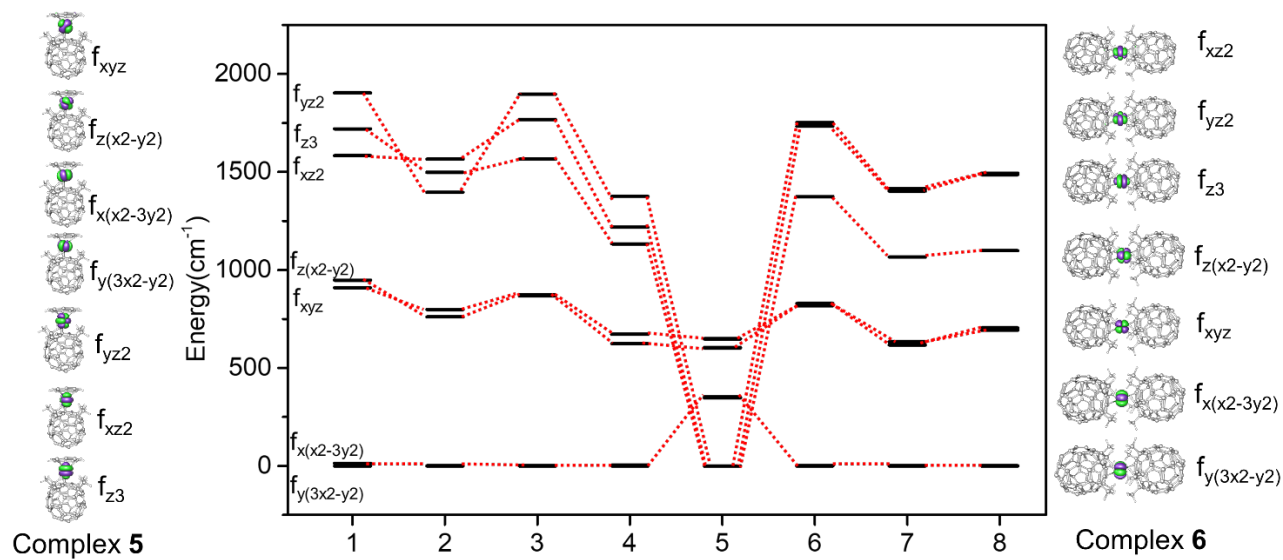
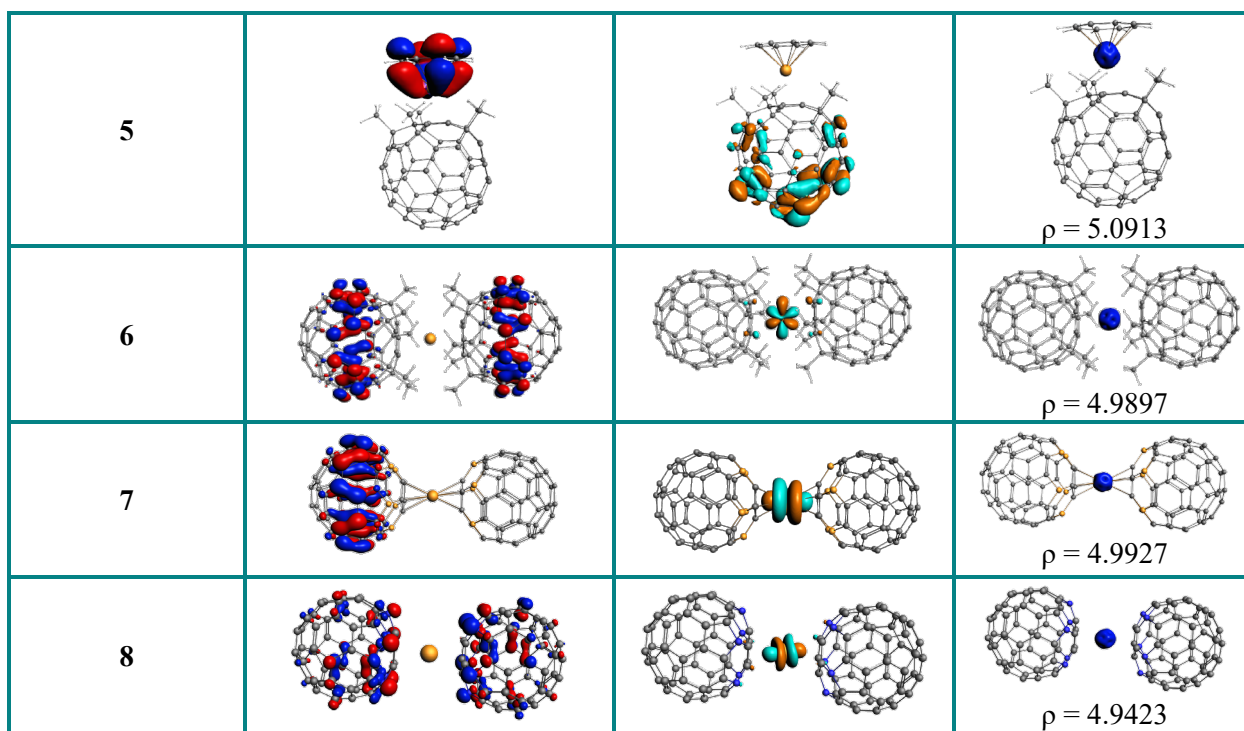


Figure S1: AILFT computed 4f-orbital splitting pattern for complexes 1-8.

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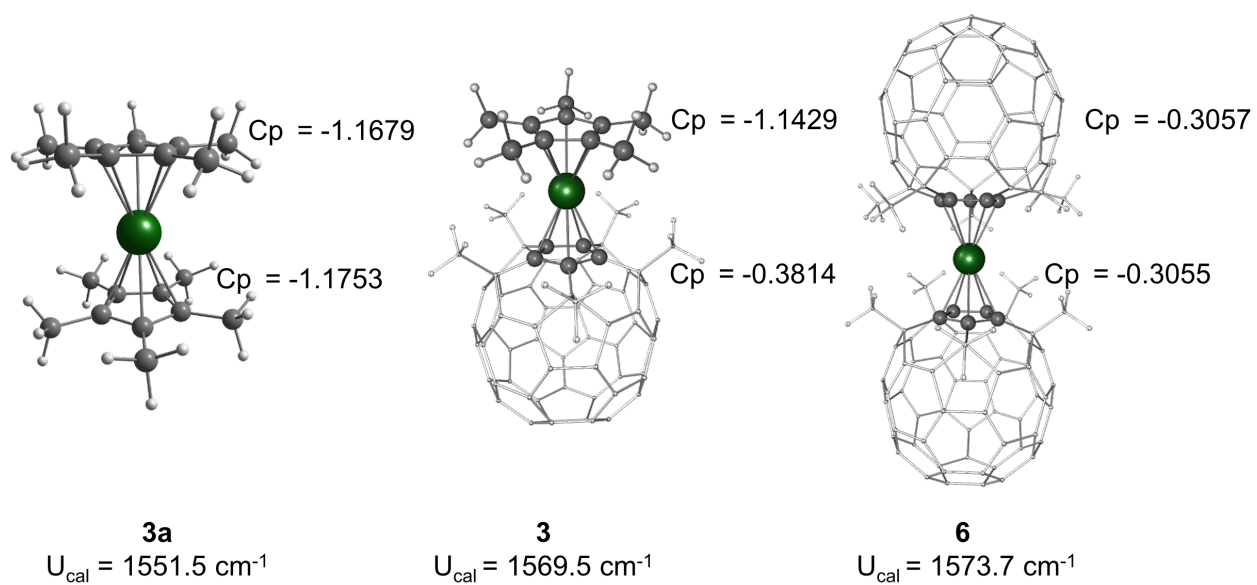


Figure S2: Comparison of CASSCF computed Mulliken charges on the five membered rings of **3a**, **3** and **6** with their corresponding U_{cal} .

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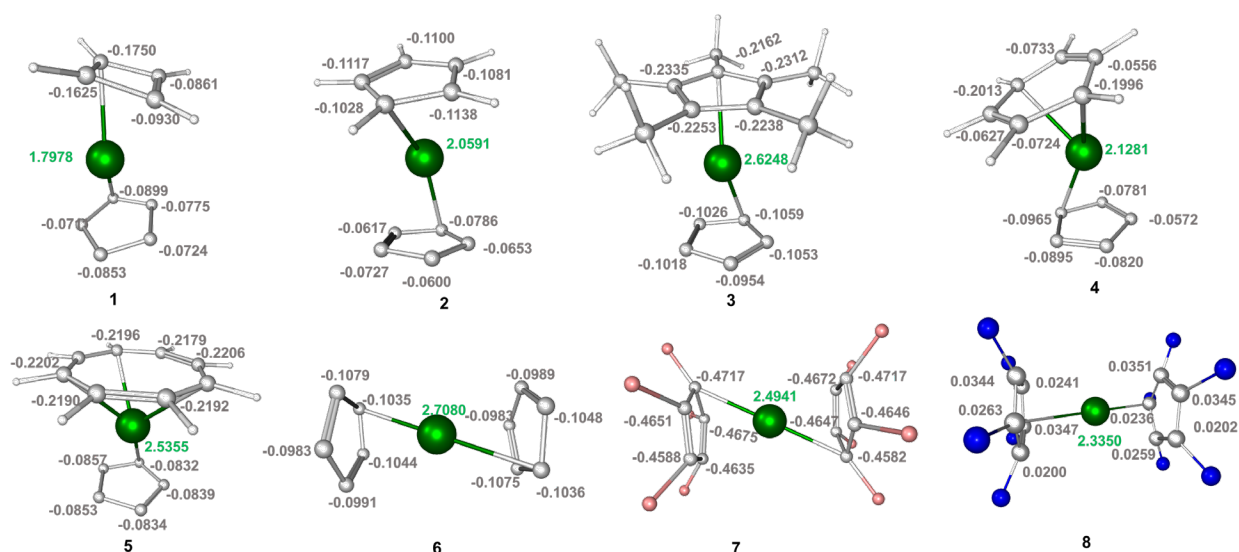


Figure S3: CASSCF computed Mulliken charges on the first coordination sphere for complexes **1-8**. Colour code: green (Dy), blue (N), pink (B), grey (C), white (H).

Thermodynamic Analysis

The gas phase energies, enthalpies, and free energies for the formation of complexes **1-8** are computed at the PBE0 level of theory. Here, we have extracted the thermodynamic parameters by performing the single-point energy calculations at the PBE0 level of theory on the DFT-optimized geometry of complexes **1-8**, while the thermal energy and entropy corrections were taken from the BP86 level of theory (see Computational Methodology).

Table S3: PBE0-D3(BJ)/DKH-def2-TZVP computed gas phase formation energies (ΔE), enthalpies (ΔH), and free energies (ΔG) for complexes **1-8** at 298.15 K.

| Complexes | ΔE kcal/mol | ΔH kcal/mol | ΔG kcal/mol |
|---|------------------------|------------------------|------------------------|
| 1 Dy(III)+ {C ₅₅ X ₅ } ⁻ + C ₄ H ₄ ²⁺ → [Dy(η^5 -C ₅₅ X ₅) (η^4 -C ₄ H ₄)] | -1346.6 | -1347.8 | -1339.1 |
| 2 Dy(III)+ {C ₅₅ X ₅ } ⁻ + Cp ⁻ → [Dy(η^5 -C ₅₅ X ₅) (η^5 -Cp)] ⁺ | -1167.4 | -1168.6 | -1158.9 |
| 3 Dy(III)+{C ₅₅ X ₅ } ⁻ + Cp* ⁻ → [Dy(η^5 -C ₅₅ X ₅) (η^5 -Cp*)] ⁺ | -1174.4 | -1175.6 | -1164.4 |
| 4 Dy(III)+{C ₅₅ X ₅ } ⁻ + C ₆ H ₆ → [Dy(η^5 -C ₅₅ X ₅) (η^6 -C ₆ H ₆)] ²⁺ | -874.8 | -876.0 | -867.3 |
| 5 Dy(III)+{C ₅₅ X ₅ } ⁻ + C ₈ H ₈ ²⁺ → [Dy(η^5 -C ₅₅ X ₅) (η^8 -C ₈ H ₈)] | -1427.1 | -1428.2 | -1416.5 |
| 6 Dy(III)+ 2 {C ₅₅ X ₅ } ⁻ → [Dy(η^5 -C ₅₅ X ₅) ₂] ⁺ | -1122.9 | -1124.1 | -1111.1 |
| 7 Dy(III)+ 2 {C ₅₅ B ₅ } ⁻ → [Dy(η^5 -C ₅₅ B ₅) ₂] ⁺ | -1067.6 | -1068.8 | -1057.9 |
| 8 Dy(III)+ 2 {C ₅₅ N ₅ } ⁻ → [Dy(η^5 -C ₅₅ N ₅) ₂] ⁺ | -1056.0 | -1057.2 | -1045.3 |

$\Delta E/\Delta H/\Delta G/ = E/H/G_{\text{complex}} - E/H/G_{\text{Dy(III)}} - E/H/G_{(\eta^5\text{-C}_{55}\text{X}_5)^{-}} - E/H/G_{(\text{CmHm})}$

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Table S4: BP86-D3(BJ)/DKH-def2-TZVP computed gas phase formation energies(ΔE), enthalpies(ΔH), and free energies (ΔG) for complexes **1-8** at 298.15 K.

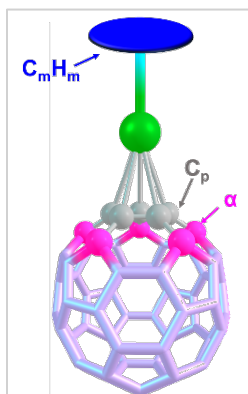
| Complexes | ΔE kcal/mol | ΔH kcal/mol | ΔG kcal/mol |
|--|------------------------|------------------------|------------------------|
| 1 Dy (III)+ {C ₅₅ X ₅ } ⁻ + C ₄ H ₄ ²⁺ → [Dy(η^5 -C ₅₅ X ₅) (η^4 -C ₄ H ₄)] | -1181.1 | -1182.2 | -1173.5 |
| 2 Dy (III)+ {C ₅₅ X ₅ } ⁻ + Cp ⁻ → [Dy(η^5 -C ₅₅ X ₅) (η^5 -Cp)] ⁺ | -919.7 | -920.9 | -911.2 |
| 3 Dy (III)+{C ₅₅ X ₅ } ⁻ + Cp* ⁻ → [Dy(η^5 -C ₅₅ X ₅) (η^5 -Cp*)] ⁺ | -927.6 | -928.8 | -917.5 |
| 4 Dy (III)+{C ₅₅ X ₅ } ⁻ + C ₆ H ₆ → [Dy(η^5 -C ₅₅ X ₅) (η^6 -C ₆ H ₆)] ²⁺ | -684.8 | -686.0 | -677.3 |
| 5 Dy (III)+{C ₅₅ X ₅ } ⁻ + C ₈ H ₈ ²⁺ → [Dy(η^5 -C ₅₅ X ₅) (η^8 -C ₈ H ₈)] | -1174.3 | -1175.5 | -1163.8 |
| 6 Dy (III)+ 2 {C ₅₅ X ₅ } ⁻ → [Dy(η^5 -C ₅₅ X ₅) ₂] ⁺ | -888.6 | -889.8 | -876.7 |
| 7 Dy (III)+ 2 {C ₅₅ B ₅ } ⁻ → [Dy(η^5 -C ₅₅ B ₅) ₂] ⁺ | -825.1 | -826.3 | -815.4 |
| 8 Dy (III)+ 2 {C ₅₅ N ₅ } ⁻ → [Dy(η^5 -C ₅₅ N ₅) ₂] ⁺ | -810.5 | -811.7 | -799.8 |

$$\Delta E/\Delta H/\Delta G/ = E/H/G_{\text{complex}} - E/H/G_{\text{Dy(III)}} - E/H/G_{(\eta^5\text{-C}_{55}\text{X}_5)^{-}} - E/H/G_{(\text{C}_m\text{H}_m)}$$

Table S5: Contribution (%) of decomposition energies to Total Binding Energy for complexes **1-8**.

| Complexes | Covalency (%) | E_{Pauli} (%) | E_{elstat} (%) | E_{orb} (%) | E_{disp} (%) |
|-----------|---------------|------------------------|-------------------------|----------------------|-----------------------|
| 1 | 49.7 | 15.7 | -57.9 | -57.2 | -0.6 |
| 2 | 50.5 | 20.2 | -59.1 | -60.4 | -0.7 |
| 3 | 51.9 | 21.6 | -58.0 | -62.7 | -0.9 |
| 4 | 63.3 | 27.3 | -46.4 | -80.0 | -0.9 |
| 5 | 50.2 | 20.0 | -59.5 | -59.9 | -0.6 |
| 6 | 54.9 | 19.4 | -53.3 | -64.9 | -1.1 |
| 7 | 59.9 | 20.0 | -47.9 | -71.5 | -0.5 |
| 8 | 61.0 | 17.7 | -45.6 | -71.3 | -0.8 |

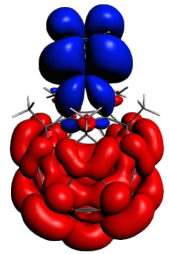
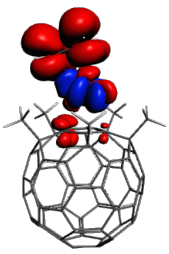
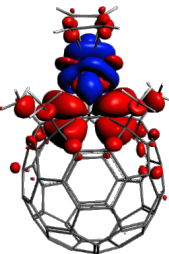
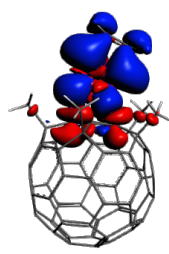
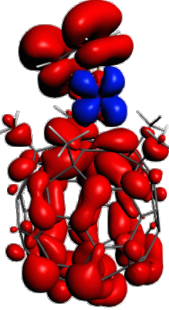
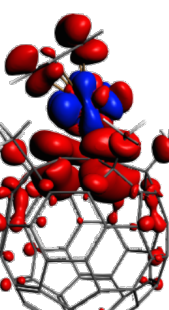
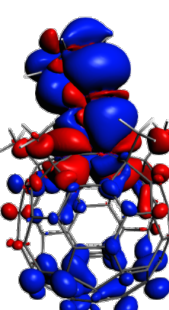
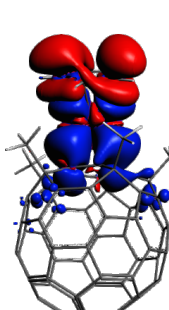
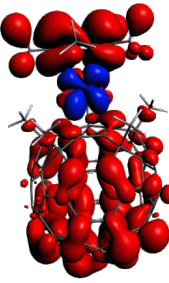
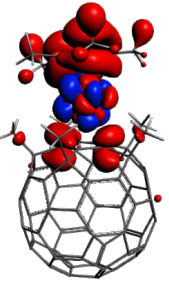
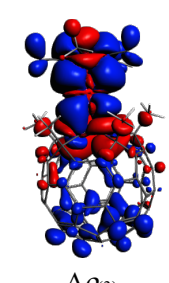
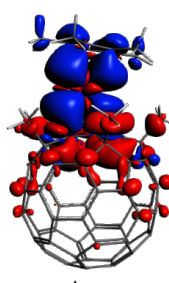
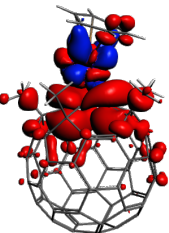
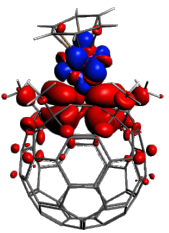
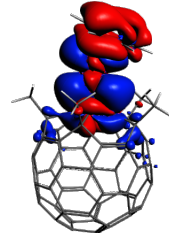
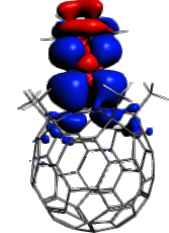
Table S6: PBE0 computed NPA charges on the coordinated C_mH_m, five-membered ring and subsequent neighbour atoms in complexes **1-8**.



