Electronic Supplementary Information

Is Lanthanide-Transition Metal Direct Bond a Route to Achieving New Generation {3d-4f} SMMs?

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Energy between the HS-LS state of TM.

Table **S1**. DFT Computed energy gap between the Low spin state of V and Mn with their high spin states.

Complexes	ΔE(LS-HS) $kJmol^{-1}$
V(0)	-105
Mn(0)	-178.7
Fe(+)	367.4 wrt to Fe(0)

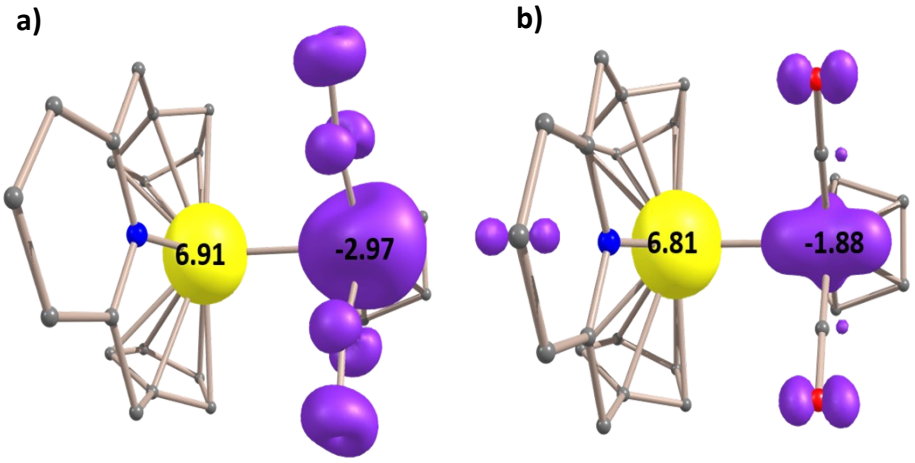

Figure **S1**. DFT computed spin density plot for Gd-V_{hs},(a) and **Gd-Mn**$_{hs}$.(b)

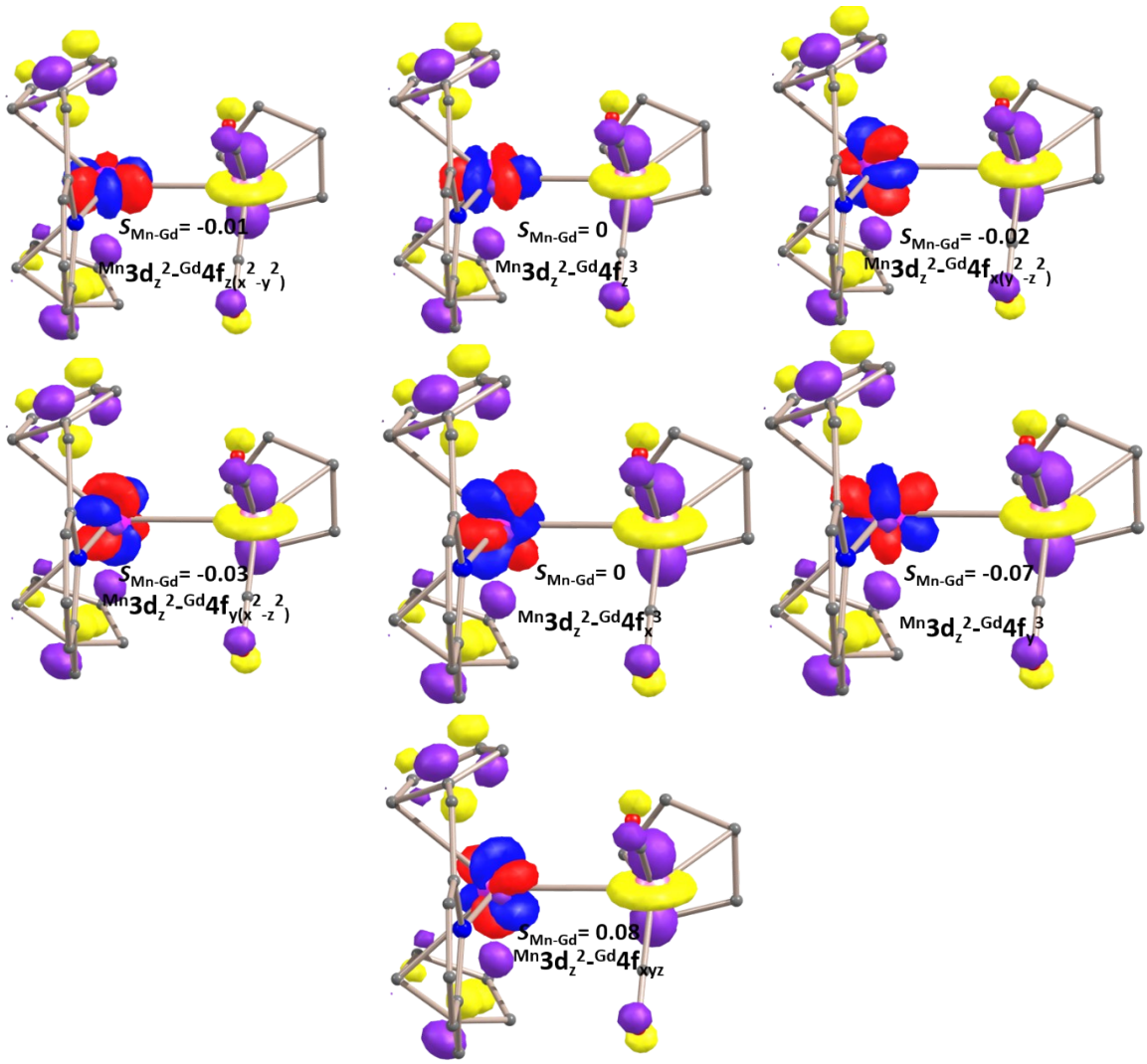

Figure **S2a**. Calculated Orbital overlap diagram for the complex **Gd-Mn** between the Mn-$3d_{z^2}$ and the Gd-4f orbitals.

