

A Structure and Magnetism Study of $\{\text{Mn}^{\text{II}}_3\text{Mn}^{\text{IV}}\text{Ln}^{\text{III}}_3\}$ Coordination Complexes with Ln = Dy, Yb

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S.1 Crystallographic data

Compound $[\text{Mn}^{\text{II}}_3\text{Mn}^{\text{IV}}\text{Dy}^{\text{III}}_3\text{O}_3(\text{OH})(\text{L}\cdot\text{SMe})_3(\text{OOCMe})_9]\cdot 4\text{MeOH}\cdot 2\text{H}_2\text{O}$ crystallizes the monoclinic space group $P2_1/c$. The formal oxidation states of the metal centers were established by bond valence sum calculations [$\Sigma_{\text{bv}}(\text{Mn}^{\text{II}}) = 1.60\text{--}1.66$, $\Sigma_{\text{bv}}(\text{Dy}^{\text{III}}) = 3.04\text{--}3.12$, $\Sigma_{\text{bv}}(\text{O}^{\text{II-}}) = -2.05\text{--}(-)2.07$ and $\Sigma_{\text{bv}}(\text{OH}^{\text{I-}}) = -1.13$] and they are in good agreement with charge neutrality arguments of the complex. Three mono-deprotonated Schiff base ligands ($\text{L}\cdot\text{SMe-}$), nine acetate ligands, three discrete μ_4 -oxygen atoms and one μ_3 -hydroxyl group bridge the metal centers of this neutral and heptanuclear coordination complex. The acetate ligands can be separated into three different coordination groups in this molecular structure. Three μ_2 -acetate ligands bridge two Dy(III)-ions each, further three μ_2 -acetate ligands connect one Dy(III)- with one Mn(II)-ion each, third group consists of two acetate ligands, which coordinate in a μ_3 -bridging fashion and link two Mn(II)-ions with one Mn(IV)-ion each. The ninth and last carboxylic group bridges one Mn(II)- with the central Mn(IV)-ion in a μ_2 -fashion.

All four manganese ions are coordinated in a distorted octahedral fashion, where the three Mn(II)-ions are in a NO_5 coordination mode and form a triangle with non-binding $\text{Mn}^{\text{II}}\cdots\text{Mn}^{\text{II}}$ distances of $5.5129(18)\text{--}5.7492(20)$ Å. The Mn(IV) ion is in the center of this triangle, its coordination environment is saturated by six oxygen atoms and the non-binding $\text{Mn}^{\text{II}}\cdots\text{Mn}^{\text{IV}}$ distances range from $3.1816(15)$ Å to $3.3067(17)$ Å, which means they are very similar to those of $\text{Dy}\cdots\text{Mn}^{\text{IV}}$ ($3.0427(12)\text{--}3.2973(9)$ Å). The eightfold O_8 -coordinated Dy(III)-ions form a triangle above the Mn(II)-triangle, which is shifted and smaller with non-binding $\text{Dy}\cdots\text{Dy}$ distances of $3.7661(7)\text{--}3.8606(7)$ Å. This Dy-triangle is capped by a discrete hydroxyl-group with Dy–O(H) bond lengths between $2.361(4)\text{--}2.458(6)$ Å. The three μ_4 -oxygen atoms form a triangle between the manganese and dysprosium layer and connect these. As it is expected, the Dy– $\mu_4\text{O}$ bond lengths are slightly shorter ($2.270(5)\text{--}2.411(4)$ Å) as the Dy–O(H) bond lengths. The bond distances of these μ_4 -oxygen atoms to the manganese(II)-ions are shorter and range

from 2.067(5) Å to 2.183(4) Å. The shortest bond lengths of these μ_4 -oxygen atoms are between the Mn(IV)-ion and them (1.797(5)–1.880(4) Å).

The distances from the central manganese(IV)-ion to the μ_3 -acetates are slightly longer (1.954(5)–2.048(4) Å). The same oxygen atom of the μ_3 -acetates has a longer distance of 2.481(5)–2.528(4) Å to the manganese(II)-ions. The other oxygen atom of each μ_3 -acetate ligand has a shorter distance of 2.067(5)–2.219(4) Å. The acetates linking the manganese(II)-ions with the dysprosium(III)-ions have a shorter distance to the manganese(II)-ions (2.113(5)–2.198(6) Å) than to the dysprosium(III)-ions (2.295(6)–2.489(6) Å). The distances of dysprosium(III) to the oxygen atoms of acetates bridging two dysprosium(III)-ions, respectively, are 2.221(5)–2.405(6) Å. They are quite similar for the two oxygen atoms of each acetate. The Schiff base ligands (L·SMe[−]) are both bridging and chelating.