| Complex | Cp { η^5 -C ₅₅ X ₅ } ⁻ | α -C/B/N | C _m H _m |
|----------|--|-----------------|-------------------------------|
| 1 | -0.4276 | -0.1188 | -1.1127 |
| 2 | -0.4239 | -0.1275 | -0.9934 |
| 3 | -0.4470 | -0.1221 | -0.4378 |
| 4 | -0.4099 | -0.1272 | -0.7377 |
| 5 | -0.3651 | -0.1075 | -1.5749 |
| 6 | -0.4532 | -0.1271 | -0.4533 |
| 7 | -1.1785 | 2.0986 | -1.1785 |
| 8 | 0.0174 | -1.0695 | 0.0174 |

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Table S7: ETS-NOCV derived first four strongest electron deformation densities ($\Delta E_{\text{orb}(1)}$ to $\Delta E_{\text{orb}(4)}$) at the PBE0-D3(BJ)/TZP level. Isosurface values are 0.0001 au. The direction of the charge flow of the deformation densities is from red to blue. The ΔE_{orb} energies are in kcal/mol. The eigenvalues v_i give the size of the charge migration.

| Complex | $\Delta E_{\text{orb}(1)}$ | $\Delta E_{\text{orb}(2)}$ | $\Delta E_{\text{orb}(3)}$ | $\Delta E_{\text{orb}(4)}$ |
|---------|---|--|--|---|
| 1 |  $\Delta\rho_{(1)}$ $\Delta E_{\text{orb}(1)} = -138.8$; $ v_1 = 0.9$ |  $\Delta\rho_{(2)}$ $\Delta E_{\text{orb}(2)} = -177.0$; $ v_2 = 0.4$ |  $\Delta\rho_{(3)}$ $\Delta E_{\text{orb}(3)} = -171.4$; $ v_3 = 0.34$ |  $\Delta\rho_{(4)}$ $\Delta E_{\text{orb}(4)} = -10.3$; $ v_4 = 0.31$ |
| 2 |  $\Delta\rho_{(1)}$ $\Delta E_{\text{orb}(1)} = 208.9$; $ v_1 = 0.48$ |  $\Delta\rho_{(2)}$ $\Delta E_{\text{orb}(2)} = -195.4$ $ v_2 = 0.38$ |  $\Delta\rho_{(3)}$ $\Delta E_{\text{orb}(3)} = -47.1$; $ v_3 = 0.36$ |  $\Delta\rho_{(4)}$ $\Delta E_{\text{orb}(4)} = -13.7$; $ v_4 = 0.34$ |
| 3 |  $\Delta\rho_{(1)}$ $\Delta E_{\text{orb}(1)} = -203.0$; $ v_1 = 0.5$ |  $\Delta\rho_{(2)}$ $\Delta E_{\text{orb}(2)} = -186.8$; $ v_2 = 0.39$ |  $\Delta\rho_{(3)}$ $\Delta E_{\text{orb}(3)} = -56.7$; $ v_3 = 0.37$ |  $\Delta\rho_{(4)}$ $\Delta E_{\text{orb}(4)} = -10.3$; $ v_4 = 0.37$ |
| 4 |  $\Delta\rho_{(1)}$ |  $\Delta\rho_{(2)}$ |  $\Delta\rho_{(3)}$ |  $\Delta\rho_{(4)}$ |

SUPPORTING INFORMATION

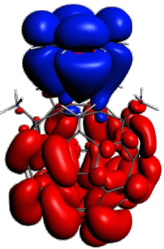
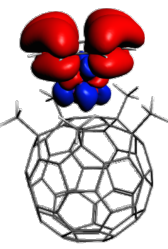
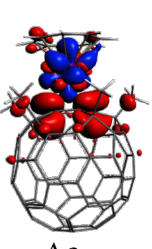
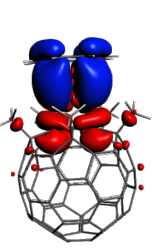
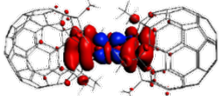
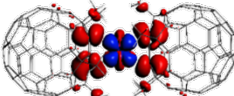
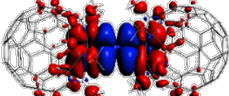
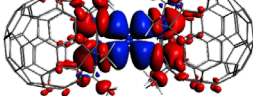
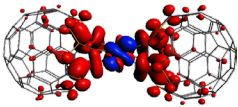
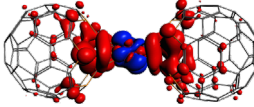
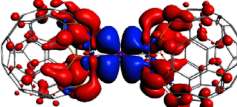
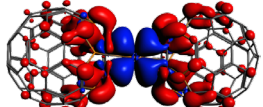
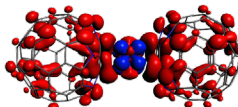
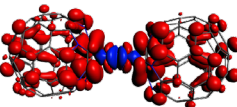
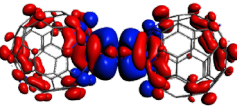
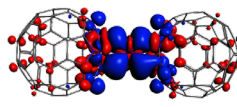
| | | | | |
|---|--|--|--|---|
| | $\Delta E_{\text{orb}(1)} = -229.3;$ $ v_1 = 0.37$ | $\Delta E_{\text{orb}(2)} = -226.7;$ $ v_2 = 0.36$ | $\Delta E_{\text{orb}(3)} = -5.6;$ $ v_3 = 0.31$ | $\Delta E_{\text{orb}(4)} = -1.0;$ $ v_4 = 0.30$ |
| 5 |  $\Delta\rho(1)$ $\Delta E_{\text{orb}(1)} = -111.6;$ $ v_1 = 0.77$ |  $\Delta\rho(2)$ $\Delta E_{\text{orb}(2)} = -172.7;$ $ v_2 = 0.38$ |  $\Delta\rho(3)$ $\Delta E_{\text{orb}(3)} = -174.6;$ $ v_3 = 0.33$ |  $\Delta\rho(4)$ $\Delta E_{\text{orb}(4)} = -0.73;$ $ v_4 = 0.32$ |
| 6 |  $\Delta\rho(1)$ $\Delta E_{\text{orb}(1)} = -188.4;$ $ v_1 = 0.39$ |  $\Delta\rho(2)$ $\Delta E_{\text{orb}(2)} = -189.7;$ $ v_2 = 0.35$ |  $\Delta\rho(3)$ $\Delta E_{\text{orb}(3)} = -41.5;$ $ v_3 = 0.35$ |  $\Delta\rho(4)$ $\Delta E_{\text{orb}(4)} = -40.9;$ $ v_4 = 0.35$ |
| 7 |  $\Delta\rho(1)$ $\Delta E_{\text{orb}(1)} = -197.4;$ $ v_1 = 0.40$ |  $\Delta\rho(2)$ $\Delta E_{\text{orb}(2)} = -197.8;$ $ v_2 = 0.39$ |  $\Delta\rho(3)$ $\Delta E_{\text{orb}(3)} = -48.9;$ $ v_3 = 0.39$ |  $\Delta\rho(4)$ $\Delta E_{\text{orb}(4)} = -48.8;$ $ v_4 = 0.39$ |
| 8 |  $\Delta\rho(1)$ $\Delta E_{\text{orb}(1)} = -185.9;$ $ v_1 = 0.48$ |  $\Delta\rho(2)$ $\Delta E_{\text{orb}(1)} = -241.6;$ $ v_2 = 0.40$ |  $\Delta\rho(3)$ $\Delta E_{\text{orb}(3)} = -49.4;$ $ v_3 = 0.39$ |  $\Delta\rho(4)$ $\Delta E_{\text{orb}(4)} = -13.2;$ $ v_4 = 0.39$ |

Table S8: Natural Population Analysis of Dy(III) ion complex **1-8** along with the Dy(III) free ion.

| Complex | Dy(III) {free} | Dy(III) {complex} |
|---------|--------------------------|--|
| 1 | | [core]6s(0.02)4f(2.10)5d(0.30)6p(0.01)7s(0.01)6d(0.02) |
| 2 | | [core]6s(0.02)4f(2.05)5d(0.26)6p(0.01)7s(0.01)6d(0.03) |
| 3 | | [core]6s(0.02)4f(2.07)5d(0.19)6p(0.01)7s(0.01)6d(0.07) |
| 4 | [core]4f(1.99)5f(0.01) | [core]6s(0.02)4f(2.03)5d(0.22)6p(0.01)7s(0.01)6d(0.03) |
| 5 | | [core]6s(0.03)4f(2.03)5d(0.52)6p(0.02)7s(0.01)6d(0.02) |
| 6 | | [core]6s(0.02)4f(2.07)5d(0.18)6p(0.01)7s(0.01)6d(0.08) |
| 7 | | [core]6s(0.02)4f(2.07)5d(0.24)6p(0.01)7s(0.01)6d(0.02) |
| 8 | | [core]6s(0.02)4f(2.14)5d(0.26)6p(0.01)7s(0.01)6d(0.03) |

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Table S9: Topological parameters obtained through QTAIM analysis for the Dy-C_{ligand} bonds in complexes **1-8**. ^aThe electron density at the bond critical density (BCP), ^bThe Laplacian of the electron density at the BCP, ^cThe Virial Field function, ^dThe electronic kinetic energy density, ^eRatio of Virial field function to Electronic kinetic energy, ^fThe total energy density at the BCP.

| Complex | $\rho(r)^a$ | $\nabla^2\rho(r)^b$ | $ V(r) ^c$ | $G(r)^d$ | $-(G(r)/V(r))^e$ | $H(r)^f$ |
|----------|-------------|---------------------|------------|----------|------------------|----------|
| 1 | 0.0382 | 0.1270 | 0.0355 | 0.0336 | 0.9465 | -0.0019 |
| | 0.0408 | 0.1190 | 0.0377 | 0.0337 | 0.8939 | -0.0040 |
| | 0.0392 | 0.1164 | 0.0356 | 0.0324 | 0.9101 | -0.0033 |
| | 0.0384 | 0.1182 | 0.0349 | 0.0322 | 0.9226 | -0.0027 |
| | 0.0394 | 0.1207 | 0.0362 | 0.0332 | 0.9171 | -0.0030 |
| | 0.0435 | 0.1040 | 0.0396 | 0.0328 | 0.8283 | -0.0068 |
| | 0.0465 | 0.1036 | 0.0431 | 0.0345 | 0.8005 | -0.0086 |
| | 0.0419 | 0.1040 | 0.0377 | 0.0319 | 0.8462 | -0.0059 |
| 0.0486 | 0.1026 | 0.0458 | 0.0357 | 0.7795 | -0.0101 | |
| 2 | 0.0442 | 0.1206 | 0.0418 | 0.0360 | 0.8612 | -0.0058 |
| | 0.0421 | 0.1135 | 0.0387 | 0.0335 | 0.8656 | -0.0052 |
| | 0.0452 | 0.1222 | 0.0431 | 0.0368 | 0.8538 | -0.0063 |
| | 0.0425 | 0.1160 | 0.0393 | 0.0342 | 0.8702 | -0.0052 |
| | 0.0427 | 0.1162 | 0.0397 | 0.0344 | 0.8665 | -0.0053 |
| | 0.0436 | 0.1175 | 0.0409 | 0.0351 | 0.8582 | -0.0057 |
| | 0.0417 | 0.1161 | 0.0385 | 0.0338 | 0.8779 | -0.0047 |
| | 0.0417 | 0.1163 | 0.0385 | 0.0338 | 0.8779 | -0.0047 |
| 0.0428 | 0.1196 | 0.0401 | 0.0350 | 0.8728 | -0.0051 | |
| 3 | 0.0445 | 0.1293 | 0.0428 | 0.0376 | 0.8785 | -0.0053 |
| | 0.0450 | 0.1299 | 0.0435 | 0.0380 | 0.8736 | -0.0055 |
| | 0.0496 | 0.1324 | 0.0495 | 0.0413 | 0.8343 | -0.0082 |
| | 0.0478 | 0.1301 | 0.0470 | 0.0398 | 0.8468 | -0.0072 |
| | 0.0479 | 0.1286 | 0.0470 | 0.0396 | 0.8426 | -0.0074 |
| 4 | 0.0436 | 0.1211 | 0.0412 | 0.0357 | 0.8665 | -0.0054 |
| | 0.0403 | 0.1141 | 0.0367 | 0.0326 | 0.8883 | -0.0041 |
| | 0.0434 | 0.1240 | 0.0411 | 0.0361 | 0.8783 | -0.0051 |
| | 0.0414 | 0.1192 | 0.0384 | 0.0341 | 0.8880 | -0.0043 |
| | 0.0413 | 0.1088 | 0.0374 | 0.0323 | 0.8636 | -0.0051 |
| | 0.0407 | 0.1075 | 0.0366 | 0.0318 | 0.8689 | -0.0049 |
| | 0.0436 | 0.1211 | 0.0412 | 0.0357 | 0.8665 | -0.0054 |
| | 0.0403 | 0.1141 | 0.0367 | 0.0326 | 0.8883 | -0.0041 |
| 5 | 0.0375 | 0.1149 | 0.0337 | 0.0312 | 0.9258 | -0.0025 |
| | 0.0372 | 0.1145 | 0.0333 | 0.0310 | 0.9309 | -0.0024 |
| | 0.0374 | 0.1143 | 0.0335 | 0.0310 | 0.9254 | -0.0025 |
| | 0.0374 | 0.1150 | 0.0336 | 0.0312 | 0.9286 | -0.0024 |
| | 0.0371 | 0.1141 | 0.0333 | 0.0309 | 0.9279 | -0.0024 |
| | 0.0444 | 0.1417 | 0.0438 | 0.0396 | 0.9041 | -0.0042 |
| | 0.0453 | 0.1389 | 0.0446 | 0.0397 | 0.8901 | -0.0050 |
| | 0.0444 | 0.1421 | 0.0438 | 0.0397 | 0.9064 | -0.0042 |
| | 0.0450 | 0.1388 | 0.0442 | 0.0395 | 0.8937 | -0.0047 |
| | 0.0449 | 0.1391 | 0.0442 | 0.0395 | 0.8937 | -0.0047 |
| | 0.0450 | 0.1402 | 0.0444 | 0.0397 | 0.8941 | -0.0047 |
| | 0.0447 | 0.1411 | 0.0441 | 0.0397 | 0.9002 | -0.0044 |
| | 0.0453 | 0.1386 | 0.0446 | 0.0396 | 0.8879 | -0.0050 |
| 6 | 0.0391 | 0.1054 | 0.0347 | 0.0305 | 0.8790 | -0.0042 |
| | 0.0405 | 0.1083 | 0.0364 | 0.0317 | 0.8709 | -0.0047 |
| | 0.0379 | 0.0997 | 0.0328 | 0.0289 | 0.8811 | -0.0040 |
| | 0.0405 | 0.1038 | 0.0361 | 0.0310 | 0.8587 | -0.0050 |
| | 0.0403 | 0.1080 | 0.0362 | 0.0316 | 0.8729 | -0.0046 |
| | 0.0392 | 0.1054 | 0.0348 | 0.0306 | 0.8793 | -0.0042 |
| | 0.0403 | 0.1034 | 0.0358 | 0.0308 | 0.8603 | -0.0050 |
| | 0.0381 | 0.1002 | 0.0331 | 0.0291 | 0.8792 | -0.0040 |
| | 0.0376 | 0.1065 | 0.0331 | 0.0298 | 0.9003 | -0.0032 |
| | 7 | 0.0396 | 0.1177 | 0.0362 | 0.0328 | 0.9061 |
| 0.0392 | | 0.1179 | 0.0358 | 0.0326 | 0.9106 | -0.0032 |
| 0.0410 | | 0.1216 | 0.0381 | 0.0342 | 0.8976 | -0.0039 |
| 0.0412 | | 0.1220 | 0.0383 | 0.0344 | 0.8982 | -0.0039 |
| 0.0418 | | 0.1253 | 0.0393 | 0.0353 | 0.8982 | -0.0040 |
| 0.0416 | | 0.1250 | 0.0391 | 0.0352 | 0.9003 | -0.0039 |
| 0.0410 | | 0.1216 | 0.0381 | 0.0343 | 0.9003 | -0.0039 |
| 0.0410 | | 0.1215 | 0.0381 | 0.0342 | 0.8976 | -0.0039 |

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|----------|--------|--------|--------|--------|--------|---------|
| | 0.0392 | 0.1179 | 0.0358 | 0.0326 | 0.9106 | -0.0032 |
| | 0.0398 | 0.1179 | 0.0364 | 0.0329 | 0.9038 | -0.0035 |
| 8 | 0.0373 | 0.0940 | 0.0317 | 0.0276 | 0.8707 | -0.0041 |
| | 0.0384 | 0.0943 | 0.0329 | 0.0282 | 0.8571 | -0.0047 |
| | 0.0356 | 0.0898 | 0.0296 | 0.0260 | 0.8784 | -0.0036 |
| | 0.0355 | 0.0901 | 0.0296 | 0.0260 | 0.8784 | -0.0035 |
| | 0.0372 | 0.0941 | 0.0317 | 0.0276 | 0.8707 | -0.0041 |
| | 0.0356 | 0.0896 | 0.0296 | 0.0260 | 0.8784 | -0.0036 |
| | 0.0371 | 0.0937 | 0.0315 | 0.0275 | 0.8730 | -0.0040 |
| | 0.0356 | 0.0902 | 0.0297 | 0.0261 | 0.8788 | -0.0036 |
| | 0.0382 | 0.0940 | 0.0327 | 0.0281 | 0.8593 | -0.0046 |
| | 0.0373 | 0.0939 | 0.0317 | 0.0276 | 0.8707 | -0.0041 |

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Table S10: CASSCF computed spin-free and SOC states and corresponding g-tensor values for the low-lying eight KDs for complexes **1** and **2**. All the energies are reported in cm^{-1} .