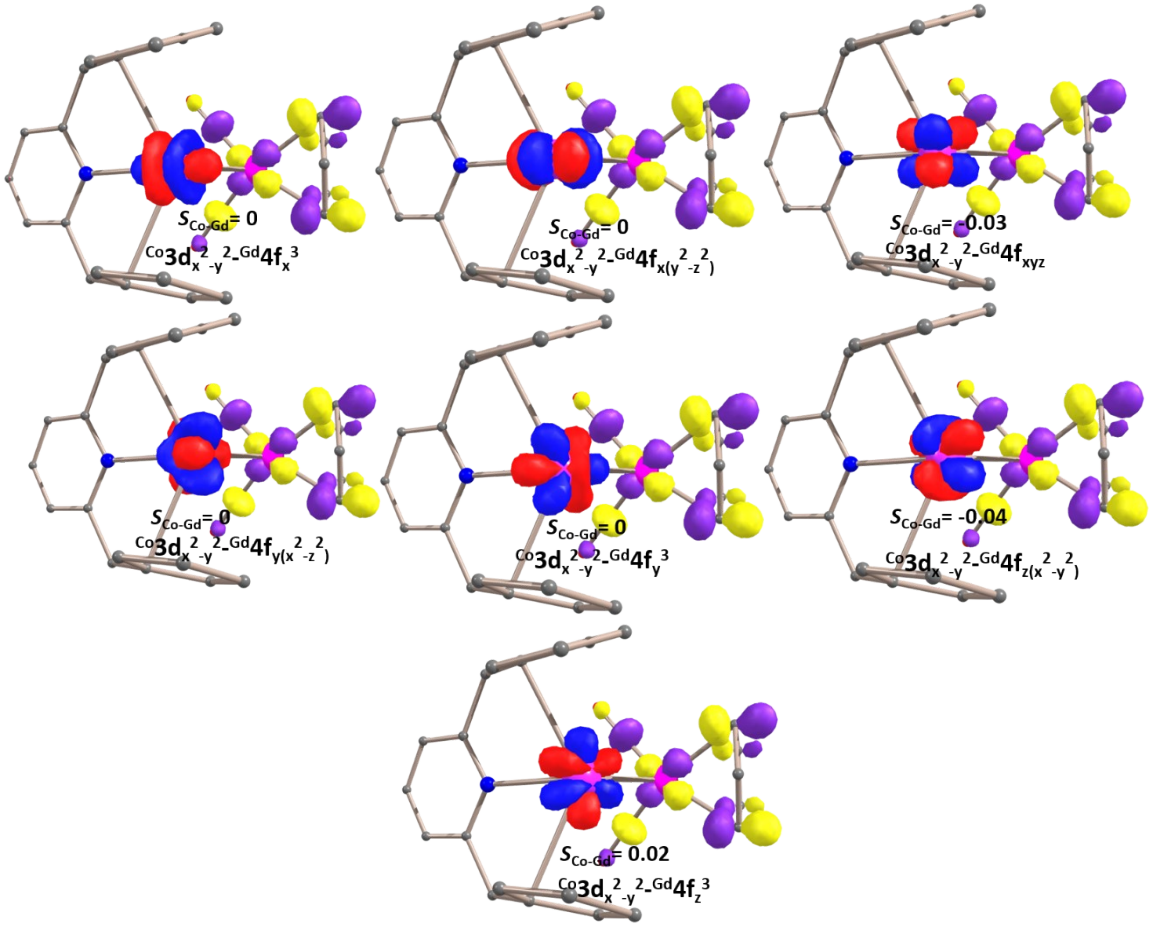

Figure **S2b**. Calculated Orbital overlap diagram for the complex **Gd-Co** between the CO-$3d_{x^2-y^2}$ and the Gd-4f orbitals.

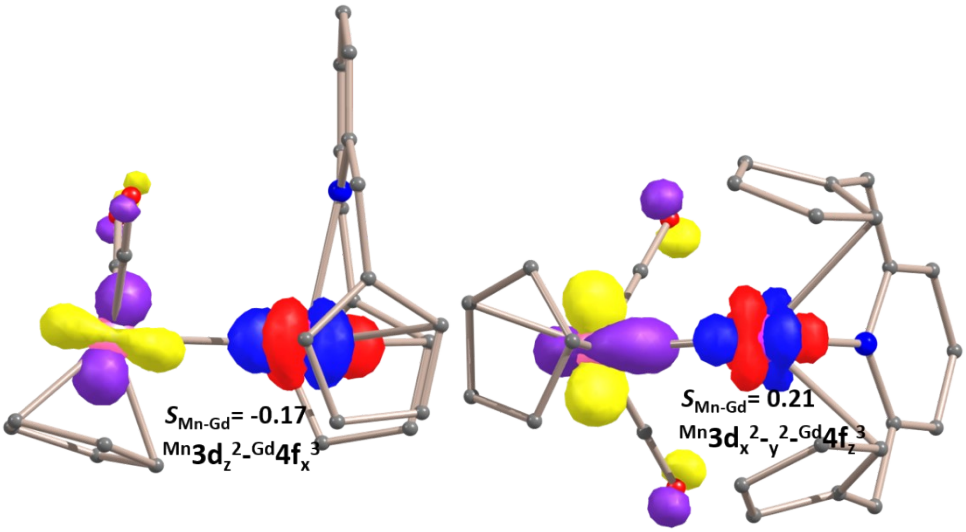

Figure **S2c**. Calculated Orbital overlap diagram for the complex **Gd-Mn**$_{hs}$ between the Mn-$3d_z^2$ and the Gd-$4f_x^3$,Mn-$3d_{x^2-y^2}$ and the Gd-$4f_z^3$ orbitals. Such a strong exchange is due to 35 possible 3d-4f overlaps that are opened up in the high-spin case. Among these, eighteen of them showing dominant overlaps, with $3d_z^2$-$4f_y^3$ being the strongest. Such a large direct overlap enhances the J_{AF} term significantly, and the J_F term remains moderate due to the absence of a strong σ-σ (example $5d_z^2$-$3d_z^2$) interaction. These two factors contribute to a very large antiferromagnetic exchange. For the **Gd-Mn$_{hs}$** example, the exchange is even larger. Although the number of overlap integrals is smaller here, some of the strongest 3d-4f overlaps are witnessed. This is due to the much shorter Gd—Mn distance than the corresponding Gd—V counterpart, enabling stronger overlap and a record-high antiferromagnetic exchange. The details of the exchange mechanism are represented in figure **5a**.