| | 1 | | | | | | 2 | | | | | |
|----------------|------------------|--------------------------------------|----------|----------|----------|----------------|------------------|--------------------------------------|----------|----------|----------|----------------|
| | Spin-free states | SOC states (${}^6\text{H}_{15/2}$) | g-values | | | | Spin-free states | SOC states (${}^6\text{H}_{15/2}$) | g-values | | | |
| | | | g_{xx} | g_{yy} | g_{zz} | Θ° | | | g_{xx} | g_{yy} | g_{zz} | Θ° |
| ${}^6\text{H}$ | 0 | 0.0 | 0.000 | 0.000 | 19.980 | 0.0 | 0.0 | 0.0 | 0.000 | 0.000 | 19.944 | 0.0 |
| | 0.0 | 487.4 | 0.000 | 0.000 | 17.014 | 4.0 | 0.2 | 409.6 | 0.000 | 0.000 | 17.047 | 0.3 |
| | 808.7 | 785.0 | 0.009 | 0.010 | 14.326 | 6.2 | 679.6 | 689.2 | 0.004 | 0.005 | 14.392 | 0.8 |
| | 812.5 | 999.4 | 0.096 | 0.105 | 11.598 | 1.9 | 679.7 | 889.1 | 0.001 | 0.007 | 11.718 | 1.4 |
| | 1005.9 | 1198.5 | 0.469 | 0.635 | 8.988 | 4.6 | 921.7 | 1062.4 | 0.035 | 0.037 | 9.043 | 2.1 |
| | 1019 | 1385.7 | 1.341 | 2.304 | 6.342 | 11.8 | 922.1 | 1208.9 | 0.969 | 1.336 | 6.263 | 3.4 |
| | 1319.7 | 1538.6 | 3.227 | 4.480 | 7.803 | 94.3 | 1170.6 | 1305.0 | 8.519 | 8.157 | 2.690 | 0.6 |
| | 1343.4 | 1649.2 | 0.863 | 4.151 | 16.490 | 90.4 | 1178.3 | 1423.5 | 0.297 | 0.954 | 17.841 | 90.0 |
| | 1602.2 | | | | | | 1311.2 | | | | | |
| | 1649.6 | | | | | | 1464.9 | | | | | |
| 1728.3 | | | | | | 1477.7 | | | | | | |
| ${}^6\text{F}$ | 8208.8 | | | | | | 8093.7 | | | | | |
| | 8290.6 | | | | | | 8182.9 | | | | | |
| | 8395.4 | | | | | | 8193.9 | | | | | |
| | 8431.3 | | | | | | 8285.3 | | | | | |
| | 8441.2 | | | | | | 8300.8 | | | | | |
| | 8653.5 | | | | | | 8465.3 | | | | | |
| 8657.2 | | | | | | 8465.4 | | | | | | |
| ${}^6\text{P}$ | 34119.0 | | | | | | 34139.0 | | | | | |
| | 35790.9 | | | | | | 35637.8 | | | | | |
| | 35986.0 | | | | | | 35691.5 | | | | | |

Table S11: CASSCF computed spin-free and SOC states and corresponding g-tensor values for the low-lying eight KDs for complexes **2a** and **3a**. All the energies are reported in cm^{-1} .

| | 2a | | | | | | 3a | | | | | | |
|----------------|------------------|--------------------------------------|----------|----------|----------|----------------|------------------|--------------------------------------|----------|----------|----------|----------------|--|
| | Spin-free states | SOC states (${}^6\text{H}_{15/2}$) | g-values | | | | Spin-free states | SOC states (${}^6\text{H}_{15/2}$) | g-values | | | | |
| | | | g_{xx} | g_{yy} | g_{zz} | Θ° | | | g_{xx} | g_{yy} | g_{zz} | Θ° | |
| ${}^6\text{H}$ | 0.0 | 0.0 | 0.000 | 0.000 | 19.890 | 0.0 | 0.0 | 0.0 | 0.000 | 0.000 | 19.970 | 0.0 | |
| | 0.5 | 310.1 | 0.000 | 0.000 | 17.098 | 0.0 | 0.2 | 497.6 | 0.000 | 0.000 | 16.992 | 0.1 | |
| | 500.4 | 606.9 | 0.001 | 0.002 | 14.422 | 0.1 | 846.7 | 825.2 | 0.003 | 0.004 | 14.334 | 0.2 | |
| | 502.1 | 837.3 | 0.001 | 0.005 | 11.696 | 0.2 | 847.4 | 1050.5 | 0.008 | 0.014 | 11.674 | 0.2 | |
| | 937.6 | 1016.3 | 0.379 | 0.459 | 9.016 | 0.9 | 1074.3 | 1249.2 | 0.057 | 0.081 | 9.003 | 0.6 | |
| | 941.7 | 1111.2 | 4.089 | 4.876 | 11.240 | 90.9 | 1077.4 | 1426.0 | 0.410 | 0.528 | 6.323 | 0.8 | |
| | 1106.5 | 1167.4 | 0.096 | 0.280 | 13.522 | 90.7 | 1378.8 | 1551.5 | 7.945 | 6.819 | 3.024 | 0.5 | |
| | 1133.0 | 1323.4 | 0.136 | 0.293 | 18.945 | 90.0 | 1385.0 | 1668.5 | 0.548 | 2.190 | 16.972 | 89.0 | |
| | 1149.1 | | | | | | 1570.1 | | | | | | |
| | 1347.0 | | | | | | 1709.5 | | | | | | |
| | 1374.2 | | | | | | 1735.5 | | | | | | |
| | ${}^6\text{F}$ | 8009.8 | | | | | | 8233.5 | | | | | |
| | | 8039.4 | | | | | | 8356.8 | | | | | |
| | | 8168.9 | | | | | | 8381.5 | | | | | |
| | | 8212.6 | | | | | | 8470.7 | | | | | |
| 8249.9 | | | | | | | 8480.8 | | | | | | |
| 8368.0 | | | | | | | 8681.4 | | | | | | |
| 8371.4 | | | | | | 8682.8 | | | | | | | |
| ${}^6\text{P}$ | 34117.5 | | | | | | 34114.3 | | | | | | |
| | 35482.6 | | | | | | 35904.9 | | | | | | |
| | 35618.2 | | | | | | 35929.5 | | | | | | |

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Table S12: CASSCF computed spin-free and SOC states and corresponding g-tensor values for the low-lying eight KDs for complexes **3** and **4**. All the energies are reported in cm^{-1} .

| 3 | | | | | | | 4 | | | | | |
|----------------|------------------|--------------------------------------|----------|----------|----------|----------------|------------------|--------------------------------------|----------|----------|----------|----------------|
| | Spin-free states | SOC states (${}^6\text{H}_{15/2}$) | g-values | | | | Spin-free states | SOC states (${}^6\text{H}_{15/2}$) | g-values | | | |
| | | | g_{xx} | g_{yy} | g_{zz} | Θ° | | | g_{xx} | g_{yy} | g_{zz} | Θ° |
| ${}^6\text{H}$ | 0.0 | 0.0 | 0.000 | 0.000 | 19.986 | 0.0 | 0.0 | 0.0 | 0.000 | 0.000 | 19.976 | 0.0 |
| | 0.3 | 541.7 | 0.000 | 0.000 | 16.963 | 0.6 | 0.1 | 373.2 | 0.000 | 0.000 | 17.137 | 5.3 |
| | 940.7 | 845.2 | 0.005 | 0.006 | 14.370 | 0.9 | 592.1 | 584.1 | 0.001 | 0.001 | 14.484 | 7.8 |
| | 941.0 | 1033.6 | 0.001 | 0.011 | 11.742 | 0.5 | 594.1 | 733.4 | 0.034 | 0.037 | 11.729 | 4.2 |
| | 1007.4 | 1215.3 | 0.056 | 0.067 | 9.025 | 1.5 | 737.4 | 879.0 | 0.237 | 0.312 | 9.107 | 1.1 |
| | 1009.7 | 1404.1 | 0.047 | 0.161 | 6.316 | 1.7 | 744.7 | 1016.5 | 1.289 | 1.955 | 6.472 | 6.2 |
| | 1321.6 | 1569.5 | 2.742 | 3.097 | 3.618 | 10.4 | 960.1 | 1124.8 | 3.309 | 3.384 | 7.521 | 82.3 |
| | 1325.6 | 1675.4 | 13.295 | 7.481 | 1.119 | 0.1 | 983.2 | 1200.5 | 0.922 | 4.677 | 15.285 | 89.7 |
| | 1632.9 | | | | | | 1149.4 | | | | | |
| | 1690.5 | | | | | | 1229.9 | | | | | |
| | 1774.1 | | | | | | 1274.7 | | | | | |
| | ${}^6\text{F}$ | 8246.3 | | | | | | 7945.3 | | | | |
| | | 8310.9 | | | | | | 8029.2 | | | | |
| 8460.0 | | | | | | | 8090.4 | | | | | |
| 8466.8 | | | | | | | 8115.9 | | | | | |
| 8476.5 | | | | | | | 8137.1 | | | | | |
| 8690.6 | | | | | | | 8283.6 | | | | | |
| 8691.7 | | | | | | | 8284.5 | | | | | |
| ${}^6\text{P}$ | 34151.4 | | | | | | 34160.9 | | | | | |
| | 35916.6 | | | | | | 35394.2 | | | | | |
| | 35939.2 | | | | | | 35443.9 | | | | | |

Table S13: CASSCF computed spin-free and SOC states and corresponding g-tensor values for the low-lying eight KDs for complexes **5** and **6**. All the energies are reported in cm^{-1} .

| 5 | | | | | | | 6 | | | | | |
|----------------|------------------|--------------------------------------|----------|----------|----------|----------------|------------------|--------------------------------------|----------|----------|----------|----------------|
| | Spin-free states | SOC states (${}^6\text{H}_{15/2}$) | g-values | | | | Spin-free states | SOC states (${}^6\text{H}_{15/2}$) | g-values | | | |
| | | | g_{xx} | g_{yy} | g_{zz} | Θ° | | | g_{xx} | g_{yy} | g_{zz} | Θ° |
| ${}^6\text{H}$ | 0.0 | 0.0 | 0.194 | 0.315 | 9.745 | 0.0 | 0.0 | 0.0 | 0.000 | 0.000 | 19.998 | 0.0 |
| | 1.6 | 14.9 | 0.015 | 0.122 | 12.038 | 23.3 | 0.5 | 520.4 | 0.000 | 0.000 | 16.987 | 1.2 |
| | 20.3 | 29.8 | 0.110 | 0.361 | 6.676 | 20.3 | 871.3 | 778.5 | 0.009 | 0.009 | 14.439 | 1.8 |
| | 21.2 | 73.7 | 1.680 | 1.940 | 3.861 | 17.7 | 872.1 | 932.0 | 0.005 | 0.012 | 11.816 | 2.0 |
| | 138.5 | 97.9 | 1.806 | 2.985 | 11.261 | 19.0 | 911.0 | 1096.5 | 0.006 | 0.013 | 9.058 | 3.3 |
| | 144.7 | 108.4 | 4.750 | 6.936 | 9.358 | 99.2 | 911.2 | 1284.8 | 0.208 | 0.221 | 6.301 | 3.0 |
| | 211.5 | 272.3 | 0.000 | 0.000 | 17.424 | 16.7 | 1180.9 | 1461.9 | 0.857 | 1.298 | 3.660 | 3.2 |
| | 229.2 | 489.7 | 0.000 | 0.000 | 19.991 | 17.8 | 1187.9 | 1573.7 | 11.607 | 9.451 | 1.188 | 0.5 |
| | 229.5 | | | | | | 1557.3 | | | | | |
| | 539.7 | | | | | | 1568.4 | | | | | |
| | 540.2 | | | | | | 1693.3 | | | | | |
| | ${}^6\text{F}$ | 7419.7 | | | | | | 8192.3 | | | | |
| | | 7420.4 | | | | | | 8198.9 | | | | |
| | | 7460.8 | | | | | | 8370.8 | | | | |
| | | 7461.6 | | | | | | 8374.4 | | | | |
| 7570.3 | | | | | | | 8420.2 | | | | | |
| 7572.0 | | | | | | | 8604.7 | | | | | |
| 7717.0 | | | | | | | 8604.7 | | | | | |
| ${}^6\text{P}$ | 34211.8 | | | | | | 34185.9 | | | | | |
| | 34221.4 | | | | | | 35824.8 | | | | | |
| | 34645.9 | | | | | | 35848.7 | | | | | |

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Table S14: CASSCF computed spin-free and SOC states and corresponding g-tensor values for the low-lying eight KDs for complexes **7** and **8**. All the energies are reported in cm^{-1} .

| 7 | | | | | | | 8 | | | | | | | |
|----------------|------------------|--------------------------------------|----------|----------|----------|--------|----------------|------------------|--------------------------------------|----------|----------|----------|--|----------------|
| | Spin-free states | SOC states (${}^6\text{H}_{15/2}$) | g-values | | | | Θ° | Spin-free states | SOC states (${}^6\text{H}_{15/2}$) | g-values | | | | Θ° |
| | | | g_{xx} | g_{yy} | g_{zz} | | | | | g_{xx} | g_{yy} | g_{zz} | | |
| ${}^6\text{H}$ | 0.0 | 0.0 | 0.000 | 0.000 | 19.996 | 0.0 | 0.0 | 0.0 | 0.000 | 0.000 | 19.998 | 0.0 | | |
| | 1.2 | 452.3 | 0.000 | 0.000 | 17.040 | 1.6 | 0.3 | 457.9 | 0.000 | 0.000 | 17.041 | 1.6 | | |
| | 707.0 | 650.6 | 0.033 | 0.034 | 14.500 | 2.8 | 702.5 | 654.8 | 0.008 | 0.008 | 14.509 | 2.8 | | |
| | 708.7 | 760.6 | 0.028 | 0.035 | 11.882 | 2.8 | 703.5 | 768.8 | 0.005 | 0.010 | 11.889 | 2.9 | | |
| | 771.0 | 887.4 | 0.033 | 0.041 | 9.124 | 3.8 | 781.5 | 906.7 | 0.020 | 0.024 | 9.109 | 3.8 | | |
| | 771.1 | 1041.3 | 0.346 | 0.403 | 6.365 | 3.1 | 781.6 | 1076.4 | 0.251 | 0.287 | 6.334 | 3.1 | | |
| | 938.4 | 1189.9 | 0.396 | 1.136 | 3.713 | 3.3 | 965.5 | 1241.5 | 0.374 | 0.910 | 3.686 | 3.2 | | |
| | 948.3 | 1284.1 | 11.322 | 9.789 | 1.212 | 0.4 | 972.7 | 1347.0 | 11.189 | 9.907 | 1.201 | 0.5 | | |
| | 1271.6 | | | | | | 1332.0 | | | | | | | |
| | 1278.3 | | | | | | 1338.9 | | | | | | | |
| 1397.1 | | | | | | 1471.7 | | | | | | | | |
| ${}^6\text{F}$ | 8022.5 | | | | | | 8042.7 | | | | | | | |
| | 8026.5 | | | | | | 8045.4 | | | | | | | |
| | 8176.5 | | | | | | 8195.9 | | | | | | | |
| | 8181.4 | | | | | | 8199.3 | | | | | | | |
| | 8222.9 | | | | | | 8258.8 | | | | | | | |
| | 8353.6 | | | | | | 8400.3 | | | | | | | |
| | 8353.8 | | | | | | 8400.4 | | | | | | | |
| ${}^6\text{P}$ | 34217.0 | | | | | | 34207.1 | | | | | | | |
| | 35520.8 | | | | | | 35571.8 | | | | | | | |
| | 35535.0 | | | | | | 35582.3 | | | | | | | |

Table S15: SINGLE_ANISO computed wave function decomposition analysis of complexes **1-8**.

| $\pm mJ$ | Complex 1 | Complex 2 |
|----------|---|--|
| KD1 | 100 % $ \pm 15/2\rangle$ | 99.6 % $ \pm 15/2\rangle$ |
| KD2 | 99.2 % $ \pm 13/2\rangle$ | 99.8 % $ \pm 13/2\rangle$ |
| KD3 | 95.3 % $ \pm 11/2\rangle$ | 99.6 % $ \pm 11/2\rangle$ |
| KD4 | 91.4 % $ \pm 9/2\rangle$ | 99.5 % $ \pm 9/2\rangle$ |
| KD5 | 90.8 % $ \pm 7/2\rangle$ | 99.8 % $ \pm 7/2\rangle$ |
| KD6 | 91.4 % $ \pm 5/2\rangle$ | 96.9 % $ \pm 5/2\rangle$ |
| KD7 | 86.9 % $ \pm 3/2\rangle$ + 8.7% $ \pm 1/2\rangle$ | 79 % $ \pm 3/2\rangle$ + 19.5 % $ \pm 1/2\rangle$ |
| KD8 | 88 % $ \pm 1/2\rangle$ + 10 % $ \pm 3/2\rangle$ | 78.1 % $ \pm 1/2\rangle$ + 20.5% $ \pm 3/2\rangle$ |

| $\pm mJ$ | Complex 3 | Complex 4 |
|----------|---------------------------|---|
| KD1 | 100 % $ \pm 15/2\rangle$ | 99.8 % $ \pm 15/2\rangle$ |
| KD2 | 100 % $ \pm 13/2\rangle$ | 98.9 % $ \pm 13/2\rangle$ |
| KD3 | 99.7 % $ \pm 11/2\rangle$ | 93.5 % $ \pm 11/2\rangle$ |
| KD4 | 99.6 % $ \pm 9/2\rangle$ | 88.4 % $ \pm 9/2\rangle$ + 6.7% $ \pm 7/2\rangle$ |
| KD5 | 99.6 % $ \pm 7/2\rangle$ | 88 % $ \pm 7/2\rangle$ + 5.6 % $ \pm 5/2\rangle$ |
| KD6 | 99.7 % $ \pm 5/2\rangle$ | 90.2 % $ \pm 5/2\rangle$ |

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| | | |
|-----|--------------------------|--|
| KD7 | 98.9 % $ \pm 3/2\rangle$ | 87.9 % $ \pm 3/2\rangle$ + 7.6 % $ \pm 1/2\rangle$ |
| KD8 | 98.1 % $ \pm 1/2\rangle$ | 91.9 % $ \pm 1/2\rangle$ |

| $\pm mJ$ | Complex 5 | Complex 6 |
|----------|---|--|
| KD1 | 38.8 % $ \pm 9/2\rangle$ + 27.1 % $ \pm 5/2\rangle$ + 15.1 % $ \pm 11/2\rangle$ | 100 % $ \pm 15/2\rangle$ |
| KD2 | 37.0 % $ \pm 7/2\rangle$ + 30.1 % $ \pm 11/2\rangle$ + 16.9 % $ \pm 5/2\rangle$ | 98.9 % $ \pm 13/2\rangle$ |
| KD3 | 33.1 % $ \pm 3/2\rangle$ + 30.4 % $ \pm 7/2\rangle$ + 19.4 % $ \pm 1/2\rangle$ | 78.5 % $ \pm 11/2\rangle$ + 17.5 % $ \pm 9/2\rangle$ |
| KD4 | 48.7 % $ \pm 1/2\rangle$ + 31 % $ \pm 5/2\rangle$ + 14.6 % $ \pm 7/2\rangle$ | 77.6 % $ \pm 9/2\rangle$ + 20 % $ \pm 11/2\rangle$ |
| KD5 | 25.1 % $ \pm 9/2\rangle$ + 24.5 % $ \pm 13/2\rangle$ + 13.1 % $ \pm 3/2\rangle$ + 10.7% $ \pm 7/2\rangle$ | 97.8 % $ \pm 7/2\rangle$ |
| KD6 | 34.9 % $ \pm 3/2\rangle$ + 21.1 % $ \pm 1/2\rangle$ + 16.7 % $ \pm 5/2\rangle$ | 99.8 % $ \pm 5/2\rangle$ |
| KD7 | 33.3 % $ \pm 11/2\rangle$ + 30.9 % $ \pm 13/2\rangle$ + 26.7% $ \pm 15/2\rangle$ | 99.7 % $ \pm 3/2\rangle$ |
| KD8 | 68.7 % $ \pm 15/2\rangle$ + 26.3 % $ \pm 13/2\rangle$ | 99.7 % $ \pm 1/2\rangle$ |

| $\pm mJ$ | Complex 7 | Complex 8 |
|----------|---------------------------|---------------------------|
| KD1 | 100 % $ \pm 15/2\rangle$ | 100 % $ \pm 15/2\rangle$ |
| KD2 | 99.9 % $ \pm 13/2\rangle$ | 99.9 % $ \pm 13/2\rangle$ |
| KD3 | 99.3 % $ \pm 11/2\rangle$ | 99.3 % $ \pm 11/2\rangle$ |
| KD4 | 99.3 % $ \pm 9/2\rangle$ | 99.3 % $ \pm 9/2\rangle$ |
| KD5 | 99.8 % $ \pm 7/2\rangle$ | 99.9 % $ \pm 7/2\rangle$ |
| KD6 | 99.9 % $ \pm 5/2\rangle$ | 99.9 % $ \pm 5/2\rangle$ |
| KD7 | 99.7 % $ \pm 3/2\rangle$ | 99.7 % $ \pm 3/2\rangle$ |
| KD8 | 99.7 % $ \pm 1/2\rangle$ | 99.8 % $ \pm 1/2\rangle$ |

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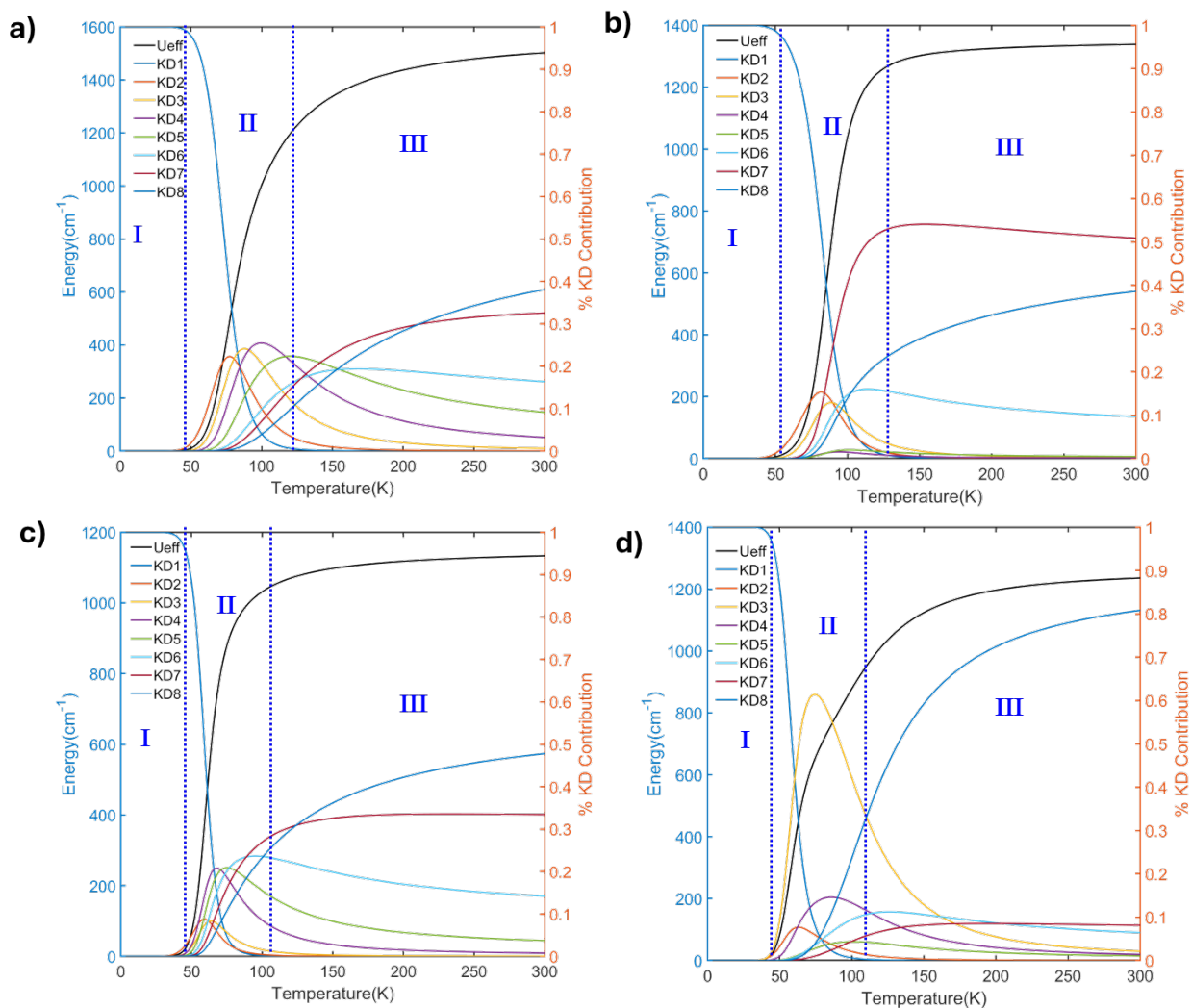


Figure S4: Temperature dependence of calculated U_{eff} and relative contribution of each Kramer's doublet to the relaxation calculated as $k_i(T)/N_k$ for complexes 1(a), 2(b), 4(c), 7(d).

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Table S16: Effective demagnetization barrier (U_{eff}) with the three most contributing KDs to the barrier heights.

| Complexes | U_{cal} (cm ⁻¹) | U_{eff} (cm ⁻¹) | k_{QTM} | % contribution from KDs |
|-----------|--------------------------------------|--------------------------------------|------------------|----------------------------|
| 1 | 1538.6 | 1501 | 2.43E-07 | KD8 37% + KD7 32%+ KD6 16% |
| 2 | 1305.0 | 1338 | 1.46E-06 | KD8 38% + KD7 50%+ KD6 39% |
| 3 | 1569.5 | 1627.5 | 6.55E-08 | KD8 68% + KD7 26%+ KD6 1% |
| 4 | 1124.8 | 1133 | 1.71E-07 | KD8 47% + KD7 33%+ KD6 14% |
| 5 | 108.4 | 95.2 | 8.48E-02 | KD6 59% + KD5 19%+ KD4 15% |
| 6 | 1573.7 | 1533 | 3.99E-09 | KD8 81% + KD7 12%+ KD6 4% |
| 7 | 1284.1 | 1235 | 2.37E-07 | KD8 80% + KD7 8%+ KD6 6% |
| 8 | 1347.0 | 1314.0 | 8.99E-08 | KD8 85% + KD7 7%+ KD6 5% |
| 3a | 1551.5 | 1589.0 | 6.02E-07 | KD8 38% + KD7 51%+ KD6 6% |

Table S17: SINGLE_ANISO computed crystal field parameters for **1–8**. The CF parameters were computed using the following equation, $\widehat{H}_{CF} = \sum_{k=-q}^q B_k^q O_k^q$ and here B_k^q and O_k^q are the crystal field parameters and Steven's operator, respectively.

| k | q | B_k^q | | | | | | | |
|---|----|------------------|------------------|------------------|------------------|-----------------|------------------|------------------|------------------|
| | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| 2 | -2 | 3.69E+00 | -1.14E-01 | 1.89E-02 | -7.27E-02 | 2.24E-01 | 1.51E-01 | 6.76E-02 | 1.09E-01 |
| 2 | -1 | 2.40E+00 | 7.33E-02 | -3.10E-01 | 3.30E+00 | 1.39E+00 | 1.96E-01 | 2.73E-01 | 7.24E-03 |
| 2 | 0 | -2.10E+01 | -1.83E+01 | -2.10E+01 | -1.53E+01 | 5.32E+00 | -8.51E+00 | -1.57E+01 | -1.65E+01 |
| 2 | 1 | 4.00E+00 | 2.50E-01 | 8.61E-01 | -1.80E+00 | 3.69E+00 | 3.04E-02 | -5.06E-01 | -6.21E-01 |
| 2 | 2 | 3.79E-01 | -1.41E+00 | 2.45E-01 | -8.14E-01 | -2.63E-02 | -1.28E-01 | -2.68E-01 | -1.91E-01 |
| 4 | -4 | -2.11E-02 | -1.90E-03 | -6.55E-04 | 1.44E-02 | 1.61E-05 | -3.03E-04 | -3.04E-03 | -1.49E-03 |
| 4 | -3 | -3.66E-03 | 7.71E-03 | -1.30E-02 | -6.81E-04 | 1.02E-03 | 4.90E-04 | 4.78E-03 | -4.03E-04 |
| 4 | -2 | 1.97E-02 | 4.39E-03 | -1.03E-02 | -1.28E-02 | 6.69E-03 | 1.28E-04 | 1.49E-04 | 1.31E-05 |
| 4 | -1 | -4.16E-03 | 1.44E-03 | -1.72E-03 | -4.17E-02 | 3.79E-02 | 8.73E-04 | 2.44E-03 | 2.82E-04 |
| 4 | 0 | -1.27E-02 | -1.38E-02 | -1.80E-02 | -8.55E-03 | 4.75E-02 | -1.50E-04 | -8.93E-03 | -2.05E-03 |
| 4 | 1 | -1.99E-02 | 1.69E-02 | 4.26E-03 | 2.67E-02 | 1.04E-01 | 1.47E-04 | -4.77E-03 | -7.38E-03 |
| 4 | 2 | -6.68E-03 | 1.25E-02 | 1.56E-02 | -9.61E-03 | 6.94E-03 | -1.24E-04 | -1.11E-03 | 4.23E-04 |
| 4 | 3 | 1.6E-04 | 4.95E-03 | 7.03E-03 | 3.00E-03 | 5.40E-04 | 8.06E-04 | -1.40E-03 | 4.51E-03 |
| 4 | 4 | 1.28E-02 | -3.21E-05 | -3.95E-04 | -7.57E-03 | -4.31E-04 | -5.16E-05 | 2.18E-03 | 3.67E-03 |
| 6 | -6 | -1.01E-04 | 2.60E-05 | 7.10E-05 | 7.89E-05 | 1.87E-04 | 1.62E-06 | -5.47E-05 | -1.48E-05 |
| 6 | -5 | 1.03E-04 | -3.10E-03 | 5.41E-03 | -4.35E-04 | 3.42E-03 | -8.96E-05 | 9.96E-03 | 1.97E-03 |
| 6 | -4 | 1.14E-04 | -5.07E-05 | 2.27E-05 | -3.12E-04 | -1.33E-04 | 1.08E-05 | 2.65E-04 | 5.78E-05 |
| 6 | -3 | -1.26E-04 | -8.12E-04 | 8.65E-04 | -1.26E-04 | 3.43E-05 | -5.39E-06 | -1.20E-04 | 1.91E-05 |
| 6 | -2 | -2.63E-03 | -1.21E-03 | 1.58E-03 | 4.30E-03 | -9.15E-05 | -1.74E-06 | 9.41E-06 | -4.10E-06 |
| 6 | -1 | -1.93E-03 | 1.21E-05 | 1.92E-04 | -2.38E-03 | -6.23E-04 | -4.30E-05 | -4.74E-04 | -2.91E-05 |
| 6 | 0 | -1.26E-03 | -6.86E-04 | -1.70E-03 | -9.76E-04 | -5.18E-04 | -7.00E-05 | -1.80E-03 | -1.94E-03 |

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| | | | | | | | | | |
|----|-----|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 6 | 1 | -2.68E-03 | -2.86E-05 | -2.88E-04 | 1.23E-03 | -2.08E-03 | -6.90E-06 | 9.07E-04 | 1.19E-03 |
| 6 | 2 | -9.32E-04 | -5.98E-03 | -2.50E-03 | 2.33E-03 | -2.57E-04 | 1.91E-06 | 2.21E-05 | -1.91E-05 |
| 6 | 3 | -5.80E-04 | 2.68E-04 | -6.83E-04 | -1.58E-03 | -3.49E-05 | -9.56E-06 | 1.36E-05 | -1.79E-04 |
| 6 | 4 | 1.01E-04 | -6.48E-04 | 1.54E-04 | 5.23E-04 | -1.08E-04 | 1.74E-06 | -1.78E-04 | -1.63E-04 |
| 6 | 5 | -1.37E-03 | 3.50E-03 | -1.85E-03 | -1.55E-03 | 1.89E-03 | 2.72E-04 | -1.02E-03 | -4.80E-03 |
| 6 | 6 | -3.82E-04 | 4.77E-05 | -7.81E-05 | -1.88E-04 | -4.01E-05 | 8.31E-07 | -2.25E-05 | 3.51E-05 |
| 8 | -8 | 6.79E-07 | 2.09E-09 | 3.26E-09 | 1.24E-08 | 3.46E-07 | 3.77E-11 | -8.93E-09 | 4.88E-09 |
| 8 | -7 | 1.34E-06 | -6.69E-07 | -4.54E-07 | 7.13E-07 | -1.01E-06 | 4.71E-09 | 5.35E-07 | 1.77E-07 |
| 8 | -6 | -3.02E-07 | -6.55E-08 | 7.39E-08 | 1.42E-07 | -8.43E-07 | -1.36E-09 | 2.45E-08 | 5.31E-09 |
| 8 | -5 | 7.28E-07 | -2.24E-05 | 4.26E-05 | -4.42E-06 | -1.29E-05 | 2.50E-07 | 5.87E-05 | 1.15E-05 |
| 8 | -4 | -1.26E-06 | -4.85E-07 | -4.22E-08 | -1.76E-07 | 5.68E-07 | -3.22E-08 | 1.08E-06 | 1.28E-07 |
| 8 | -3 | 3.95E-06 | -7.30E-06 | 9.42E-06 | -1.33E-06 | -5.21E-07 | 2.49E-08 | -8.41E-07 | 1.15E-07 |
| 8 | -2 | -2.18E-05 | -1.07E-05 | 1.63E-05 | 2.99E-05 | -4.93E-07 | -5.73E-10 | 1.48E-07 | 1.30E-07 |
| 8 | -1 | -3.47E-06 | 6.96E-08 | 2.67E-07 | -3.12E-06 | -2.31E-07 | 3.11E-08 | -5.64E-07 | -3.91E-08 |
| 8 | 0 | -2.06E-06 | -1.02E-06 | -2.72E-06 | -1.10E-06 | -3.50E-08 | 2.62E-08 | -2.00E-06 | -2.27E-06 |
| 8 | 1 | -4.64E-06 | 1.12E-07 | -2.67E-07 | 1.61E-06 | -5.11E-07 | 5.21E-09 | 1.08E-06 | 1.54E-06 |
| 8 | 2 | -9.99E-06 | -5.31E-05 | -2.54E-05 | 1.53E-05 | -4.65E-07 | -1.31E-09 | -2.55E-07 | -3.74E-07 |
| 8 | 3 | -8.25E-06 | 1.87E-06 | -7.47E-06 | -8.68E-06 | -4.50E-07 | 4.54E-08 | 1.09E-07 | -1.39E-06 |
| 8 | 4 | 1.68E-06 | -4.62E-06 | 1.24E-06 | 2.13E-06 | 5.48E-07 | -5.19E-09 | -7.14E-07 | -4.43E-07 |
| 8 | 5 | -9.41E-06 | 2.54E-05 | -1.47E-05 | -9.23E-06 | -7.37E-06 | -7.58E-07 | -5.99E-06 | -2.80E-05 |
| 8 | 6 | -5.16E-07 | -5.85E-08 | -2.26E-07 | 1.96E-07 | -2.07E-08 | -7.87E-10 | 1.54E-09 | -8.08E-09 |
| 8 | 7 | 7.01E-07 | 8.53E-07 | 4.98E-08 | -5.37E-07 | 8.09E-07 | -1.94E-09 | 6.55E-08 | -1.34E-07 |
| 8 | 8 | 6.84E-08 | 2.22E-08 | 2.16E-08 | -2.56E-08 | -4.08E-07 | 1.63E-10 | -1.74E-08 | -8.21E-09 |
| 10 | -10 | 8.80E-09 | -1.52E-08 | -1.28E-08 | -2.60E-09 | 1.40E-08 | 1.85E-11 | -1.37E-08 | -1.58E-08 |
| 10 | -9 | 2.77E-08 | 1.31E-08 | 1.23E-08 | -1.58E-08 | -3.98E-09 | -5.35E-11 | -1.45E-09 | 8.04E-09 |
| 10 | -8 | -3.05E-08 | 7.62E-09 | 1.02E-08 | 1.68E-08 | 1.03E-08 | 1.18E-12 | -8.78E-10 | 8.03E-10 |
| 10 | -7 | -6.14E-08 | -1.28E-07 | 1.83E-07 | 5.21E-08 | 3.23E-08 | 5.20E-12 | -6.28E-09 | 3.99E-10 |
| 10 | -6 | -1.05E-08 | 2.14E-09 | 6.30E-09 | 2.64E-09 | 2.69E-08 | -1.70E-11 | -1.52E-08 | -4.17E-09 |
| 10 | -5 | 1.48E-08 | -4.66E-08 | 2.61E-07 | -3.82E-08 | 7.92E-08 | 7.96E-11 | 5.11E-07 | 1.10E-07 |
| 10 | -4 | 1.61E-07 | 1.34E-07 | -4.95E-08 | 1.08E-07 | -5.40E-08 | 2.97E-11 | 1.22E-07 | 3.35E-08 |
| 10 | -3 | 2.70E-07 | -1.61E-07 | 1.47E-07 | -6.18E-09 | -1.19E-08 | -5.06E-11 | -1.96E-08 | 5.20E-09 |
| 10 | -2 | 4.06E-08 | 1.57E-08 | -2.28E-08 | -5.60E-08 | -1.22E-08 | -9.82E-12 | -1.15E-09 | 1.75E-10 |
| 10 | -1 | 8.21E-08 | -1.18E-08 | -5.76E-09 | 9.91E-08 | -2.69E-08 | -5.52E-11 | 1.97E-08 | 1.01E-09 |
| 10 | 0 | 1.67E-08 | 2.88E-09 | 3.45E-08 | 7.23E-09 | -6.15E-09 | 1.87E-11 | 3.37E-08 | 3.28E-08 |
| 10 | 1 | 1.28E-07 | -1.40E-09 | 2.82E-09 | -5.48E-08 | -7.86E-08 | -8.72E-12 | -3.75E-08 | -4.49E-08 |
| 10 | 2 | 3.36E-08 | 5.69E-08 | 3.98E-08 | -3.65E-08 | -1.72E-08 | 9.75E-12 | 1.13E-09 | 2.89E-10 |
| 10 | 3 | -1.03E-07 | 1.47E-08 | -1.43E-07 | 4.51E-07 | -6.57E-09 | -9.90E-11 | -3.07E-09 | -3.75E-08 |
| 10 | 4 | -3.98E-08 | 2.77E-07 | 7.96E-08 | -4.04E-08 | -4.92E-08 | 3.11E-12 | -8.19E-08 | -9.05E-08 |