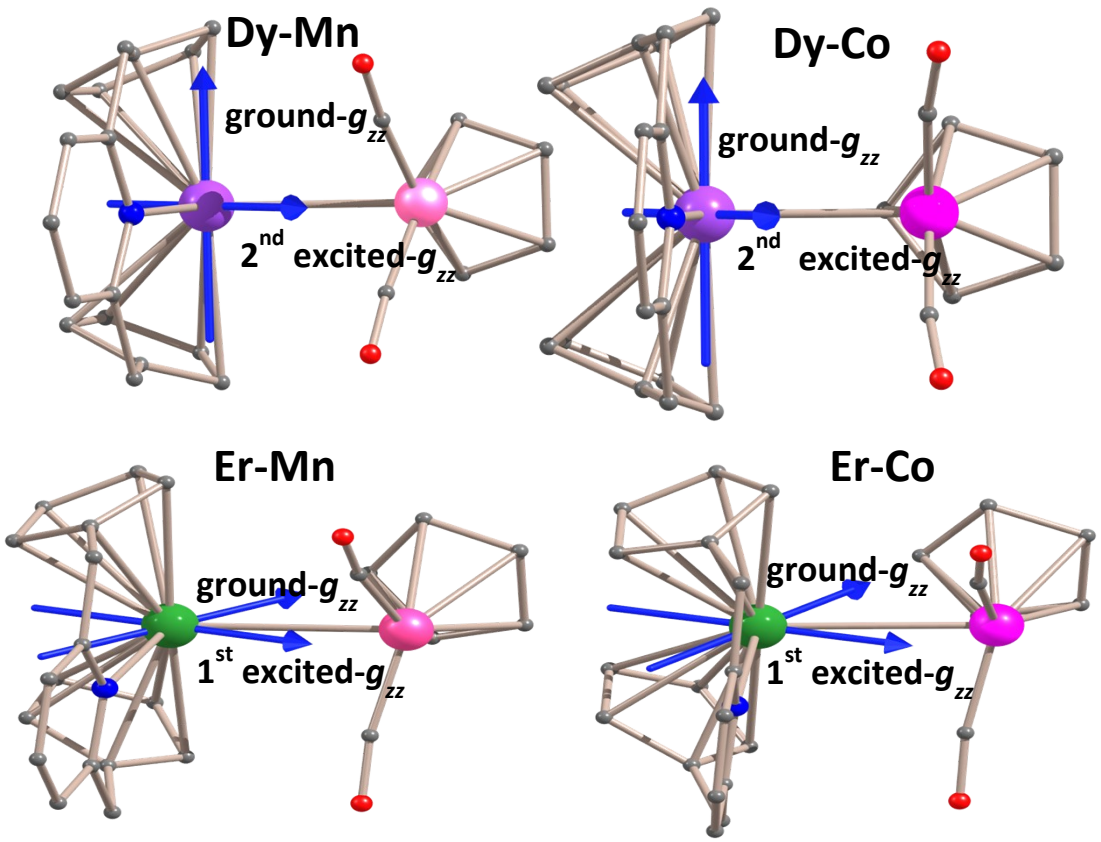

Figure **S3.** Arrangement of ground state and 2nd excited g-anisotropy axis for complex Dy-Mn, Dy-Co, ground state and 1st excited g-anisotropy axis for complex **Er-Mn** and **Er-Co**.

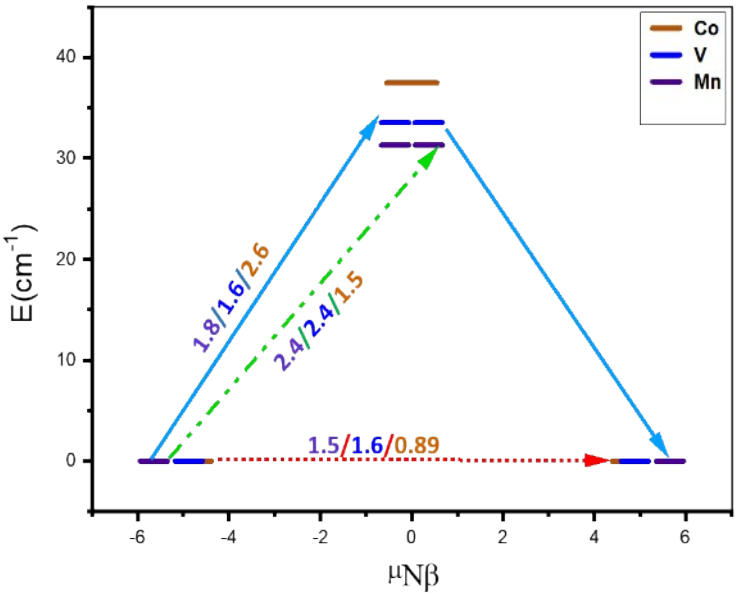

Figure **S4**. Dynamics of magnetic relaxation for complex **Er-V**, **Er-Mn** and **Er-Co**. obtained from single-aniso calculations. Red dotted line represents QTM, blue solid line represents the TA and green line represents the Raman/Orbach processes. The number at the top of the arrows indicates the mean value of the transition probability between the corresponding states.

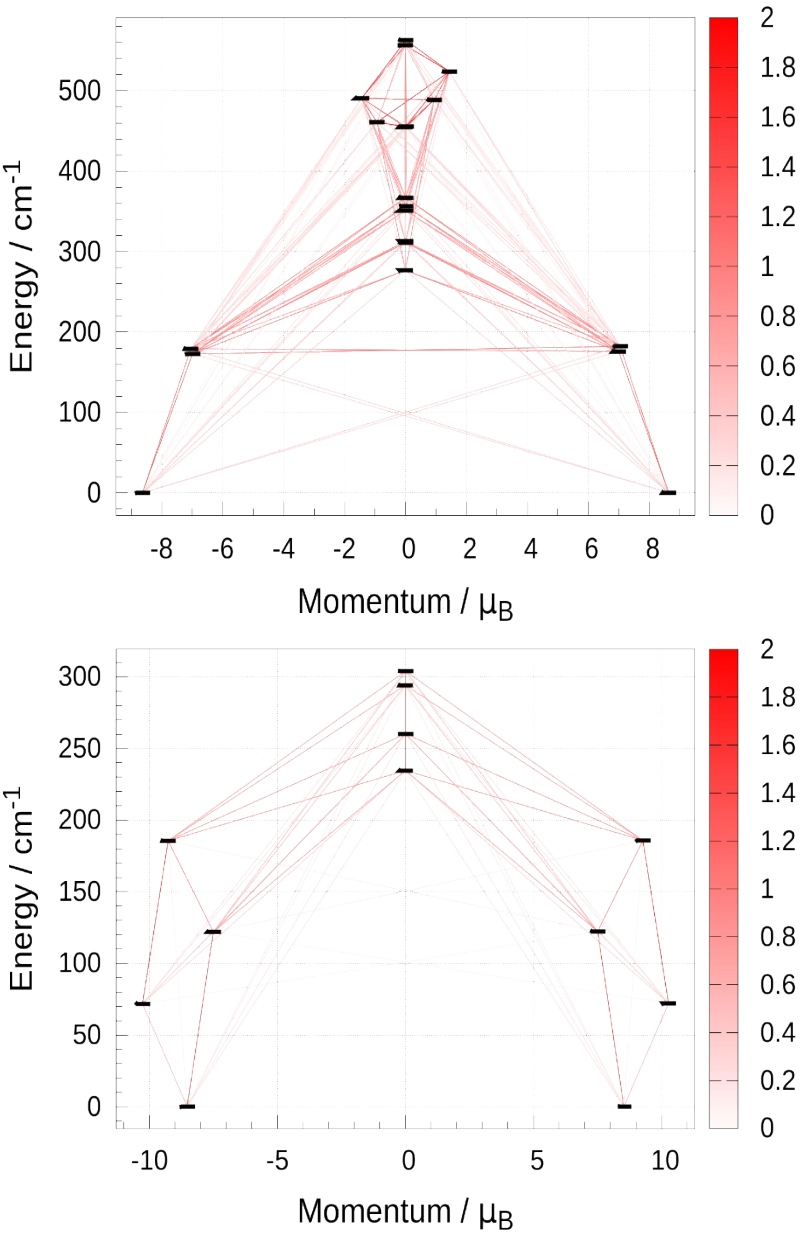

Figure **S5a**. Poly_aniso computed magnetic relaxation pathways for complex **Dy-V**$_{hs}$(top), **Dy-V**(bottom). Red dotted line represents QTM, solid blue line represents the thermal assisted mechanism and green arrow indicates Raman/Orbach process. The number on the top of the arrow indicates the transition probability.