SUPPORTING INFORMATION

| | | | | | | | | | |
|----|----|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 10 | 5 | -6.91E-08 | 5.31E-08 | -8.99E-08 | -5.16E-08 | 4.67E-08 | -2.39E-10 | -5.20E-08 | -2.69E-07 |
| 10 | 6 | -4.09E-08 | 3.17E-09 | -5.05E-09 | -1.68E-08 | 2.51E-09 | -8.86E-12 | -6.02E-09 | 9.56E-09 |
| 10 | 7 | -4.17E-08 | 2.30E-07 | 4.22E-08 | 1.24E-08 | -7.92E-09 | -7.00E-13 | 1.65E-09 | -2.48E-09 |
| 10 | 8 | 5.79E-10 | 8.67E-09 | 8.18E-10 | 1.61E-08 | -1.20E-08 | 7.40E-12 | -2.41E-09 | -1.34E-09 |
| 10 | 9 | -4.20E-08 | -3.28E-08 | -6.73E-09 | 2.65E-11 | -2.52E-08 | -2.83E-11 | -3.43E-09 | -6.95E-09 |
| 10 | 10 | -6.57E-09 | 1.40E-09 | -1.60E-08 | 3.43E-09 | -1.01E-08 | -2.51E-11 | -6.63E-08 | 1.60E-08 |

Table S18: Comparison of CASSCF computed SOC states and corresponding g-tensor values for the low-lying eight KDs for complexes **1-8** with a) 21 sextets and b) 21 sextet, 224 quartets and 490 doublets. All the energies are reported in cm^{-1} .

| a) 21 sextets | | | | b) 21 sextet, 224 quartet and 490 doublets | | | |
|---------------|--------|-------|--------|--|--------|-------|--------|
| 1 | | | | | | | |
| SOC states | gx | gy | gz | SOC states | gx | gy | gz |
| 0.0 | 0.000 | 0.000 | 19.980 | 0.0 | 0.000 | 0.000 | 19.893 |
| 487.4 | 0.000 | 0.000 | 17.014 | 484.8 | 0.000 | 0.000 | 16.988 |
| 785.0 | 0.009 | 0.010 | 14.326 | 778.5 | 0.009 | 0.010 | 14.299 |
| 999.4 | 0.096 | 0.105 | 11.598 | 995.1 | 0.098 | 0.107 | 11.585 |
| 1198.5 | 0.469 | 0.635 | 8.988 | 1194.3 | 0.498 | 0.665 | 8.976 |
| 1385.7 | 1.341 | 2.304 | 6.342 | 1377.6 | 1.509 | 2.504 | 6.314 |
| 1538.6 | 3.227 | 4.480 | 7.803 | 1524.2 | 3.183 | 4.617 | 8.205 |
| 1649.2 | 0.863 | 4.151 | 16.490 | 1631.6 | 0.822 | 3.778 | 16.690 |
| 2 | | | | | | | |
| 0.0 | 0.000 | 0.000 | 19.944 | 0.0 | 0.000 | 0.000 | 19.859 |
| 409.6 | 0.000 | 0.000 | 17.047 | 408.2 | 0.000 | 0.000 | 17.014 |
| 689.2 | 0.004 | 0.005 | 14.392 | 684.9 | 0.004 | 0.004 | 14.366 |
| 889.1 | 0.001 | 0.007 | 11.718 | 885.3 | 0.000 | 0.007 | 11.701 |
| 1062.4 | 0.035 | 0.037 | 9.043 | 1057.7 | 0.034 | 0.038 | 9.041 |
| 1208.9 | 0.969 | 1.336 | 6.263 | 1201.2 | 1.001 | 1.364 | 6.263 |
| 1305.0 | 8.519 | 8.157 | 2.690 | 1294.8 | 8.461 | 8.099 | 2.699 |
| 1423.5 | 0.297 | 0.954 | 17.841 | 1407.4 | 0.306 | 0.989 | 17.769 |
| 3 | | | | | | | |
| 0.0 | 0.000 | 0.000 | 19.986 | 0.0 | 0.000 | 0.000 | 19.900 |
| 541.7 | 0.000 | 0.000 | 16.963 | 539.7 | 0.000 | 0.000 | 16.946 |
| 845.2 | 0.005 | 0.006 | 14.370 | 837.3 | 0.005 | 0.006 | 14.346 |
| 1033.6 | 0.001 | 0.011 | 11.742 | 1029.6 | 0.001 | 0.010 | 11.718 |
| 1215.3 | 0.056 | 0.067 | 9.025 | 1213.0 | 0.055 | 0.066 | 9.025 |
| 1404.1 | 0.047 | 0.161 | 6.316 | 1398.2 | 0.051 | 0.162 | 6.340 |
| 1569.5 | 2.742 | 3.097 | 3.618 | 1556.3 | 2.672 | 3.024 | 3.650 |
| 1675.4 | 13.295 | 7.481 | 1.119 | 1655.2 | 13.197 | 7.523 | 1.136 |
| 4 | | | | | | | |

SUPPORTING INFORMATION

| | | | | | | | |
|----------|--------|-------|--------|--------|--------|-------|--------|
| 0.0 | 0.000 | 0.000 | 19.976 | 0.0 | 0.000 | 0.000 | 19.889 |
| 373.2 | 0.000 | 0.000 | 17.137 | 369.4 | 0.000 | 0.000 | 17.099 |
| 584.1 | 0.001 | 0.001 | 14.484 | 578.3 | 0.001 | 0.001 | 14.444 |
| 733.4 | 0.034 | 0.037 | 11.729 | 729.6 | 0.031 | 0.033 | 11.706 |
| 879.0 | 0.237 | 0.312 | 9.107 | 874.9 | 0.235 | 0.304 | 9.092 |
| 1016.5 | 1.289 | 1.955 | 6.472 | 1009.6 | 1.340 | 1.993 | 6.457 |
| 1124.8 | 3.309 | 3.384 | 7.521 | 1114.2 | 3.148 | 3.411 | 7.350 |
| 1200.5 | 0.922 | 4.677 | 15.285 | 1185.1 | 0.945 | 4.821 | 15.122 |
| 5 | | | | | | | |
| 0.0 | 0.194 | 0.315 | 9.745 | 0.0 | 0.168 | 0.304 | 9.733 |
| 14.9 | 0.015 | 0.122 | 12.038 | 13.4 | 0.023 | 0.125 | 12.009 |
| 29.8 | 0.110 | 0.361 | 6.676 | 31.0 | 0.093 | 0.350 | 6.629 |
| 73.7 | 1.680 | 1.940 | 3.861 | 75.4 | 1.641 | 1.904 | 3.857 |
| 97.9 | 1.806 | 2.985 | 11.261 | 95.3 | 0.746 | 1.433 | 12.962 |
| 108.4 | 4.750 | 6.936 | 9.358 | 109.0 | 10.831 | 7.987 | 2.980 |
| 272.3 | 0.000 | 0.000 | 17.424 | 265.8 | 0.000 | 0.001 | 17.332 |
| 489.7 | 0.000 | 0.000 | 19.991 | 484.7 | 0.000 | 0.000 | 19.900 |
| 6 | | | | | | | |
| 0.0 | 0.000 | 0.000 | 19.998 | 0.0 | 0.000 | 0.000 | 19.911 |
| 520.4 | 0.000 | 0.000 | 16.987 | 515.9 | 0.000 | 0.000 | 16.968 |
| 778.5 | 0.009 | 0.009 | 14.439 | 768.9 | 0.009 | 0.009 | 14.404 |
| 932.0 | 0.005 | 0.012 | 11.816 | 927.8 | 0.005 | 0.011 | 11.782 |
| 1096.5 | 0.006 | 0.013 | 9.058 | 1094.8 | 0.006 | 0.012 | 9.053 |
| 1284.8 | 0.208 | 0.221 | 6.301 | 1280.0 | 0.211 | 0.223 | 6.327 |
| 1461.9 | 0.857 | 1.298 | 3.660 | 1449.1 | 0.915 | 1.366 | 3.696 |
| 1573.7 | 11.607 | 9.451 | 1.188 | 1553.4 | 11.634 | 9.354 | 1.204 |
| 7 | | | | | | | |
| 0.0 | 0.000 | 0.000 | 19.996 | 0.0 | 0.000 | 0.000 | 19.909 |
| 452.3 | 0.000 | 0.000 | 17.040 | 446.6 | 0.000 | 0.000 | 17.012 |
| 650.6 | 0.033 | 0.034 | 14.500 | 641.7 | 0.031 | 0.031 | 14.454 |
| 760.6 | 0.028 | 0.035 | 11.882 | 756.4 | 0.025 | 0.033 | 11.838 |
| 887.4 | 0.033 | 0.041 | 9.124 | 885.1 | 0.033 | 0.040 | 9.110 |
| 1041.3 | 0.346 | 0.403 | 6.365 | 1036.0 | 0.355 | 0.412 | 6.382 |
| 1189.9 | 0.396 | 1.136 | 3.713 | 1177.9 | 0.431 | 1.191 | 3.741 |
| 1284.1 | 11.322 | 9.789 | 1.212 | 1266.1 | 11.329 | 9.707 | 1.226 |
| 8 | | | | | | | |

SUPPORTING INFORMATION

| | | | | | | | |
|--------|--------|-------|--------|--------|--------|-------|--------|
| 0.0 | 0.000 | 0.000 | 19.998 | 0.0 | 0.000 | 0.000 | 19.911 |
| 457.9 | 0.000 | 0.000 | 17.041 | 451.4 | 0.000 | 0.000 | 17.014 |
| 654.8 | 0.008 | 0.008 | 14.509 | 645.9 | 0.007 | 0.007 | 14.461 |
| 768.8 | 0.005 | 0.010 | 11.889 | 765.8 | 0.005 | 0.009 | 11.842 |
| 906.7 | 0.020 | 0.024 | 9.109 | 906.4 | 0.020 | 0.024 | 9.096 |
| 1076.4 | 0.251 | 0.287 | 6.334 | 1073.4 | 0.263 | 0.299 | 6.355 |
| 1241.5 | 0.374 | 0.910 | 3.686 | 1231.2 | 0.410 | 0.971 | 3.719 |
| 1347.0 | 11.189 | 9.907 | 1.201 | 1329.8 | 11.202 | 9.823 | 1.217 |

Table S19: DFT optimized coordinates of complexes 1-8.

| <i>Complex 1</i> | | | | <i>Complex 2</i> | | | |
|------------------|-----------------|-----------------|-----------------|------------------|-----------------|-----------------|-----------------|
| Dy | 0.000000000000 | 0.000000000000 | 0.000000000000 | Dy | 0.000000000000 | 0.000000000000 | 0.000000000000 |
| C | 0.631249000000 | -1.171237000000 | -2.264617000000 | C | -0.682416000000 | -1.098949000000 | -2.233554000000 |
| C | 1.859401000000 | -0.648065000000 | -1.751772000000 | C | -0.157339000000 | -2.168769000000 | -1.454978000000 |
| C | 1.774261000000 | 0.766969000000 | -1.771127000000 | C | 1.248006000000 | -1.938455000000 | -1.279810000000 |
| C | 0.494993000000 | 1.125825000000 | -2.296794000000 | C | 1.574566000000 | -0.723216000000 | -1.948067000000 |
| C | -0.201122000000 | -0.073492000000 | -2.611613000000 | C | 0.380036000000 | -0.201442000000 | -2.528903000000 |
| C | 0.471850000000 | -2.568643000000 | -2.818229000000 | C | -2.001619000000 | -1.123581000000 | -2.965794000000 |
| C | 3.152247000000 | -1.422207000000 | -1.673853000000 | C | -0.826762000000 | -3.521781000000 | -1.338592000000 |
| C | 2.963824000000 | 1.693404000000 | -1.713333000000 | C | 2.254432000000 | -3.033796000000 | -0.987247000000 |
| C | 0.167448000000 | 2.480909000000 | -2.879964000000 | C | 2.964127000000 | -0.331640000000 | -2.396433000000 |
| C | -1.372982000000 | -0.155102000000 | -3.562211000000 | C | 0.336351000000 | 0.843492000000 | -3.617366000000 |
| C | 1.877450000000 | -3.021305000000 | -3.281730000000 | C | -2.273864000000 | -2.608431000000 | -3.299542000000 |
| C | 3.071462000000 | -2.510729000000 | -2.773063000000 | C | -1.744014000000 | -3.672532000000 | -2.578455000000 |
| C | 4.251210000000 | -0.495268000000 | -2.249060000000 | C | 0.264732000000 | -4.572995000000 | -1.652025000000 |
| C | 4.167673000000 | 0.892976000000 | -2.265871000000 | C | 1.628870000000 | -4.353152000000 | -1.501262000000 |
| C | 2.754909000000 | 2.739749000000 | -2.836399000000 | C | 3.415320000000 | -2.852490000000 | -1.995811000000 |
| C | 1.508411000000 | 3.090610000000 | -3.355436000000 | C | 3.736777000000 | -1.654036000000 | -2.616053000000 |
| C | -0.542160000000 | 2.212953000000 | -4.230619000000 | C | 2.829761000000 | 0.175873000000 | -3.853639000000 |
| C | -1.230930000000 | 1.041325000000 | -4.533260000000 | C | 1.665031000000 | 0.706518000000 | -4.396148000000 |
| C | -1.085883000000 | -1.347556000000 | -4.504758000000 | C | -0.684162000000 | 0.335566000000 | -4.698607000000 |
| C | -0.262171000000 | -2.420837000000 | -4.174727000000 | C | -1.726182000000 | -0.540203000000 | -4.373364000000 |
| C | 1.812755000000 | -3.435914000000 | -4.661457000000 | C | -2.492007000000 | -2.745385000000 | -4.719609000000 |
| C | 4.224742000000 | -2.408748000000 | -3.631317000000 | C | -1.426243000000 | -4.903803000000 | -3.261930000000 |
| C | 4.944812000000 | -1.180627000000 | -3.313561000000 | C | -0.200283000000 | -5.449844000000 | -2.698607000000 |
| C | 4.774583000000 | 1.631090000000 | -3.348001000000 | C | 2.561793000000 | -5.016391000000 | -2.385297000000 |
| C | 3.913131000000 | 2.756922000000 | -3.693764000000 | C | 3.648391000000 | -4.099275000000 | -2.689303000000 |
| C | 1.395936000000 | 3.459254000000 | -4.744995000000 | C | 4.293117000000 | -1.670311000000 | -3.950933000000 |
| C | 0.144575000000 | 2.928469000000 | -5.278111000000 | C | 3.743536000000 | -0.554257000000 | -4.703403000000 |
| C | -1.244405000000 | 0.556414000000 | -5.893010000000 | C | 1.377907000000 | 0.510650000000 | -5.796424000000 |
| C | -1.155534000000 | -0.899965000000 | -5.875246000000 | C | -0.051755000000 | 0.288064000000 | -5.961057000000 |
| C | 0.507213000000 | -3.072641000000 | -5.205734000000 | C | -2.157845000000 | -1.486762000000 | -5.372428000000 |
| C | 2.952208000000 | -3.403799000000 | -5.492886000000 | C | -2.247293000000 | -3.967053000000 | -5.384281000000 |
| C | 4.194034000000 | -2.878591000000 | -4.963579000000 | C | -1.701653000000 | -5.073730000000 | -4.635970000000 |
| C | 5.604454000000 | -0.466471000000 | -4.336194000000 | C | 0.704500000000 | -6.153571000000 | -3.526945000000 |
| C | 5.516565000000 | 0.977259000000 | -4.354040000000 | C | 2.122644000000 | -5.932769000000 | -3.363659000000 |
| C | 3.827342000000 | 3.186337000000 | -5.037520000000 | C | 4.262448000000 | -4.130971000000 | -3.961899000000 |
| C | 2.531924000000 | 3.546549000000 | -5.577367000000 | C | 4.593836000000 | -2.882672000000 | -4.669727000000 |
| C | 0.078970000000 | 2.502849000000 | -6.622266000000 | C | 3.511382000000 | -0.686693000000 | -6.089159000000 |
| C | -0.635817000000 | 1.284010000000 | -6.937202000000 | C | 2.296297000000 | -0.142768000000 | -6.650334000000 |
| C | -0.462153000000 | -1.573042000000 | -6.902914000000 | C | -0.513254000000 | -0.584463000000 | -6.969633000000 |
| C | 0.393201000000 | -2.690084000000 | -6.560270000000 | C | -1.591148000000 | -1.495896000000 | -6.667465000000 |
| C | 2.835926000000 | -2.990603000000 | -6.886507000000 | C | -1.643839000000 | -3.974654000000 | -6.715650000000 |
| C | 4.853636000000 | -2.125834000000 | -6.021855000000 | C | -0.752555000000 | -5.779465000000 | -5.494838000000 |
| C | 5.547988000000 | -0.940053000000 | -5.717349000000 | C | 0.426798000000 | -6.313915000000 | -4.949753000000 |
| C | 5.405977000000 | 1.407315000000 | -5.746142000000 | C | 2.739211000000 | -5.947309000000 | -4.686768000000 |
| C | 4.574901000000 | 2.494650000000 | -6.078275000000 | C | 3.791993000000 | -5.063095000000 | -4.980248000000 |
| C | 2.467952000000 | 3.087945000000 | -6.959600000000 | C | 4.330252000000 | -3.027227000000 | -6.037648000000 |
| C | 1.259758000000 | 2.573066000000 | -7.475086000000 | C | 3.798312000000 | -1.948727000000 | -6.764489000000 |

SUPPORTING INFORMATION

| | | | | | | | |
|---|-----------------|-----------------|-----------------|---|-----------------|-----------------|-----------------|
| C | 3.273777000000 | -2.899393000000 | -4.232819000000 | C | 3.721681000000 | 2.005078000000 | -2.389261000000 |
| C | 4.747313000000 | -0.532386000000 | -3.832740000000 | C | 1.782865000000 | 3.049693000000 | -3.294083000000 |
| C | 4.667075000000 | 0.923380000000 | -3.851006000000 | C | 0.544410000000 | 2.806045000000 | -3.866721000000 |
| C | 2.946072000000 | 3.107273000000 | -4.303272000000 | C | -0.960741000000 | 1.079076000000 | -4.540786000000 |
| C | 1.582985000000 | 3.479878000000 | -4.666480000000 | C | -1.138556000000 | -0.297416000000 | -4.603542000000 |
| C | -0.954863000000 | 2.463124000000 | -5.351452000000 | C | -0.120234000000 | -2.398666000000 | -4.107032000000 |
| C | -1.720021000000 | 1.238134000000 | -5.560361000000 | C | 1.011783000000 | -2.999593000000 | -3.574910000000 |
| C | -1.567800000000 | -1.577048000000 | -5.527410000000 | C | 3.140165000000 | -2.576243000000 | -2.598928000000 |
| C | 0.217640000000 | -3.120122000000 | -6.302945000000 | C | 4.011460000000 | -1.574233000000 | -2.209561000000 |
| C | 1.569602000000 | -3.489463000000 | -5.940655000000 | C | 5.281820000000 | 0.230478000000 | -3.021541000000 |
| C | 4.148060000000 | -2.456320000000 | -5.247061000000 | C | 4.088808000000 | 2.700239000000 | -3.604456000000 |
| C | 4.906711000000 | -1.241041000000 | -5.040926000000 | C | 2.912892000000 | 3.332857000000 | -4.154495000000 |
| C | 4.751056000000 | 1.617768000000 | -5.074781000000 | C | 0.406911000000 | 2.835037000000 | -5.307726000000 |
| C | 3.865830000000 | 2.739252000000 | -5.307563000000 | C | -0.506283000000 | 1.791734000000 | -5.715701000000 |
| C | 1.190311000000 | 3.469128000000 | -6.021066000000 | C | -0.860763000000 | -0.989913000000 | -5.842622000000 |
| C | -0.113238000000 | 2.948674000000 | -6.373331000000 | C | -0.243694000000 | -2.261922000000 | -5.541780000000 |
| C | -1.610894000000 | 0.542702000000 | -6.782286000000 | C | 2.042443000000 | -3.484187000000 | -4.471193000000 |
| C | -1.531634000000 | -0.901755000000 | -6.764751000000 | C | 3.333315000000 | -3.225240000000 | -3.879697000000 |
| C | 0.266183000000 | -2.408178000000 | -7.574823000000 | C | 5.100152000000 | -1.200225000000 | -3.878113000000 |
| C | 2.466475000000 | -3.009243000000 | -6.985204000000 | C | 5.704870000000 | 0.940385000000 | -4.175169000000 |
| C | 3.733001000000 | -2.501096000000 | -6.644295000000 | C | 5.094722000000 | 2.203679000000 | -4.473442000000 |
| C | 4.967979000000 | -0.522367000000 | -6.309875000000 | C | 2.771276000000 | 3.446757000000 | -5.562213000000 |
| C | 4.891955000000 | 0.881159000000 | -6.326756000000 | C | 1.490198000000 | 3.191072000000 | -6.152064000000 |
| C | 3.449299000000 | 2.705926000000 | -6.704748000000 | C | -0.309247000000 | 1.131133000000 | -6.956334000000 |
| C | 2.135324000000 | 3.066217000000 | -7.055846000000 | C | -0.490646000000 | -0.290172000000 | -7.021032000000 |
| C | 0.013525000000 | 2.216988000000 | -7.629360000000 | C | 0.724253000000 | -2.802059000000 | -6.428331000000 |
| C | -0.720799000000 | 1.034849000000 | -7.829032000000 | C | 1.892874000000 | -3.427732000000 | -5.881113000000 |
| C | -0.591840000000 | -1.317567000000 | -7.800412000000 | C | 4.441891000000 | -2.921606000000 | -4.711460000000 |
| C | 1.659673000000 | -2.339286000000 | -7.997717000000 | C | 5.347069000000 | -1.885679000000 | -4.306029000000 |
| C | 4.241170000000 | -1.303778000000 | -7.303268000000 | C | 5.945431000000 | 0.238365000000 | -5.435301000000 |
| C | 4.085037000000 | 1.556033000000 | -7.336348000000 | C | 4.945762000000 | 2.310659000000 | -5.924377000000 |
| C | 1.407227000000 | 2.290063000000 | -8.052261000000 | C | 3.801860000000 | 2.919008000000 | -6.459711000000 |
| C | -0.090495000000 | -0.118272000000 | -8.460146000000 | C | 1.699674000000 | 2.502181000000 | -7.427276000000 |
| C | 2.147228000000 | -1.179574000000 | -8.632566000000 | C | 0.814985000000 | 1.490364000000 | -7.822741000000 |
| C | 3.460836000000 | -0.652710000000 | -8.279276000000 | C | 0.517921000000 | -0.839734000000 | -7.927027000000 |
| C | 3.381404000000 | 0.801822000000 | -8.296268000000 | C | 1.115106000000 | -2.075261000000 | -7.635274000000 |
| C | 2.018921000000 | 1.175201000000 | -8.660888000000 | C | 3.032589000000 | -3.101416000000 | -6.740536000000 |
| C | 1.256431000000 | -0.049621000000 | -8.868833000000 | C | 4.284790000000 | -2.851677000000 | -6.165205000000 |
| C | -2.162343000000 | -2.292091000000 | -2.159105000000 | C | 5.767838000000 | -1.151544000000 | -5.500187000000 |
| C | 1.827265000000 | -3.423219000000 | -1.116990000000 | C | 5.472062000000 | 1.089226000000 | -6.519096000000 |
| C | 4.139665000000 | 0.215568000000 | -0.525906000000 | C | 3.134735000000 | 2.334395000000 | -7.615291000000 |
| C | 1.459758000000 | 3.539926000000 | -1.194567000000 | C | 1.326818000000 | 0.265353000000 | -8.422118000000 |
| C | -2.400529000000 | 1.958081000000 | -2.214561000000 | C | 2.547195000000 | -2.261075000000 | -7.827416000000 |
| C | -0.372890000000 | -1.163072000000 | 2.248895000000 | C | 5.107268000000 | -1.751777000000 | -6.651431000000 |
| C | 0.996755000000 | -0.708099000000 | 2.311050000000 | C | 4.824018000000 | 0.513939000000 | -7.630431000000 |
| C | 0.987483000000 | 0.724428000000 | 2.312083000000 | C | 3.634789000000 | 1.148366000000 | -8.189395000000 |
| C | -0.387136000000 | 1.156648000000 | 2.248046000000 | C | 2.714668000000 | 0.095131000000 | -8.598097000000 |
| C | -1.224212000000 | -0.009905000000 | 2.222744000000 | C | 3.336165000000 | -1.190888000000 | -8.294902000000 |
| H | -1.651609000000 | -2.897332000000 | -1.386350000000 | C | 4.638823000000 | -0.932412000000 | -7.697605000000 |
| H | -2.870121000000 | -2.953681000000 | -2.687046000000 | C | 4.137685000000 | -0.503982000000 | 0.124617000000 |
| H | -2.754057000000 | -1.495933000000 | -1.667505000000 | C | 2.226033000000 | 3.343778000000 | -0.756951000000 |
| H | 2.420144000000 | -2.970269000000 | -0.302589000000 | C | -1.642738000000 | 2.527945000000 | -2.492944000000 |
| H | 2.281801000000 | -4.394736000000 | -1.375610000000 | C | -2.187189000000 | -1.717205000000 | -2.690194000000 |
| H | 0.802152000000 | -3.616055000000 | -0.748630000000 | C | 1.336806000000 | -3.644180000000 | -1.086501000000 |
| H | 3.900521000000 | -0.678376000000 | 0.075980000000 | H | 3.897322000000 | 0.403522000000 | 0.702584000000 |
| H | 3.817610000000 | 1.115941000000 | 0.025943000000 | H | 5.231741000000 | -0.641860000000 | 0.139332000000 |
| H | 5.234354000000 | 0.263536000000 | -0.654081000000 | H | 3.674683000000 | -1.378632000000 | 0.611895000000 |
| H | 2.117370000000 | 3.176884000000 | -0.384252000000 | H | 1.181786000000 | 3.634851000000 | -0.548350000000 |
| H | 0.426988000000 | 3.621240000000 | -0.808324000000 | H | 2.811857000000 | 4.261597000000 | -0.934680000000 |
| H | 1.795383000000 | 4.551262000000 | -1.480881000000 | H | 2.637975000000 | 2.839242000000 | 0.134328000000 |
| H | -2.909763000000 | 1.111886000000 | -1.713944000000 | H | -1.239380000000 | 3.065511000000 | -1.614994000000 |
| H | -3.168304000000 | 2.529713000000 | -2.763196000000 | H | -2.384987000000 | 1.781629000000 | -2.154032000000 |
| H | -1.967437000000 | 2.628524000000 | -1.448538000000 | H | -2.173838000000 | 3.260877000000 | -3.123021000000 |
| C | 2.181537000000 | 1.619627000000 | 2.498992000000 | H | -2.728485000000 | -0.847183000000 | -2.273050000000 |
| C | 2.292993000000 | 1.900989000000 | 3.563831000000 | H | -1.937655000000 | -2.419111000000 | -1.873397000000 |
| H | 3.118442000000 | 1.124090000000 | 2.196031000000 | H | -2.875125000000 | -2.235690000000 | -3.379415000000 |
| H | 2.096726000000 | 2.560973000000 | 1.928679000000 | H | 1.844259000000 | -3.341025000000 | -0.153836000000 |
| C | 2.197178000000 | -1.592716000000 | 2.504005000000 | H | 1.684757000000 | -4.655874000000 | -1.356170000000 |
| H | 2.382678000000 | -1.761711000000 | 3.582330000000 | H | 0.249551000000 | -3.690384000000 | -0.900072000000 |
| H | 2.060077000000 | -2.587508000000 | 2.046759000000 | H | -2.282849000000 | -1.044748000000 | 2.357109000000 |

SUPPORTING INFORMATION

| | | | | | | |
|------------------|-----------------|-----------------|-----------------|------------------|-----------------|-----------------|
| H | 3.116121000000 | -1.149230000000 | 2.086949000000 | | | |
| C | -0.870569000000 | 2.582048000000 | 2.237138000000 | | | |
| H | -1.689733000000 | 2.752707000000 | 1.511309000000 | | | |
| H | -1.275783000000 | 2.868692000000 | 3.226982000000 | | | |
| H | -0.060124000000 | 3.292491000000 | 2.003415000000 | | | |
| C | -2.728576000000 | -0.008060000000 | 2.148228000000 | | | |
| H | -3.130142000000 | -0.946086000000 | 1.725209000000 | | | |
| H | -3.176101000000 | 0.100185000000 | 3.154923000000 | | | |
| H | -3.123358000000 | 0.831786000000 | 1.545817000000 | | | |
| C | -0.814473000000 | -2.602154000000 | 2.245308000000 | | | |
| H | -0.093108000000 | -3.258522000000 | 1.724706000000 | | | |
| H | -0.905315000000 | -2.991599000000 | 3.278391000000 | | | |
| H | -1.802969000000 | -2.737934000000 | 1.770829000000 | | | |
| <i>Complex 5</i> | | | | <i>Complex 6</i> | | |
| Dy | 0.000000000000 | 0.000000000000 | 0.000000000000 | Dy | 0.000000000000 | 0.000000000000 |
| C | 1.081411000000 | -0.594057000000 | -2.325301000000 | C | 1.051780000000 | 0.606196000000 |
| C | 0.917539000000 | 0.820408000000 | -2.328089000000 | C | -0.256812000000 | 1.189150000000 |
| C | -0.478478000000 | 1.100532000000 | -2.338155000000 | C | -1.209468000000 | 0.129348000000 |
| C | -1.176397000000 | -0.139760000000 | -2.339298000000 | C | -0.490115000000 | -1.111132000000 |
| C | -0.212487000000 | -1.187123000000 | -2.332093000000 | C | 0.904615000000 | -0.813561000000 |
| C | 2.344680000000 | -1.304675000000 | -2.751667000000 | C | 2.314171000000 | 1.322160000000 |
| C | 1.982586000000 | 1.801234000000 | -2.759317000000 | C | -0.544148000000 | 2.595354000000 |
| C | -1.080758000000 | 2.415751000000 | -2.772740000000 | C | -2.632919000000 | 0.270504000000 |
| C | -2.613747000000 | -0.308320000000 | -2.771887000000 | C | -1.064097000000 | -2.437880000000 |
| C | -0.496099000000 | -2.607572000000 | -2.759750000000 | C | 1.989921000000 | -1.784787000000 |
| C | 3.080611000000 | -0.346786000000 | -3.720131000000 | C | 1.882388000000 | 2.423085000000 |
| C | 2.919439000000 | 1.035111000000 | -3.723949000000 | C | 0.612608000000 | 2.986597000000 |
| C | 1.300409000000 | 2.792339000000 | -3.733132000000 | C | -1.720955000000 | 2.494058000000 |
| C | -0.063108000000 | 3.065647000000 | -3.739297000000 | C | -2.648668000000 | 1.462540000000 |
| C | -2.235694000000 | 2.069920000000 | -3.743917000000 | C | -2.886857000000 | -0.910415000000 |
| C | -2.917379000000 | 0.857019000000 | -3.744180000000 | C | -2.194463000000 | -2.114666000000 |
| C | -2.640318000000 | -1.517470000000 | -3.737460000000 | C | -0.016877000000 | -3.085721000000 |
| C | -1.697810000000 | -2.540726000000 | -3.732267000000 | C | 1.340532000000 | -2.796883000000 |
| C | 0.645671000000 | -3.010846000000 | -3.723683000000 | C | 2.935076000000 | -1.021745000000 |
| C | 1.909649000000 | -2.429905000000 | -3.720447000000 | C | 3.078801000000 | 0.359106000000 |
| C | 3.353521000000 | -1.034479000000 | -4.959542000000 | C | 2.644513000000 | 2.294768000000 |
| C | 3.027368000000 | 1.760574000000 | -4.966963000000 | C | 0.070274000000 | 3.438150000000 |
| C | 2.039185000000 | 2.833220000000 | -4.972666000000 | C | -1.355226000000 | 3.136637000000 |
| C | -0.719988000000 | 3.387902000000 | -4.983633000000 | C | -3.236649000000 | 1.042620000000 |
| C | -2.045455000000 | 2.778941000000 | -4.986755000000 | C | -3.384149000000 | -0.407198000000 |
| C | -3.425458000000 | 0.325439000000 | -4.986208000000 | C | -1.975227000000 | -2.845283000000 |
| C | -3.256077000000 | -1.123464000000 | -4.981854000000 | C | -0.643981000000 | -3.438806000000 |
| C | -1.349306000000 | -3.194469000000 | -4.971051000000 | C | 2.109158000000 | -2.852207000000 |
| C | 0.081144000000 | -3.481719000000 | -4.965799000000 | C | 3.084041000000 | -1.768791000000 |
| C | 2.638879000000 | -2.306192000000 | -4.959510000000 | C | 3.374481000000 | 1.032710000000 |
| C | 3.532240000000 | -0.328757000000 | -6.168121000000 | C | 2.151191000000 | 2.788259000000 |
| C | 3.364053000000 | 1.108270000000 | -6.171974000000 | C | 0.828985000000 | 3.377179000000 |
| C | 1.423197000000 | 3.215838000000 | -6.183322000000 | C | -1.970779000000 | 2.781165000000 |
| C | 0.004539000000 | 3.501325000000 | -6.189138000000 | C | -2.938799000000 | 1.705202000000 |
| C | -2.598868000000 | 2.304914000000 | -6.195319000000 | C | -3.233741000000 | -1.143034000000 |
| C | -3.307469000000 | 1.043466000000 | -6.194988000000 | C | -2.508957000000 | -2.396265000000 |
| C | -2.975417000000 | -1.801513000000 | -6.186906000000 | C | 0.107514000000 | -3.559598000000 |
| C | -1.995680000000 | -2.866159000000 | -6.181699000000 | C | 1.523004000000 | -3.259800000000 |
| C | 0.812967000000 | -3.429812000000 | -6.171093000000 | C | 3.436199000000 | -1.129650000000 |
| C | 2.127986000000 | -2.826157000000 | -6.167839000000 | C | 3.584131000000 | 0.309958000000 |
| C | 2.978911000000 | -0.854552000000 | -7.412266000000 | C | 2.347778000000 | 2.027583000000 |
| C | 2.705847000000 | 1.486818000000 | -7.418166000000 | C | 0.195735000000 | 2.985573000000 |
| C | 1.752833000000 | 2.520757000000 | -7.423552000000 | C | -1.178969000000 | 2.691874000000 |
| C | -0.558058000000 | 2.985333000000 | -7.433409000000 | C | -2.754316000000 | 0.939397000000 |
| C | -1.835851000000 | 2.397637000000 | -7.436009000000 | C | -2.901134000000 | -0.459343000000 |
| C | -2.990926000000 | 0.343159000000 | -7.435424000000 | C | -1.719975000000 | -2.498495000000 |
| C | -2.827385000000 | -1.053453000000 | -7.431024000000 | C | -0.434326000000 | -3.070112000000 |
| C | -1.231458000000 | -2.787624000000 | -7.423119000000 | C | 1.870630000000 | -2.581431000000 |
| C | 0.147217000000 | -3.063277000000 | -7.417089000000 | C | 2.810046000000 | -1.535549000000 |
| C | 2.289592000000 | -2.080342000000 | -7.411985000000 | C | 3.050969000000 | 0.808916000000 |
| C | 2.466795000000 | 0.270450000000 | -8.186484000000 | C | 1.136490000000 | 2.148750000000 |
| C | 0.525402000000 | 2.377608000000 | -8.198021000000 | C | -1.665045000000 | 1.551253000000 |