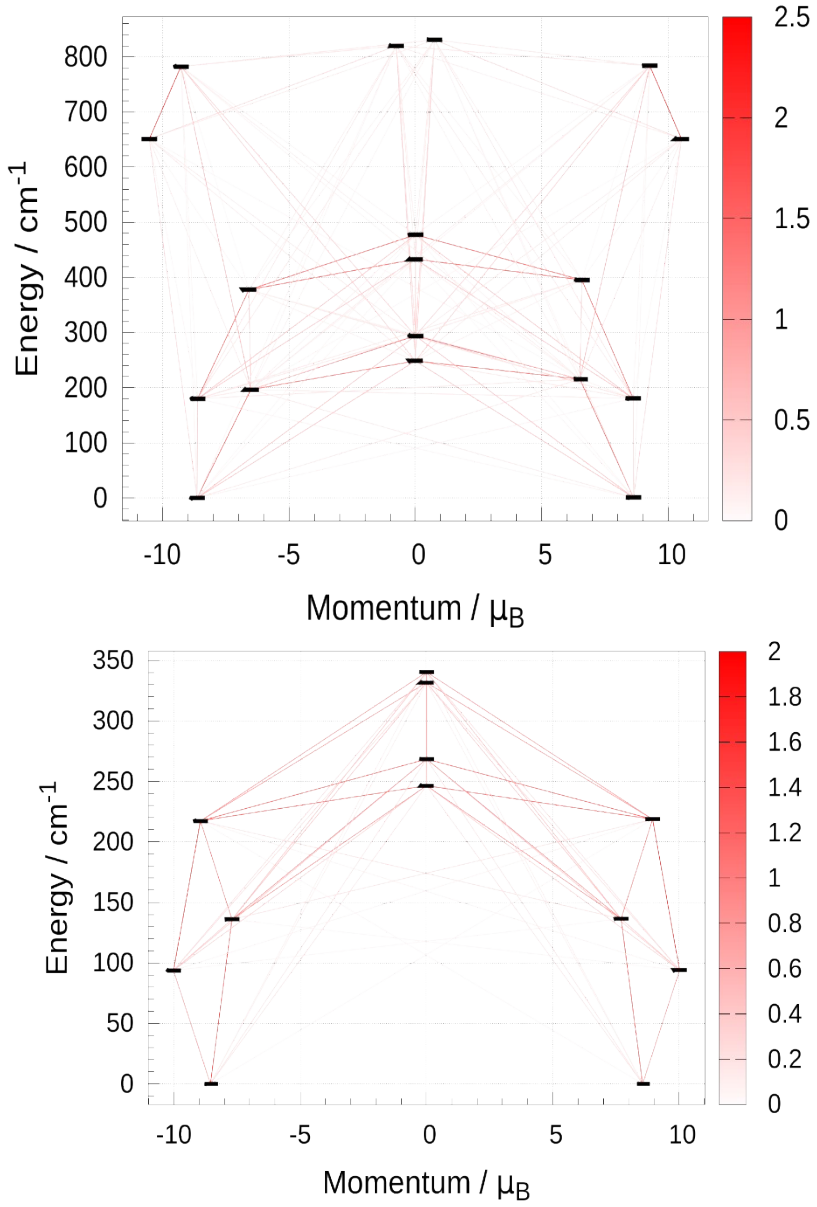

Figure **S5b**. Poly_aniso computed magnetic relaxation pathways for complex **Dy-Mn**$_{hs}$(top), **Dy-Mn**(bottom). Red dotted line represents QTM, solid blue line represents the thermal assisted mechanism and green arrow indicates Raman/Orbach process. The number on the top of the arrow indicates the transition probability.

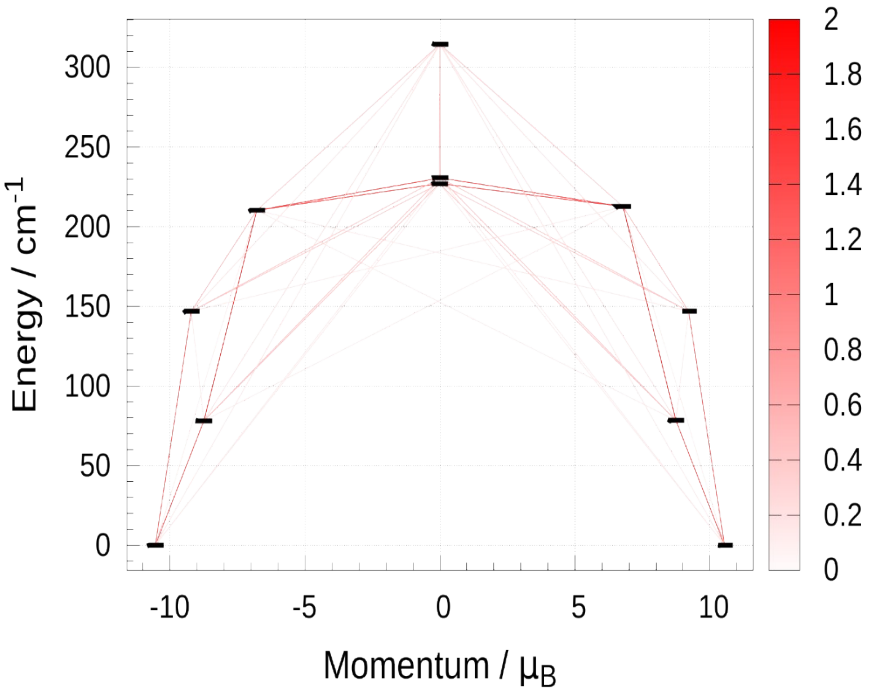

Figure **S5c**. Poly_aniso computed magnetic relaxation pathways for complex **Dy-Co**. Red dotted line represents QTM, solid blue line represents the thermal assisted mechanism and green arrow indicates Raman/Orbach process. The number on the top of the arrow indicates the transition probability.

Table **S2a**. The computed overlap integral for **Gd-V**, **Gd-Mn** and **Gd-Co**.

Gd-4f-V-3d	V-$3d_{xy}$ (x 10^{-2})	Gd-4f	Mn-$3d_{z^2}$ (x 10^{-2})	Gd-4f	Co-$3d_{x2-y2}$ (x 10^{-2})
$x(y^2-z^2)$	-1.2	$z(x^2-y^2)$	0	x^3	0
x^3	0.0	z^3	0	$x(y^2-z^2)$	0
$y(x^2-z^2)$	-1.8	$x(y^2-z^2)$	0	xyz	-3.0
$z(x^2-y^2)$	-1.1	$y(x^2-z^2)$	-2.8	$y(x^2-z^2)$	0
y^3	0.0	x^3	0	y^3	0
xyz	-1.2	Y^3	-7.0	$z(x^2-y^2)$	-4.6
z^3	0.0	xyz	8.3	z^3	1.9

Table **S2b**. The computed overlap integral for **Gd-V_{hs}**.