SUPPORTING INFORMATION

| | | | | | | | |
|---|-----------------|-----------------|-----------------|---|-----------------|-----------------|-----------------|
| C | -2.078847000000 | 1.182317000000 | -8.204521000000 | C | -1.962377000000 | -1.299120000000 | -8.270434000000 |
| C | -1.747169000000 | -1.664293000000 | -8.197370000000 | C | 0.657377000000 | -2.464437000000 | -8.192345000000 |
| C | 1.061754000000 | -2.226649000000 | -8.185140000000 | C | 2.571780000000 | -0.333220000000 | -8.171600000000 |
| C | 1.280282000000 | 0.129988000000 | -8.935301000000 | C | 0.668368000000 | 1.044313000000 | -8.978693000000 |
| C | 0.292308000000 | 1.202157000000 | -8.940378000000 | C | -0.756883000000 | 0.740703000000 | -9.011477000000 |
| C | -1.032955000000 | 0.594159000000 | -8.944400000000 | C | -0.907165000000 | -0.708962000000 | -8.993915000000 |
| C | -0.864301000000 | -0.854632000000 | -8.941097000000 | C | 0.425475000000 | -1.302003000000 | -8.955678000000 |
| C | 0.565353000000 | -1.141130000000 | -8.934953000000 | C | 1.399053000000 | -0.218475000000 | -8.944836000000 |
| C | 3.227979000000 | -1.800969000000 | -1.585468000000 | C | 3.181171000000 | 1.855912000000 | -1.610230000000 |
| C | 2.722418000000 | 2.495645000000 | -1.594326000000 | C | -0.785406000000 | 3.636624000000 | -1.740813000000 |
| C | -1.506264000000 | 3.340413000000 | -1.611538000000 | C | -3.708641000000 | 0.380214000000 | -1.774441000000 |
| C | -3.624915000000 | -0.419016000000 | -1.609945000000 | C | -1.516254000000 | -3.370755000000 | -1.659418000000 |
| C | -0.694194000000 | -3.601588000000 | -1.594413000000 | C | 2.725685000000 | -2.457640000000 | -1.560752000000 |
| H | 3.532596000000 | -0.949081000000 | -0.952877000000 | H | 2.615312000000 | 2.593153000000 | -1.014422000000 |
| H | 4.135546000000 | -2.303569000000 | -1.962383000000 | H | 4.088568000000 | 2.353923000000 | -1.992229000000 |
| H | 2.664256000000 | -2.512566000000 | -0.957875000000 | H | 3.500965000000 | 1.026141000000 | -0.953902000000 |
| H | 1.999493000000 | 3.033071000000 | -0.955115000000 | H | -1.663480000000 | 3.356249000000 | -1.132435000000 |
| H | 3.466526000000 | 3.218335000000 | -1.972388000000 | H | -0.975024000000 | 4.634715000000 | -2.171624000000 |
| H | 3.244930000000 | 1.746767000000 | -0.973192000000 | H | 0.099482000000 | 3.713671000000 | -1.084413000000 |
| H | -0.634288000000 | 3.583587000000 | -0.978268000000 | H | -3.536847000000 | 1.273195000000 | -1.148565000000 |
| H | -2.259275000000 | 2.836088000000 | -0.980875000000 | H | -3.695155000000 | -0.520329000000 | -1.134532000000 |
| H | -1.938555000000 | 4.282157000000 | -1.992190000000 | H | -4.715489000000 | 0.465286000000 | -2.217950000000 |
| H | -3.597515000000 | 0.498395000000 | -0.995541000000 | H | -2.325596000000 | -2.899019000000 | -1.075125000000 |
| H | -3.370789000000 | -1.276600000000 | -0.962771000000 | H | -0.667943000000 | -3.596175000000 | -0.988726000000 |
| H | -4.651671000000 | -0.556472000000 | -1.991091000000 | H | -1.897244000000 | -4.326516000000 | -2.057921000000 |
| H | 0.211856000000 | -3.629275000000 | -0.963480000000 | H | 3.210048000000 | -1.695141000000 | -0.925450000000 |
| H | -0.892330000000 | -4.620888000000 | -1.970186000000 | H | 3.507144000000 | -3.147765000000 | -1.922032000000 |
| H | -1.544604000000 | -3.287872000000 | -0.963504000000 | H | 2.014893000000 | -3.039909000000 | -0.948592000000 |
| C | -0.054384000000 | -1.860186000000 | 1.739905000000 | C | 1.196178000000 | -0.128984000000 | 2.377163000000 |
| H | -0.087588000000 | -2.952619000000 | 1.643056000000 | C | 0.244254000000 | -1.188973000000 | 2.367308000000 |
| C | 1.276333000000 | -1.355169000000 | 1.738336000000 | C | -1.064624000000 | -0.606638000000 | 2.334159000000 |
| H | 2.027523000000 | -2.150031000000 | 1.642617000000 | C | -0.917925000000 | 0.813342000000 | 2.324278000000 |
| C | 1.858998000000 | -0.053997000000 | 1.746613000000 | C | 0.476897000000 | 1.111253000000 | 2.349656000000 |
| H | 2.952658000000 | -0.085624000000 | 1.656979000000 | C | 2.619609000000 | -0.269621000000 | 2.878414000000 |
| C | 1.354243000000 | 1.276425000000 | 1.748899000000 | C | 0.532014000000 | -2.595181000000 | 2.854744000000 |
| H | 2.150331000000 | 2.026232000000 | 1.656763000000 | C | -2.326908000000 | -1.323154000000 | 2.766285000000 |
| C | 0.054624000000 | 1.860006000000 | 1.739439000000 | C | -2.003604000000 | 1.784265000000 | 2.736260000000 |
| H | 0.087271000000 | 2.952777000000 | 1.641755000000 | C | 1.050342000000 | 2.438107000000 | 2.803417000000 |
| C | -1.276402000000 | 1.354519000000 | 1.739477000000 | C | 2.635401000000 | -1.461798000000 | 3.864779000000 |
| H | -2.027363000000 | 2.149552000000 | 1.644176000000 | C | 1.707834000000 | -2.493599000000 | 3.855093000000 |
| C | -1.858942000000 | 0.054417000000 | 1.748629000000 | C | -0.625569000000 | -2.986995000000 | 3.802882000000 |
| H | -2.951527000000 | 0.086899000000 | 1.653455000000 | C | -1.895333000000 | -2.423531000000 | 3.762928000000 |
| C | -1.354470000000 | -1.276015000000 | 1.745666000000 | C | -3.092439000000 | -0.360171000000 | 3.703889000000 |
| H | -2.151026000000 | -2.026754000000 | 1.656158000000 | C | -2.949010000000 | 1.020635000000 | 3.690681000000 |
| | | | | C | -1.355173000000 | 2.796128000000 | 3.708402000000 |
| | | | | C | 0.001986000000 | 3.085724000000 | 3.738441000000 |
| | | | | C | 2.179833000000 | 2.115387000000 | 3.808477000000 |
| | | | | C | 2.872864000000 | 0.911472000000 | 3.843885000000 |
| | | | | C | 3.221768000000 | -1.041584000000 | 5.116295000000 |
| | | | | C | 1.340980000000 | -3.136269000000 | 5.095690000000 |
| | | | | C | -0.084454000000 | -3.438193000000 | 5.062985000000 |
| | | | | C | -2.658957000000 | -2.295629000000 | 4.980557000000 |
| | | | | C | -3.389177000000 | -1.033782000000 | 4.945219000000 |
| | | | | C | -3.099688000000 | 1.767713000000 | 4.917482000000 |
| | | | | C | -2.125200000000 | 2.851373000000 | 4.928461000000 |
| | | | | C | 0.627599000000 | 3.438969000000 | 4.990258000000 |
| | | | | C | 1.959071000000 | 2.846059000000 | 5.032478000000 |
| | | | | C | 3.368716000000 | 0.408361000000 | 5.101865000000 |
| | | | | C | 2.922673000000 | -1.704177000000 | 6.324259000000 |
| | | | | C | 1.955019000000 | -2.780414000000 | 6.313685000000 |
| | | | | C | -0.844504000000 | -3.377326000000 | 6.248931000000 |
| | | | | C | -2.166906000000 | -2.788968000000 | 6.206875000000 |
| | | | | C | -3.600473000000 | -0.311085000000 | 6.137092000000 |
| | | | | C | -3.453104000000 | 1.128612000000 | 6.123257000000 |
| | | | | C | -1.540643000000 | 3.259343000000 | 6.144632000000 |
| | | | | C | -0.125250000000 | 3.559558000000 | 6.176287000000 |
| | | | | C | 2.491589000000 | 2.397271000000 | 6.259062000000 |
| | | | | C | 3.216594000000 | 1.144208000000 | 6.294509000000 |
| | | | | C | 2.736464000000 | -0.938323000000 | 7.552603000000 |
| | | | | C | 1.161768000000 | -2.691307000000 | 7.535362000000 |

SUPPORTING INFORMATION

| | | | | | | | |
|---|-----------------|-----------------|-----------------|---|-----------------|-----------------|-----------------|
| C | -1.410871000000 | -3.210600000000 | 5.278915000000 | C | 2.988097000000 | 1.663575000000 | -5.038105000000 |
| C | -2.599683000000 | -2.333321000000 | 5.292715000000 | C | 2.013414000000 | 2.739708000000 | -5.057995000000 |
| C | -3.467547000000 | 0.392785000000 | 5.299913000000 | C | -0.748110000000 | 3.316726000000 | -5.058387000000 |
| C | -2.545625000000 | 2.379186000000 | 6.488213000000 | C | -2.654016000000 | 2.225427000000 | -6.233092000000 |
| C | -1.359953000000 | 3.230845000000 | 6.471896000000 | C | -3.374445000000 | 0.975427000000 | -6.200848000000 |
| C | 1.500045000000 | 3.210772000000 | 6.435549000000 | C | -3.057253000000 | -1.889674000000 | -6.132018000000 |
| C | 2.675475000000 | 2.343992000000 | 6.420911000000 | C | -2.087369000000 | -2.962316000000 | -6.111300000000 |
| C | 3.544513000000 | -0.384163000000 | 6.414392000000 | C | 0.734513000000 | -3.551305000000 | -6.111493000000 |
| C | 3.087077000000 | -1.771160000000 | 6.423744000000 | C | 2.051570000000 | -2.955487000000 | -6.131251000000 |
| C | 0.761669000000 | -3.438134000000 | 6.455864000000 | C | 3.486043000000 | -0.454322000000 | -6.199320000000 |
| C | -0.697835000000 | -3.428378000000 | 6.473740000000 | C | 3.326939000000 | 0.979000000000 | -6.231994000000 |
| C | -3.001122000000 | -1.729128000000 | 6.500497000000 | C | 1.387766000000 | 3.115056000000 | -6.273381000000 |
| C | -3.443439000000 | -0.337169000000 | 6.503695000000 | C | -0.024215000000 | 3.408794000000 | -6.273220000000 |
| C | -2.528970000000 | 1.614819000000 | 7.727236000000 | C | -1.891935000000 | 2.286096000000 | -7.475443000000 |
| C | -0.618209000000 | 2.986536000000 | 7.701832000000 | C | -3.064397000000 | 0.237760000000 | -7.419125000000 |
| C | 0.789072000000 | 2.978402000000 | 7.684476000000 | C | -2.911540000000 | -1.162907000000 | -7.387281000000 |
| C | 2.681715000000 | 1.580960000000 | 7.659270000000 | C | -1.325171000000 | -2.911865000000 | -7.351411000000 |
| C | 3.108989000000 | 0.237328000000 | 7.655937000000 | C | 0.055842000000 | -3.199869000000 | -7.351409000000 |
| C | 2.372057000000 | -1.997322000000 | 7.672469000000 | C | 2.209017000000 | -2.229977000000 | -7.386680000000 |
| C | 1.228409000000 | -2.817746000000 | 7.688617000000 | C | 2.909361000000 | -1.007292000000 | -7.418565000000 |
| C | -1.124043000000 | -2.800418000000 | 7.716172000000 | C | 2.653145000000 | 1.339532000000 | -7.474994000000 |
| C | -2.259029000000 | -1.964618000000 | 7.729228000000 | C | 1.705427000000 | 2.382274000000 | -7.493713000000 |
| C | -2.972213000000 | 0.277860000000 | 7.734645000000 | C | -0.606795000000 | 2.862934000000 | -7.492832000000 |
| C | -1.339863000000 | 1.989456000000 | 8.479242000000 | C | -2.149053000000 | 1.053649000000 | -8.211757000000 |
| C | 1.518375000000 | 1.971828000000 | 8.442545000000 | C | -1.838982000000 | -1.799042000000 | -8.144050000000 |
| C | 2.385828000000 | -0.757312000000 | 8.434837000000 | C | 0.971886000000 | -2.384216000000 | -8.143167000000 |
| C | 0.064059000000 | -2.423929000000 | 8.469263000000 | C | 2.396937000000 | 0.106716000000 | -8.211882000000 |
| C | -2.240679000000 | -0.725692000000 | 8.494071000000 | C | 0.467279000000 | 2.229425000000 | -8.251215000000 |
| C | -0.634356000000 | 1.019999000000 | 9.223262000000 | C | -1.110342000000 | 0.438495000000 | -8.937365000000 |
| C | 0.820311000000 | 1.010232000000 | 9.203041000000 | C | -0.952246000000 | -1.010098000000 | -8.902791000000 |
| C | 1.261793000000 | -0.379298000000 | 9.199266000000 | C | 0.474415000000 | -1.306740000000 | -8.901770000000 |
| C | 0.080733000000 | -1.227187000000 | 9.217998000000 | C | 1.198468000000 | -0.042250000000 | -8.937758000000 |
| C | -1.092384000000 | -0.362440000000 | 9.229093000000 | C | 0.218773000000 | 1.036803000000 | -8.958314000000 |
| C | -1.158780000000 | -0.373937000000 | -2.272130000000 | C | 0.246351000000 | 1.186213000000 | 2.365054000000 |
| C | 0.012405000000 | -1.235968000000 | -2.279731000000 | C | 1.208199000000 | 0.129112000000 | 2.379226000000 |
| C | 1.187514000000 | -0.390807000000 | -2.293488000000 | C | 0.499156000000 | -1.103813000000 | 2.410970000000 |
| C | 0.747626000000 | 0.994806000000 | -2.292483000000 | C | -0.896869000000 | -0.813089000000 | 2.411661000000 |
| C | -0.701924000000 | 1.005907000000 | -2.279534000000 | C | -1.056837000000 | 0.601577000000 | 2.378299000000 |
| B | -2.411800000000 | -0.774059000000 | -3.110385000000 | N | 0.512030000000 | 2.451030000000 | 2.921899000000 |
| B | 0.001106000000 | -2.551075000000 | -3.120168000000 | N | 2.496950000000 | 0.285959000000 | 2.938176000000 |
| B | 2.428563000000 | -0.808865000000 | -3.141438000000 | N | 1.038565000000 | -2.283192000000 | 2.980042000000 |
| B | 1.520027000000 | 2.048881000000 | -3.144785000000 | N | -1.858156000000 | -1.679905000000 | 2.984982000000 |
| B | -1.469202000000 | 2.067133000000 | -3.127499000000 | N | -2.176949000000 | 1.259675000000 | 2.941998000000 |
| C | -2.391540000000 | -2.083867000000 | -3.980119000000 | C | 1.708191000000 | 2.516664000000 | 3.706025000000 |
| C | -1.258355000000 | -2.918232000000 | -3.985282000000 | C | 2.652832000000 | 1.473489000000 | 3.718607000000 |
| C | 1.245376000000 | -2.938206000000 | -3.998249000000 | C | 2.905966000000 | -0.821851000000 | 3.758891000000 |
| C | 2.386786000000 | -2.119423000000 | -4.007932000000 | C | 2.203367000000 | -2.037531000000 | 3.783590000000 |
| C | 3.169135000000 | 0.259569000000 | -4.024090000000 | C | 0.099173000000 | -2.988140000000 | 3.809482000000 |
| C | 2.742392000000 | 1.601100000000 | -4.025945000000 | C | -1.275479000000 | -2.700999000000 | 3.811799000000 |
| C | 0.728909000000 | 3.090120000000 | -4.016878000000 | C | -2.826536000000 | -0.990180000000 | 3.792174000000 |
| C | -0.675867000000 | 3.097766000000 | -4.009305000000 | C | -2.984250000000 | 0.404430000000 | 3.769022000000 |
| C | -2.708776000000 | 1.636801000000 | -3.992421000000 | C | -1.838168000000 | 2.406421000000 | 3.726970000000 |
| C | -3.151399000000 | 0.302353000000 | -3.984062000000 | C | -0.557073000000 | 2.986717000000 | 3.711898000000 |
| C | -3.058649000000 | -1.759430000000 | -5.229246000000 | C | 1.419834000000 | 3.233435000000 | 4.916626000000 |
| C | -0.757164000000 | -3.458377000000 | -5.239178000000 | C | 3.322166000000 | 1.136636000000 | 4.944596000000 |
| C | 0.719482000000 | -3.467984000000 | -5.248069000000 | C | 3.479561000000 | -0.306873000000 | 4.969355000000 |
| C | 3.042044000000 | -1.801789000000 | -5.267620000000 | C | 2.073581000000 | -2.756139000000 | 5.019990000000 |
| C | 3.504824000000 | -0.398786000000 | -5.275774000000 | C | 0.749206000000 | -3.352329000000 | 5.036777000000 |
| C | 2.636693000000 | 2.327189000000 | -5.279825000000 | C | -2.012411000000 | -2.776202000000 | 5.041909000000 |
| C | 1.447761000000 | 3.204412000000 | -5.275663000000 | C | -2.987435000000 | -1.700284000000 | 5.029324000000 |
| C | -1.409896000000 | 3.223515000000 | -5.259728000000 | C | -3.301753000000 | 1.103724000000 | 4.981542000000 |
| C | -2.609295000000 | 2.362323000000 | -5.249200000000 | C | -2.581468000000 | 2.364706000000 | 4.955496000000 |
| C | -3.506618000000 | -0.351437000000 | -5.231989000000 | C | -0.002826000000 | 3.528145000000 | 4.919968000000 |
| C | -2.630772000000 | -2.352707000000 | -6.433402000000 | C | 2.087160000000 | 2.920607000000 | 6.126995000000 |
| C | -1.455202000000 | -3.219454000000 | -6.438460000000 | C | 3.057418000000 | 1.848155000000 | 6.140423000000 |
| C | 1.405006000000 | -2.239440000000 | -6.455875000000 | C | 3.375740000000 | -1.017206000000 | 6.191502000000 |
| C | 2.590698000000 | -2.387674000000 | -6.466024000000 | C | 2.655678000000 | -2.267600000000 | 6.216629000000 |
| C | 3.488528000000 | 0.328658000000 | -6.481198000000 | C | 0.026261000000 | -3.452082000000 | 6.251567000000 |
| C | 3.046054000000 | 1.720547000000 | -6.483710000000 | C | -1.385767000000 | -3.158787000000 | 6.254529000000 |
| C | 0.742609000000 | 3.419713000000 | -6.475619000000 | C | -3.325577000000 | -1.023110000000 | 6.227616000000 |