Gd-4f	V-$3d_{yz}$ (x 10^{-2})	V-$3d_{xz}$ (x 10^{-2})	V-$3d_{xy}$ (x 10^{-2})	V-$3d_{z2}$ (x 10^{-2})	V-$3d_{x2-y2}$ (x 10^{-2})
$x(y^2-z^2)$	-0.9	-0.9	-2.9	0	-0.8
x^3	-0.9	-1.5	2.8	0	-0.4
$y(x^2-z^2)$	0	0	0	-2.05	0
$z(x^2-y^2)$	-0.6	0.2	0	0	-0.7
y^3	-1.1	-0.3	1.15	0	-0.1
xyz	0	0	0	-4.2	0
z^3	0	0	0	2.2	0

Table **S2c**. The computed overlap integral for **Gd-Mn$_{hs}$**.

Gd-4f		Mn-3d_{yz} (x 10^{-2})	Mn-3d_{xz} (x 10^{-2})	Mn-3d_{xy} (x 10^{-2})	Mn-3d_{z2} (x 10^{-2})	Mn-3dx_{2-y2} (x 10^{-2})
$z(x^2-y^2)$		-4.1	3.6	0	0	5.4
z^3		-4.1	-9.1	0	0	17.2
$x(y^2-z^2)$		0	0	1.2	1.5	0
$y(x^2-z^2)$		-0.8	1.1	0	0	-7.4
x^3		0	0	-20.9	-13.8	0
Y^3		-2.1	-0.4	0	0	7.4
xyz		0	0	-1.8	2.6	0

Table **S3**. Comparison of KDs energy and g anisotropy for 21 sextet root only and 21 sextet, 122 quartet and 128 doublet roots along with Ln-V, Ln-Mn where V and Mn are in high spin.

Complexes	**Mn-Dy**	**Mn-Dy(all roots)**	**Mn$_{hs}$-Dy**	**V$_{hs}$-Dy**	**Mn$_{hs}$-Er**	**V$_{hs}$-Er**
KD1	0.00	0.00	0.0	0.0	0.0	0.0
KD2	122.16	119.52	146.7	161.6	23.1	27.4
KD3	243.65	240.12	203.7	268.8	56.5	88.7
KD4	274.93	268.25	236.7	304.2	139.2	164.5
KD5	292.84	290.14	269.4	320.5	145.9	192.5
KD6	323.21	318.56	308.4	326.7	191.4	205.7
KD7	366.13	364.92	353.3	359.6	258.0	242.5
KD8	442.95	440.21	429.0	463.8	295.1	316.1
g_{xx}	0.008	0.008	0.007	0.022	2.045	0.616
g_{yy}	0.014	0.013	0.012	0.045	3.366	2.996
g_{zz}	19.033	19.032	19.233	19.236	9.515	13.780
g_{xx}	1.407	1.410	0.253	2.254	0.516	1.097
g_{yy}	2.787	2.762	0.541	2.399	2.262	2.180
g_{zz}	15.748	15.732	18.236	15.034	7.884	12.037

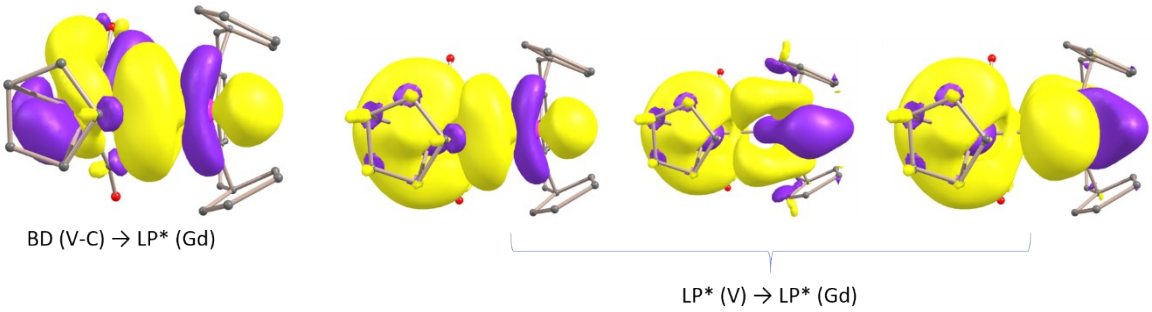

Figure **S6a**. NBO diagram for **Gd-V**.

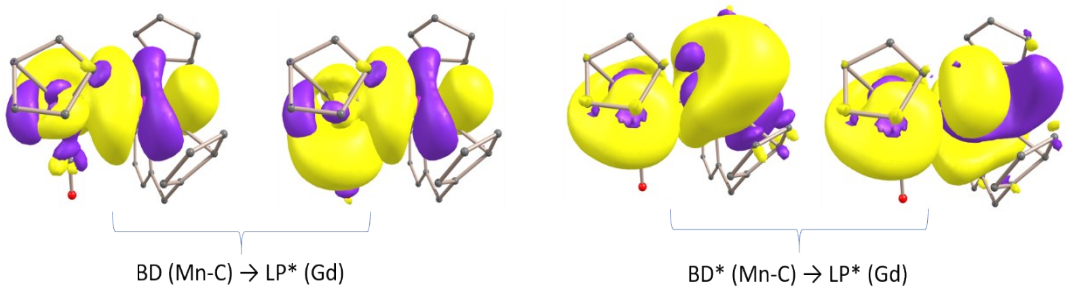

Figure **S6b**. NBO diagram for **Gd-Mn**.

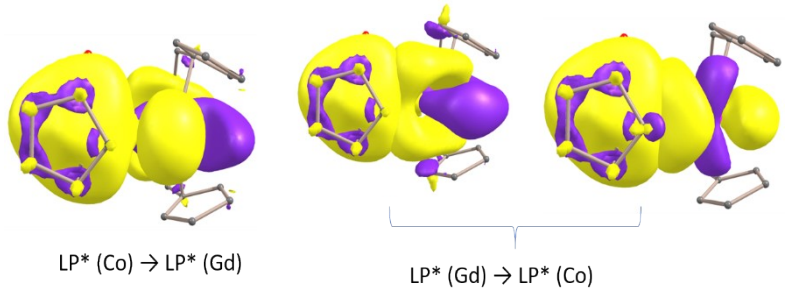

Figure **S6c**. NBO diagram for **Gd-Co**.

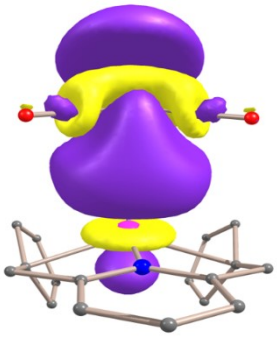

Figure **S6d**. NBO diagram for **Gd-Fe**.