SUPPORTING INFORMATION

| | | | | | | | |
|---|-----------------|-----------------|-----------------|---|-----------------|-----------------|----------------|
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| C | -3.042407000000 | 1.762383000000 | -6.447166000000 | C | -2.051760000000 | 2.912316000000 | 6.149946000000 |
| C | -3.499905000000 | 0.375415000000 | -6.438071000000 | C | -0.734920000000 | 3.508689000000 | 6.132868000000 |
| C | -2.628840000000 | -1.592170000000 | -7.673272000000 | C | 1.325928000000 | 2.862342000000 | 7.367316000000 |
| C | -0.735994000000 | -2.989631000000 | -7.683117000000 | C | 2.913012000000 | 1.113741000000 | 7.391358000000 |
| C | 0.671405000000 | -2.997679000000 | -7.691158000000 | C | 3.066315000000 | -0.287072000000 | 7.414456000000 |
| C | 2.582226000000 | -1.625861000000 | -7.706698000000 | C | 1.894539000000 | -2.336145000000 | 7.459162000000 |
| C | 3.025508000000 | -0.288920000000 | -7.714003000000 | C | 0.609624000000 | -2.913558000000 | 7.474083000000 |
| C | 2.312092000000 | 1.953496000000 | -7.717765000000 | C | -1.702748000000 | -2.433562000000 | 7.479529000000 |
| C | 1.177014000000 | 2.789252000000 | -7.713946000000 | C | -2.650770000000 | -1.391011000000 | 7.467908000000 |
| C | -1.175503000000 | 2.806442000000 | -7.701852000000 | C | -2.907829000000 | 0.955988000000 | 7.425977000000 |
| C | -2.319199000000 | 1.986026000000 | -7.691615000000 | C | -2.207961000000 | 2.179069000000 | 7.401055000000 |
| C | -3.056230000000 | -0.248565000000 | -7.675524000000 | C | -0.055183000000 | 3.149914000000 | 7.370134000000 |
| C | -1.460324000000 | -1.984591000000 | -8.448005000000 | C | 1.840767000000 | 1.744893000000 | 8.152745000000 |
| C | 1.398114000000 | -2.002063000000 | -8.465740000000 | C | 2.151746000000 | -1.108089000000 | 8.202710000000 |
| C | 2.298806000000 | 0.713020000000 | -8.480171000000 | C | -0.464089000000 | -2.284906000000 | 8.237029000000 |
| C | -0.006065000000 | 2.411206000000 | -8.474119000000 | C | -2.394486000000 | -0.162655000000 | 8.212160000000 |
| C | -2.327975000000 | 0.744537000000 | -8.451668000000 | C | -0.970358000000 | 2.329135000000 | 8.157575000000 |
| C | -0.757272000000 | -1.024497000000 | -9.205806000000 | C | 0.954844000000 | 0.951037000000 | 8.907325000000 |
| C | 0.697512000000 | -1.034214000000 | -9.216437000000 | C | 1.113448000000 | -0.497701000000 | 8.932887000000 |
| C | 1.155446000000 | 0.348226000000 | -9.222055000000 | C | -0.215447000000 | -1.096538000000 | 8.951187000000 |
| C | -0.017775000000 | 1.212946000000 | -9.220567000000 | C | -1.195540000000 | -0.017722000000 | 8.938100000000 |
| C | -1.198873000000 | 0.364990000000 | -9.207836000000 | C | -0.471902000000 | 1.247196000000 | 8.909181000000 |

Reference

1. S.D. Jiang, S.S. Liu, L.N. Zhou, B.W. Wang, Z.M. Wang and S. Gao, *Inorg. Chem.*, 2012, **51**, 3079–3087.

SUPPORTING INFORMATION

Input files

Optimization:

```
!DKH2 DKH-def2-SVP OPT BP86 D3BJ numfreq slowconv tightSCF  
!KDIIS
```

```
%pal nprocs 32  
end
```

```
%scf  
maxiter 1000  
end
```

```
%basis newgto Dy  
0 6  
1 1205955.486947000027 0.008165729207  
2 535980.216420999961 -0.004019299653  
3 238213.429520000005 0.016042861724  
4 105872.635341999994 0.006534642408  
5 47054.504596999999 0.032501357805  
6 20913.113153999999 0.044343203836  
0 1  
7 9294.716957000001 1.000000000000  
0 1  
8 4130.985314000000 1.000000000000  
0 1  
9 1835.993473000000 1.000000000000  
0 1  
10 815.997099000000 1.000000000000  
0 1  
11 362.665377000000 1.000000000000  
0 1  
12 161.184612000000 1.000000000000  
0 1  
13 71.637605000000 1.000000000000  
0 1  
14 31.838936000000 1.000000000000  
0 1  
15 14.150638000000 1.000000000000  
0 1  
16 6.289172000000 1.000000000000  
0 1  
17 2.795188000000 1.000000000000  
0 1  
18 1.242306000000 1.000000000000  
0 1  
19 0.552136000000 1.000000000000
```

SUPPORTING INFORMATION

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21 0.109064000000 1.000000000000
0 1
22 0.048473000000 1.000000000000
0 1
23 0.021543000000 1.000000000000
1 5
1 16500.520027999999 0.004760264705
2 6600.208011000000 0.005897483480
3 2640.083204000000 0.029326527847
4 1056.033282000000 0.089161858001
5 422.413313000000 0.265122289728
1 1
6 168.965325000000 1.000000000000
1 1
7 67.586130000000 1.000000000000
1 1
8 27.034452000000 1.000000000000
1 1
9 10.813781000000 1.000000000000
1 1
10 4.325512000000 1.000000000000
1 1
11 1.730205000000 1.000000000000
1 1
12 0.692082000000 1.000000000000
1 1
13 0.276833000000 1.000000000000
1 1
14 0.110733000000 1.000000000000
1 1
15 0.044293000000 1.000000000000
1 1
16 0.017717000000 1.000000000000
2 4
1 1185.048662000000 0.004734300415
2 430.926786000000 0.026490774838
3 156.700650000000 0.145474353692
4 56.982054000000 0.463452784138
2 1
5 20.720747000000 1.000000000000
2 1
6 7.534817000000 1.000000000000
2 1
7 2.739933000000 1.000000000000
2 1
8 0.996339000000 1.000000000000
2 1
9 0.362305000000 1.000000000000

SUPPORTING INFORMATION

```
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10 0.131747000000 1.000000000000
2 1
11 0.047908000000 1.000000000000
2 1
12 0.017421000000 1.000000000000
3 4
1 33.836944000000 0.101241740066
2 11.278981000000 0.330021330584
3 3.759660000000 0.494377985697
4 1.253220000000 0.347706969111
3 1
5 0.417740000000 0.145206846483
3 1
6 0.139247000000 1.000000000000
end
end

%scf
directresetfreq 1
diismaxeq 25
end

%method
SpecialGridAtoms 66
SpecialGridIntAcc 9
End

*xyz charge mult
*

EDA:

#!/bin/sh

# dependency: /home/netweb/KK/Fullerne/SP/Dy4/NEW/Dy4.Region_1 Dy4.Region_1.results/adf.rkf
Region_1.rkf
# dependency: /home/netweb/KK/Fullerne/SP/Dy4/NEW/Dy4.Region_2 Dy4.Region_2.results/adf.rkf
Region_2.rkf

"$AMSBIN/ams" -n 12 << eor

Task SinglePoint
System
  Atoms
    Dy 0.0 0.0 0.0 region=Region_1 adf.f=Region_1
    C 0.6312489999999999 -1.171237 -2.264617 region=Region_1 adf.f=Region_1
    C 1.859401 -0.648065 -1.751772 region=Region_1 adf.f=Region_1
    C 1.774261 0.766969 -1.771127 region=Region_1 adf.f=Region_1
    C 0.494993 1.125825 -2.296794 region=Region_1 adf.f=Region_1
    C -0.201122 -0.073492 -2.611613 region=Region_1 adf.f=Region_1
```


SUPPORTING INFORMATION

C 0.47185 -2.568643 -2.818229 region=Region_1 adf.f=Region_1
C 3.152247 -1.422207 -1.673853 region=Region_1 adf.f=Region_1
C 2.963824 1.693404 -1.713333 region=Region_1 adf.f=Region_1
C 0.167448 2.480909 -2.879964 region=Region_1 adf.f=Region_1
C -1.372982 -0.155102 -3.562211 region=Region_1 adf.f=Region_1
C 1.87745 -3.021305 -3.28173 region=Region_1 adf.f=Region_1
C 3.071462 -2.510729 -2.773063 region=Region_1 adf.f=Region_1
C 4.25121 -0.495268 -2.24906 region=Region_1 adf.f=Region_1
C 4.167673 0.892976 -2.265871 region=Region_1 adf.f=Region_1
C 2.754909 2.739749 -2.836399 region=Region_1 adf.f=Region_1
C 1.508411 3.09061 -3.355436 region=Region_1 adf.f=Region_1
C -0.54216 2.212953 -4.230619 region=Region_1 adf.f=Region_1
C -1.23093 1.041325 -4.53326 region=Region_1 adf.f=Region_1
C -1.085883 -1.347556 -4.504758 region=Region_1 adf.f=Region_1
C -0.262171 -2.420837 -4.174727 region=Region_1 adf.f=Region_1
C 1.812755 -3.435914 -4.661457 region=Region_1 adf.f=Region_1
C 4.224742 -2.408748 -3.631317 region=Region_1 adf.f=Region_1
C 4.944812 -1.180627 -3.313561 region=Region_1 adf.f=Region_1
C 4.774583 1.63109 -3.348001 region=Region_1 adf.f=Region_1
C 3.913131 2.756922 -3.693764 region=Region_1 adf.f=Region_1
C 1.395936 3.459254 -4.744995 region=Region_1 adf.f=Region_1
C 0.144575 2.928469 -5.278111 region=Region_1 adf.f=Region_1
C -1.244405 0.556414 -5.89301 region=Region_1 adf.f=Region_1
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C 0.507213 -3.072641 -5.205734 region=Region_1 adf.f=Region_1
C 2.952208 -3.403799 -5.492886 region=Region_1 adf.f=Region_1
C 4.194034 -2.878591 -4.963579 region=Region_1 adf.f=Region_1
C 5.604454 -0.466471 -4.336194 region=Region_1 adf.f=Region_1
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C 3.827342 3.186337 -5.03752 region=Region_1 adf.f=Region_1
C 2.531924 3.546549 -5.577367 region=Region_1 adf.f=Region_1
C 0.07897 2.502849 -6.622266 region=Region_1 adf.f=Region_1
C -0.635817 1.28401 -6.937202 region=Region_1 adf.f=Region_1
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C 0.393201 -2.690084 -6.56027 region=Region_1 adf.f=Region_1
C 2.835926 -2.990603 -6.886507 region=Region_1 adf.f=Region_1
C 4.853636 -2.125834 -6.021855 region=Region_1 adf.f=Region_1
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C 4.574901 2.49465 -6.078275 region=Region_1 adf.f=Region_1
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C 0.101126 0.586608 -7.986548 region=Region_1 adf.f=Region_1
C 0.186344 -0.816584 -7.969052 region=Region_1 adf.f=Region_1
C 1.574547 -2.638247 -7.412986 region=Region_1 adf.f=Region_1
C 4.010126 -2.193511 -7.212597 region=Region_1 adf.f=Region_1
C 5.42976 0.221005 -6.588218 region=Region_1 adf.f=Region_1
C 3.730869 2.430518 -7.268505 region=Region_1 adf.f=Region_1
C 1.274973 1.386915 -8.318153000000001 region=Region_1 adf.f=Region_1
C 1.449334 -1.477224 -8.281931 region=Region_1 adf.f=Region_1
C 3.892271 -1.068413 -8.055312000000001 region=Region_1 adf.f=Region_1

SUPPORTING INFORMATION

C 4.612229 0.157286 -7.742793 region=Region_1 adf.f=Region_1
C 3.749022 1.279685 -8.082916000000001 region=Region_1 adf.f=Region_1
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C 2.586356 -0.703345 -8.6012 region=Region_1 adf.f=Region_1
C -0.203647 -3.562599 -1.848564 region=Region_1 adf.f=Region_1
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C 3.218959 2.311196 -0.320182 region=Region_1 adf.f=Region_1
C -0.625424 3.405918 -1.931353 region=Region_1 adf.f=Region_1
C -2.749319 -0.228984 -2.865674 region=Region_1 adf.f=Region_1
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H -1.216072 -3.210574 -1.577994 region=Region_1 adf.f=Region_1
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H -1.586458 2.9374 -1.649915 region=Region_1 adf.f=Region_1
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4 9 1.0
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7 12 1.0
7 21 1.0
7 62 1.0

SUPPORTING INFORMATION

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11 20 1.0
11 66 1.0
12 13 1.5
12 22 1.5
13 23 1.5
14 15 1.5
14 24 1.5
15 25 1.5
16 17 1.5
16 26 1.5
17 27 1.5
18 19 1.5
18 28 1.5
19 29 1.5
20 21 1.5
20 30 1.5
21 31 1.5
22 31 1.0
22 32 1.5
23 24 1.0
23 33 1.5
24 34 1.5
25 26 1.0
25 35 1.5
26 36 1.5
27 28 1.0
27 37 1.5
28 38 1.5
29 30 1.0
29 39 1.5
30 40 1.5
31 41 1.5
32 33 1.5
32 42 1.0
33 43 1.0
34 35 1.5
34 44 1.0
35 45 1.0
36 37 1.5
36 46 1.0
37 47 1.0

SUPPORTING INFORMATION

38 39 1.5
38 48 1.0
39 49 1.0
40 41 1.5
40 50 1.0
41 51 1.0
42 51 2.0
42 52 1.0
43 44 2.0
43 52 1.0
44 53 1.0
45 46 2.0
45 53 1.0
46 54 1.0
47 48 2.0
47 54 1.0
48 55 1.0
49 50 2.0
49 55 1.0
50 56 1.0
51 56 1.0
52 57 2.0
53 58 2.0
54 59 2.0
55 60 2.0
56 61 2.0
57 58 1.0
57 61 1.0
58 59 1.0
59 60 1.0
60 61 1.0
62 67 1.0
62 68 1.0
62 69 1.0
63 70 1.0
63 71 1.0
63 72 1.0
64 73 1.0
64 74 1.0
64 75 1.0
65 76 1.0
65 77 1.0
65 78 1.0
66 79 1.0
66 80 1.0
66 81 1.0
82 83 1.5
82 84 1.5
82 88 1.0
83 85 1.5
83 87 1.0

SUPPORTING INFORMATION

84 85 1.5

84 89 1.0

85 86 1.0

End

End

Engine ADF

Basis

Core None

PerAtomType Symbol=Dy File=ZORA/TZP/Dy

PerAtomType Symbol=C File=ZORA/DZP/C

PerAtomType Symbol=H File=ZORA/DZP/H

End

SpinPolarization 5

Fragments

Region_1 =/home/netweb/KK/Fullerne/SP/Dy4/NEW/1/ams.results/adf.rkf

Region_2 =/home/netweb/KK/Fullerne/SP/Dy4/NEW/2/ams.results/adf.rkf

End

Save TAPE15

Print ETSLOWDIN-Unrestricted

XC

Hybrid PBE0

DISPERSION GRIMME3 BJDAMP

End

Symmetry NOSYM

Unrestricted Yes

BeckeGrid

Quality Good

End

LOCORB

END

NumericalQuality Good

FullFock Yes

AOMat2File Yes

UnrestrictedFragments Yes

ETSNOCV

Enabled Yes

End

QTAIM

Enabled Yes

End

SCF

DIIS

N 20

Cyc 25

End

Mixing 0.015

Mixing1 0.09

Iterations 3000

End

SUPPORTING INFORMATION

EndEngine
Eor

CASSCF calculations:

!DKH2 DKH-def2-svp slowconv tightscf autoaux

!moread

%moinp "/scratch/subhamsau.chy.iith/Fullerne_OPT/Dy_2F/DKH/CAS/Dy4/ro.gbw"

%pal nprocs 32

end

%Maxcore 15000

%basis newgto Dy

0 6

1 1205955.486947000027 0.008165729207

2 535980.216420999961 -0.004019299653

3 238213.429520000005 0.016042861724

4 105872.635341999994 0.006534642408

5 47054.504596999999 0.032501357805

6 20913.113153999999 0.044343203836

0 1

7 9294.716957000001 1.000000000000

0 1

8 4130.985314000000 1.000000000000

0 1

9 1835.993473000000 1.000000000000

0 1

10 815.997099000000 1.000000000000

0 1

11 362.665377000000 1.000000000000

0 1

12 161.184612000000 1.000000000000

0 1

13 71.637605000000 1.000000000000

0 1

14 31.838936000000 1.000000000000

0 1

15 14.150638000000 1.000000000000

0 1

16 6.289172000000 1.000000000000

0 1

17 2.795188000000 1.000000000000

0 1

18 1.242306000000 1.000000000000

0 1

19 0.552136000000 1.000000000000

0 1

SUPPORTING INFORMATION

20 0.245394000000 1.000000000000
0 1
21 0.109064000000 1.000000000000
0 1
22 0.048473000000 1.000000000000
0 1
23 0.021543000000 1.000000000000
1 5
1 16500.520027999999 0.004760264705
2 6600.208011000000 0.005897483480
3 2640.083204000000 0.029326527847
4 1056.033282000000 0.089161858001
5 422.413313000000 0.265122289728
1 1
6 168.965325000000 1.000000000000
1 1
7 67.586130000000 1.000000000000
1 1
8 27.034452000000 1.000000000000
1 1
9 10.813781000000 1.000000000000
1 1
10 4.325512000000 1.000000000000
1 1
11 1.730205000000 1.000000000000
1 1
12 0.692082000000 1.000000000000
1 1
13 0.276833000000 1.000000000000
1 1
14 0.110733000000 1.000000000000
1 1
15 0.044293000000 1.000000000000
1 1
16 0.017717000000 1.000000000000
2 4
1 1185.048662000000 0.004734300415
2 430.926786000000 0.026490774838
3 156.700650000000 0.145474353692
4 56.982054000000 0.463452784138
2 1
5 20.720747000000 1.000000000000
2 1
6 7.534817000000 1.000000000000
2 1
7 2.739933000000 1.000000000000
2 1
8 0.996339000000 1.000000000000
2 1
9 0.362305000000 1.000000000000
2 1

SUPPORTING INFORMATION

```
10 0.131747000000 1.000000000000
2 1
11 0.047908000000 1.000000000000
2 1
12 0.017421000000 1.000000000000
3 4
1 33.836944000000 0.101241740066
2 11.278981000000 0.330021330584
3 3.759660000000 0.494377985697
4 1.253220000000 0.347706969111
3 1
5 0.417740000000 0.145206846483
3 1
6 0.139247000000 1.000000000000
end
end
```

```
%method
SpecialGridAtoms 66
SpecialGridIntAcc 9
end
```

```
%casscf
nel 9
norb 7
mult 6
nroots 21
trafostep ri
maxiter 100
nevpt2 true
actorbs forbs
ci
nguessmat 4000
maxiter 100
end
```

```
rel
dosoc true
gtensor true
printlevel 3
NDoubGTensor 8
domagnetization true
dosusceptibility true
```

```
SUSTempMIN 2.0
SUSTempMAX 300.0
SUSNPoints 100
```

```
MAGTemperatureMIN 2.0
MAGTemperatureMAX 5.0
MAGTemperatureNPoints 4
```


SUPPORTING INFORMATION

MAGFieldMIN 0.0
MAGFieldMAX 70000.0
MAGNpoints 15

end

ANISO
doaniso true
MLTP 2,2,2,2,2,2,2,2
TINT 0, 300, 100
HINT 0, 7.0, 10
TMAG 2.0, 3.0, 5.0
CRYS_element "Dy"
CRYS_charge 3
PLOT true
UBAR true
end
end

*xyz 0 6
*