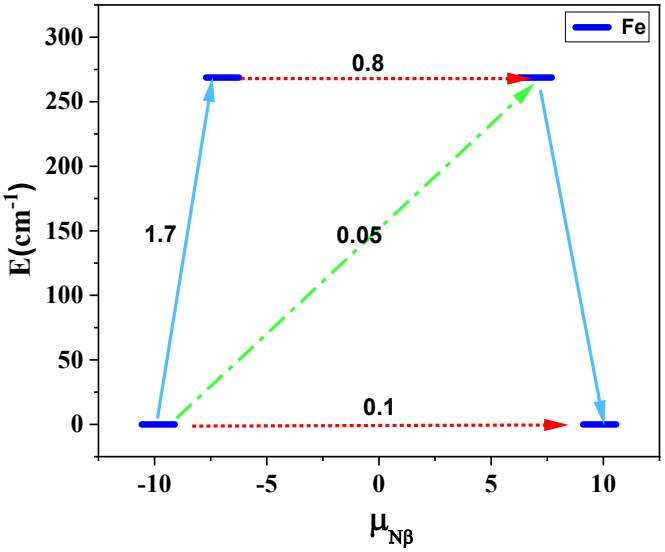

Figure **S7**. Dynamics of magnetic relaxation for complexes **Dy-Fe** obtained from SINGLE_ANISO calculations. Red dotted line represents QTM, blue solid line represents the TA and green line represents the Raman/Orbach processes. The number at the top of the arrows indicates the mean value of the transition probability between the corresponding states.

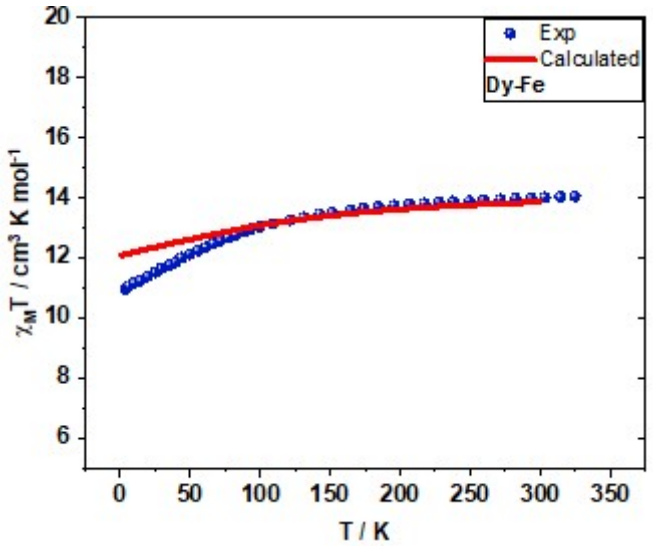

Figure **S8**. Calculated molar magnetic susceptibility for complex the Dy-Fe using the single ion CASSCF methodology.

Table **S4**. Sum of α-density matrix and β density matrix along with QTAIM performed $\nabla^2\rho$(lcp) values.

Complexes	Sum of α-density matrix	Sum of β density matrix	$\nabla^2\rho$(lcp)
Gd-V	0.045	0.050	0.043
Gd-Mn	0.042	0.051	0.039
Gd-Co	0.048	0.054	----

Optimised Coordinates of Ln-TM complexes.

Table **S5**. Y-V coordinates.

Y	-0.845544000	-0.119110000	0.000000000
V	1.301043000	2.242034000	0.000000000
O	2.140556000	0.803094000	2.583154000
N	0.598256000	-2.139120000	0.000000000
C	-0.982003000	0.064102000	2.664665000
H	-0.253790000	0.686466000	3.162915000
C	-2.277385000	0.457568000	2.242446000
H	-2.727037000	1.432878000	2.390089000
C	-2.911756000	-0.672885000	1.671137000
H	-3.921877000	-0.707538000	1.282914000
C	-2.003413000	-1.754391000	1.718680000
H	-2.188425000	-2.756703000	1.350899000
C	-0.796954000	-1.299527000	2.323963000
C	0.480012000	-2.088276000	2.472041000
H	0.363843000	-2.905037000	3.197940000
H	1.259433000	-1.428890000	2.874289000
C	0.991953000	-2.692886000	1.172797000
C	1.846308000	-3.797228000	1.199148000
H	2.142492000	-4.220909000	2.153555000
C	2.289374000	-4.346573000	0.000000000
H	2.951244000	-5.208388000	0.000000000
C	0.954288000	4.349041000	-0.717836000
H	1.655492000	4.867990000	-1.359506000
C	-0.149155000	3.574121000	-1.155009000
H	-0.429037000	3.387912000	-2.183333000
C	-0.829074000	3.073400000	0.000000000
H	-1.792579000	2.571225000	0.000000000
C	1.755846000	1.257586000	1.563806000
C	-0.982003000	0.064102000	-2.664665000
H	-0.253790000	0.686466000	-3.162915000
C	-2.277385000	0.457568000	-2.242446000
H	-2.727037000	1.432878000	-2.390089000
C	-2.911756000	-0.672885000	-1.671137000
H	-3.921877000	-0.707538000	-1.282914000
C	-2.003413000	-1.754391000	-1.718680000
H	-2.188425000	-2.756703000	-1.350899000
C	-0.796954000	-1.299527000	-2.323963000
C	0.480012000	-2.088276000	-2.472041000
H	0.363843000	-2.905037000	-3.197940000

H	1.259433000	-1.428890000	-2.874289000
C	0.991953000	-2.692886000	-1.172797000
C	1.846308000	-3.797228000	-1.199148000
H	2.142492000	-4.220909000	-2.153555000
C	0.954288000	4.349041000	0.717836000
H	1.655492000	4.867990000	1.359506000
C	-0.149155000	3.574121000	1.155009000
H	-0.429037000	3.387912000	2.183333000
O	2.140556000	0.803094000	-2.583154000
C	1.755846000	1.257586000	-1.563806000

Table **S6**. Y-Mn coordinates.

Y	0.860295000	0.085699000	0.000000000
Mn	-1.149258000	-2.145109000	0.000000000
O	-2.311810000	-0.533991000	2.175051000
N	-0.518580000	2.161249000	0.000000000
C	0.920296000	-0.121661000	2.660997000
H	0.140491000	-0.706384000	3.128346000
C	2.199388000	-0.586598000	2.262405000
H	2.587461000	-1.588387000	2.406442000
C	2.909068000	0.508216000	1.710219000
H	3.927205000	0.486880000	1.341574000
C	2.064224000	1.641812000	1.750443000
H	2.315237000	2.634967000	1.396776000
C	0.823607000	1.253677000	2.331573000
C	-0.406766000	2.112589000	2.473773000
H	-0.243901000	2.926941000	3.193181000
H	-1.222095000	1.500498000	2.878740000
C	-0.889731000	2.733336000	1.172194000
C	-1.696270000	3.872817000	1.198444000
H	-1.974704000	4.307585000	2.153174000
C	-2.116344000	4.440520000	0.000000000
H	-2.742090000	5.328884000	0.000000000
C	-1.136486000	-4.187484000	-0.713083000
H	-1.903404000	-4.599499000	-1.355668000
C	0.063924000	-3.556056000	-1.152157000
H	0.362429000	-3.408976000	-2.181352000
C	0.813670000	-3.177182000	0.000000000
H	1.815891000	-2.760695000	0.000000000
C	-1.804274000	-1.133553000	1.298028000
C	0.920296000	-0.121661000	-2.660997000
H	0.140491000	-0.706384000	-3.128346000
C	2.199388000	-0.586598000	-2.262405000
H	2.587461000	-1.588387000	-2.406442000
C	2.909068000	0.508216000	-1.710219000
H	3.927205000	0.486880000	-1.341574000
C	2.064224000	1.641812000	-1.750443000
H	2.315237000	2.634967000	-1.396776000
C	0.823607000	1.253677000	-2.331573000
C	-0.406766000	2.112589000	-2.473773000
H	-0.243901000	2.926941000	-3.193181000

H	-1.222095000	1.500498000	-2.878740000
C	-0.889731000	2.733336000	-1.172194000
C	-1.696270000	3.872817000	-1.198444000
H	-1.974704000	4.307585000	-2.153174000
C	-1.136486000	-4.187484000	0.713083000
H	-1.903404000	-4.599499000	1.355668000
C	0.063924000	-3.556056000	1.152157000
H	0.362429000	-3.408976000	2.181352000
O	-2.311810000	-0.533991000	-2.175051000
C	-1.804274000	-1.133553000	-1.298028000

Table **S7**. Y-Co coordinates.

Y	0.912362000	0.051150000	0.000000000
Co	-1.073626000	-1.911188000	0.000000000
O	-2.516661000	-0.589712000	2.200832000
N	-0.502120000	2.120533000	0.000000000
C	0.958710000	-0.146122000	2.667877000
H	0.186550000	-0.740450000	3.137072000
C	2.243824000	-0.598701000	2.275707000
H	2.639523000	-1.597170000	2.420494000
C	2.943866000	0.502588000	1.723816000
H	3.963751000	0.491197000	1.359461000
C	2.087063000	1.627549000	1.758226000
H	2.329007000	2.622802000	1.404088000
C	0.848390000	1.227190000	2.334659000
C	-0.390286000	2.074062000	2.473878000
H	-0.235781000	2.890702000	3.192530000
H	-1.201425000	1.459438000	2.884611000
C	-0.878066000	2.690444000	1.171273000
C	-1.692907000	3.824130000	1.198138000
H	-1.974130000	4.256896000	2.152988000
C	-2.117249000	4.389291000	0.000000000
H	-2.749178000	5.273208000	0.000000000
C	-1.155323000	-4.077547000	-0.715340000
H	-1.942924000	-4.467040000	-1.347529000
C	0.054180000	-3.501478000	-1.156663000
H	0.355433000	-3.357179000	-2.185682000
C	0.787273000	-3.078795000	0.000000000
H	1.817765000	-2.733422000	0.000000000
C	-1.864581000	-1.065639000	1.359902000
C	0.958710000	-0.146122000	-2.667877000
H	0.186550000	-0.740450000	-3.137072000
C	2.243824000	-0.598701000	-2.275707000
H	2.639523000	-1.597170000	-2.420494000
C	2.943866000	0.502588000	-1.723816000
H	3.963751000	0.491197000	-1.359461000
C	2.087063000	1.627549000	-1.758226000
H	2.329007000	2.622802000	-1.404088000
C	0.848390000	1.227190000	-2.334659000
C	-0.390286000	2.074062000	-2.473878000

H	-0.235781000	2.890702000	-3.192530000
H	-1.201425000	1.459438000	-2.884611000
C	-0.878066000	2.690444000	-1.171273000
C	-1.692907000	3.824130000	-1.198138000
H	-1.974130000	4.256896000	-2.152988000
C	-1.155323000	-4.077547000	0.715340000
H	-1.942924000	-4.467040000	1.347529000
C	0.054180000	-3.501478000	1.156663000
H	0.355433000	-3.357179000	2.185682000
O	-2.516661000	-0.589712000	-2.200832000
C	-1.864581000	-1.065639000	-1.359902000

Table **S8**. Y-V_{HS} coordinates.

Y	-0.914696000	-0.451975000	0.000000000
V	0.957458000	2.500061000	0.000000000
O	2.669916000	1.138546000	2.304347000
N	0.673408000	-2.154360000	0.000000000
C	-0.858085000	0.020813000	2.614903000
H	-0.126727000	0.709003000	3.021427000
C	-2.192051000	0.339599000	2.241526000
H	-2.671705000	1.306889000	2.338668000
C	-2.814752000	-0.859648000	1.811095000
H	-3.845063000	-0.962399000	1.491958000
C	-1.865037000	-1.910427000	1.915753000
H	-2.027147000	-2.949507000	1.652758000
C	-0.646366000	-1.366869000	2.407299000
C	0.679777000	-2.086688000	2.477755000
H	0.693476000	-2.820578000	3.294187000
H	1.459808000	-1.347932000	2.717954000
C	1.039278000	-2.794427000	1.183704000
C	1.705624000	-4.004549000	1.198488000
H	1.945647000	-4.454980000	2.158221000
C	2.067192000	-4.642778000	0.000000000
H	2.595553000	-5.590151000	0.000000000
C	0.687870000	4.669856000	-0.710008000
H	1.412587000	5.161788000	-1.346897000
C	-0.437876000	3.916256000	-1.150260000
H	-0.719841000	3.735340000	-2.179835000
C	-1.138962000	3.458491000	0.000000000
H	-2.052935000	2.878491000	0.000000000
C	2.023705000	1.580379000	1.457733000
C	-0.858085000	0.020813000	-2.614903000
H	-0.126727000	0.709003000	-3.021427000
C	-2.192051000	0.339599000	-2.241526000
H	-2.671705000	1.306889000	-2.338668000
C	-2.814752000	-0.859648000	-1.811095000
H	-3.845063000	-0.962399000	-1.491958000
C	-1.865037000	-1.910427000	-1.915753000
H	-2.027147000	-2.949507000	-1.652758000
C	-0.646366000	-1.366869000	-2.407299000

C	0.679777000	-2.086688000	-2.477755000
H	0.693476000	-2.820578000	-3.294187000
H	1.459808000	-1.347932000	-2.717954000
C	1.039278000	-2.794427000	-1.183704000
C	1.705624000	-4.004549000	-1.198488000
H	1.945647000	-4.454980000	-2.158221000
C	0.687870000	4.669856000	0.710008000
H	1.412587000	5.161788000	1.346897000
C	-0.437876000	3.916256000	1.150260000
H	-0.719841000	3.735340000	2.179835000
O	2.669916000	1.138546000	-2.304347000
C	2.023705000	1.580379000	-1.457733000

Table **S9**. Y-Mn_{HS} coordinates.

Y	1.030862000	0.270143000	0.000000000
Mn	-1.169556000	-2.226780000	0.000000000
O	-2.575719000	-1.124491000	2.405883000
N	-0.713273000	1.951242000	0.000000000
C	1.032953000	-0.063658000	2.638565000
H	0.345869000	-0.784725000	3.063374000
C	2.381930000	-0.300441000	2.259967000
H	2.929246000	-1.228062000	2.383364000
C	2.911193000	0.918987000	1.766559000
H	3.927481000	1.081682000	1.428795000
C	1.890205000	1.901114000	1.837191000
H	1.978175000	2.936776000	1.529531000
C	0.721119000	1.291584000	2.371495000
C	-0.647824000	1.914089000	2.474140000
H	-0.677817000	2.685178000	3.255321000
H	-1.363176000	1.140152000	2.781977000
C	-1.128709000	2.533907000	1.173818000
C	-1.968684000	3.639645000	1.195840000
H	-2.259898000	4.059076000	2.154414000
C	-2.419692000	4.204611000	0.000000000
H	-3.078533000	5.067277000	0.000000000
C	-0.597715000	-4.189660000	-0.711325000
H	-1.247771000	-4.766067000	-1.356706000
C	0.424793000	-3.292555000	-1.147859000
H	0.694275000	-3.100678000	-2.177537000
C	1.109946000	-2.794576000	0.000000000
H	2.048865000	-2.252927000	0.000000000
C	-2.063003000	-1.507524000	1.434468000
C	1.032953000	-0.063658000	-2.638565000
H	0.345869000	-0.784725000	-3.063374000
C	2.381930000	-0.300441000	-2.259967000
H	2.929246000	-1.228062000	-2.383364000
C	2.911193000	0.918987000	-1.766559000
H	3.927481000	1.081682000	-1.428795000
C	1.890205000	1.901114000	-1.837191000
H	1.978175000	2.936776000	-1.529531000
C	0.721119000	1.291584000	-2.371495000

C	-0.647824000	1.914089000	-2.474140000
H	-0.677817000	2.685178000	-3.255321000
H	-1.363176000	1.140152000	-2.781977000
C	-1.128709000	2.533907000	-1.173818000
C	-1.968684000	3.639645000	-1.195840000
H	-2.259898000	4.059076000	-2.154414000
C	-0.597715000	-4.189660000	0.711325000
H	-1.247771000	-4.766067000	1.356706000
C	0.424793000	-3.292555000	1.147859000
H	0.694275000	-3.100678000	2.177537000
O	-2.575719000	-1.124491000	-2.405883000
C	-2.063003000	-1.507524000	-1.434468000

Table **S10**. Y-Fe coordinates.

Y	0.896826000	0.063524000	0.000000000
Fe	-1.033824000	-2.033741000	0.000000000
O	-2.400998000	-0.601242000	2.123097000
N	-0.525510000	2.123654000	0.000000000
C	0.938084000	-0.141814000	2.665835000
H	0.162934000	-0.738047000	3.127526000
C	2.226712000	-0.588174000	2.277666000
H	2.627718000	-1.584684000	2.423110000
C	2.925129000	0.517734000	1.732250000
H	3.946650000	0.511499000	1.372089000
C	2.064366000	1.639462000	1.768070000
H	2.303872000	2.636437000	1.416912000
C	0.824751000	1.232479000	2.337530000
C	-0.419791000	2.071653000	2.473351000
H	-0.276733000	2.883780000	3.199432000
H	-1.229718000	1.445844000	2.869065000
C	-0.901808000	2.692904000	1.171541000
C	-1.714370000	3.828245000	1.198240000
H	-1.995717000	4.260873000	2.153095000
C	-2.136857000	4.394529000	0.000000000
H	-2.766862000	5.279865000	0.000000000
C	-1.202906000	-4.042479000	-0.707689000
H	-1.995766000	-4.406807000	-1.346975000
C	0.022425000	-3.452304000	-1.150264000
H	0.321282000	-3.315707000	-2.180728000
C	0.793583000	-3.097083000	0.000000000
H	1.822672000	-2.752194000	0.000000000
C	-1.823216000	-1.136422000	1.253686000
C	0.938084000	-0.141814000	-2.665835000
H	0.162934000	-0.738047000	-3.127526000
C	2.226712000	-0.588174000	-2.277666000
H	2.627718000	-1.584684000	-2.423110000
C	2.925129000	0.517734000	-1.732250000
H	3.946650000	0.511499000	-1.372089000
C	2.064366000	1.639462000	-1.768070000
H	2.303872000	2.636437000	-1.416912000
C	0.824751000	1.232479000	-2.337530000

C	-0.419791000	2.071653000	-2.473351000
H	-0.276733000	2.883780000	-3.199432000
H	-1.229718000	1.445844000	-2.869065000
C	-0.901808000	2.692904000	-1.171541000
C	-1.714370000	3.828245000	-1.198240000
H	-1.995717000	4.260873000	-2.153095000
C	-1.202906000	-4.042479000	0.707689000
H	-1.995766000	-4.406807000	1.346975000
C	0.022425000	-3.452304000	1.150264000
H	0.321282000	-3.315707000	2.180728000
O	-2.400998000	-0.601242000	-2.123097000
C	-1.823216000	-1.136422000	-1.253686000

Table **S11**. Y-Fe^{+} coordinates.

Y	1.021752000	0.290895000	0.000000000
Fe	-1.196421000	-2.360420000	0.000000000
O	-2.361269000	-0.776379000	2.191748000
N	-0.638833000	2.104130000	0.000000000
C	0.997477000	-0.017834000	2.613511000
H	0.275653000	-0.677725000	3.077978000
C	2.326795000	-0.355432000	2.238926000
H	2.807630000	-1.316654000	2.379885000
C	2.948378000	0.815955000	1.743139000
H	3.976464000	0.900012000	1.413691000
C	2.003449000	1.871223000	1.798359000
H	2.179884000	2.898068000	1.500017000
C	0.789608000	1.358033000	2.335982000
C	-0.508459000	2.108811000	2.482952000
H	-0.380882000	2.971163000	3.150002000
H	-1.250427000	1.464632000	2.971338000
C	-1.095453000	2.619551000	1.174193000
C	-2.074238000	3.612641000	1.198727000
H	-2.415630000	4.002785000	2.152116000
C	-2.582442000	4.103981000	0.000000000
H	-3.342127000	4.880033000	0.000000000
C	-0.760794000	-4.342871000	-0.710591000
H	-1.426906000	-4.901460000	-1.355015000
C	0.273971000	-3.460447000	-1.148860000
H	0.530535000	-3.257263000	-2.180138000
C	0.939741000	-2.934245000	0.000000000
H	1.866808000	-2.370342000	0.000000000
C	-1.879931000	-1.374300000	1.329748000
C	0.997477000	-0.017834000	-2.613511000
H	0.275653000	-0.677725000	-3.077978000
C	2.326795000	-0.355432000	-2.238926000
H	2.807630000	-1.316654000	-2.379885000
C	2.948378000	0.815955000	-1.743139000
H	3.976464000	0.900012000	-1.413691000
C	2.003449000	1.871223000	-1.798359000
H	2.179884000	2.898068000	-1.500017000
C	0.789608000	1.358033000	-2.335982000

C	-0.508459000	2.108811000	-2.482952000
H	-0.380882000	2.971163000	-3.150002000
H	-1.250427000	1.464632000	-2.971338000
C	-1.095453000	2.619551000	-1.174193000
C	-2.074238000	3.612641000	-1.198727000
H	-2.415630000	4.002785000	-2.152116000
C	-0.760794000	-4.342871000	0.710591000
H	-1.426906000	-4.901460000	1.355015000
C	0.273971000	-3.460447000	1.148860000
H	0.530535000	-3.257263000	2.180138000
O	-2.361269000	-0.776379000	-2.191748000
C	-1.879931000	-1.374300000	-1.329748000