The atomic coordinates of the {Mn^{II}₃Mn^{IV}Dy^{III}₃} complex used in the calculations are given below:

Atom	X	Y	Z
Dy	-8.54785200	44.09101200	-16.78385300
Dy	-7.98860300	47.56159400	-15.56509600
Dy	-8.00883900	46.85528400	-19.27817300
Mn	-10.47473000	46.56698800	-17.30090200
Mn	-11.10308100	45.12597900	-14.53346100
Mn	-10.15173900	49.72201900	-17.41715000
Mn	-10.84351800	44.81582300	-19.97618900
O	-9.61262100	45.91781200	-15.83329300
O	-9.20377100	47.83174400	-17.53744300
O	-9.58516300	45.40916500	-18.39039700
O	-7.19673098	45.96103842	-17.22932001
H	-8.33912100	46.40516700	-11.00398900
O	-8.09730300	41.76819900	-15.95288200
O	-10.00932900	43.37457700	-15.09289400

N	-12.51697700	43.61352300	-13.67716500
C	-6.83576800	41.12233600	-16.00036700
H	-6.91524400	40.22569700	-15.61697700
H	-6.18331500	41.64281200	-15.48507700
H	-6.53898900	41.05609300	-16.93070200
C	-9.10510600	41.19094400	-15.23182800
C	-9.17099400	39.84243800	-14.95747600
H	-8.48006100	39.25808500	-15.25469100
C	-10.26782100	39.33379100	-14.23466300
H	-10.30955300	38.40876300	-14.02362300
C	-11.26206200	40.16418700	-13.83720400
H	-11.99462300	39.80458500	-13.35181200
C	-11.24022900	41.54581400	-14.12035000
C	-10.13675600	42.08048500	-14.80974800
C	-12.32645000	42.32889400	-13.61737100
H	-13.00775500	41.83917300	-13.17594500
C	-13.73601900	44.08431700	-13.09152900
C	-14.95102200	43.42899100	-13.29025800
H	-14.97401700	42.66247100	-13.85127400
C	-16.12088700	43.86193200	-12.69231100
H	-16.93633000	43.39113800	-12.83124600
C	-16.08676800	45.00461300	-11.87804700
C	-14.87784300	45.65047700	-11.69162900
H	-14.84407200	46.41699600	-11.13061300
C	-13.72119200	45.21043800	-12.30012800
H	-12.90751600	45.68833000	-12.17350400
H	-9.63442600	47.26868400	-10.63642700
O	-8.77503700	48.87742800	-20.15785900
O	-8.90993500	50.68016800	-18.84413400
C	-8.47291500	50.04140200	-19.84833300

O	-12.35789700	46.87832700	-14.54594800
O	-6.92041700	49.21337200	-13.99372600
O	-8.91586900	49.71492100	-15.62049400
N	-10.91328100	51.61229300	-16.51917400
C	-5.72993100	49.01227900	-13.21111800
H	-5.54132600	49.81901600	-12.68879400
H	-4.97449200	48.82538000	-13.80730700
H	-5.86230000	48.25285700	-12.60437800
C	-7.60058800	50.40336900	-13.80379000
C	-7.28393500	51.31656800	-12.82069400
H	-6.58286000	51.12730400	-12.20691800
C	-7.99252000	52.51839400	-12.72572600
H	-7.77461000	53.15006300	-12.04863800
C	-8.99013000	52.77626600	-13.60154300
H	-9.45983600	53.60193100	-13.54526500
C	-9.35313400	51.83941000	-14.59870800
C	-8.64684500	50.61865700	-14.69895200
C	-10.44838800	52.22976700	-15.47276600
H	-10.88271100	53.04360200	-15.24941500
C	-7.48474000	50.75350700	-20.73822000
H	-7.22298200	50.16442300	-21.47510200
H	-6.69058800	50.99718500	-20.21589500
C	-12.23540000	47.87669500	-15.27931200
C	-13.08976100	49.09744700	-15.02254700
H	-13.64896900	48.94367000	-14.23466300
H	-13.65880300	49.26541900	-15.80163700
H	-12.51161000	49.87343000	-14.86602500
H	-7.89818400	51.56497700	-21.10050500
O	-11.46019200	47.97369200	-16.28878800
O	-11.50650600	47.06522500	-18.91799800

O	-11.77582600	49.30090600	-18.78258000
C	-12.05161000	48.17242000	-19.23455800
C	-13.13473500	48.03756900	-20.29855200
C	-13.98610100	44.14346200	-16.88673500
H	-14.57649900	43.69159400	-17.52513200
H	-14.46152300	44.89815200	-16.48224200
H	-13.72155600	43.51179400	-16.18502700
H	-7.16262023	45.22447443	-15.00949223
O	-7.04982300	47.10544400	-21.60700200
O	-9.34942100	46.01007800	-21.00202000
N	-11.84379300	44.89105500	-21.97632200
C	-5.71445200	47.46504500	-21.92708000
H	-5.60777500	47.48870300	-22.90138200
H	-5.09801400	46.80262100	-21.54896600
H	-5.51473600	48.34748900	-21.55248300
C	-7.91419900	46.89725300	-22.65692700
C	-7.61456900	47.16458900	-23.96185900
H	-6.77889200	47.55494600	-24.19224500
C	-8.56185300	46.85466900	-24.96957600
H	-8.37225500	47.05103000	-25.87880800
C	-9.73436300	46.27978000	-24.63015300
H	-10.35338200	46.06922300	-25.31779300
C	-10.06953100	45.98405500	-23.31115200
C	-9.13044100	46.28451100	-22.28760700
C	-11.33821500	45.35475200	-23.07549000
H	-11.89255800	45.26248600	-23.84227000
H	-13.84071300	47.44138700	-19.97319900
H	-12.74298300	47.66140700	-21.11633300
O	-11.91308400	45.26012000	-16.83573400
H	-6.59476951	48.20008025	-17.46820920

H	-7.18557311	44.44909362	-18.80681345
O	-12.60390200	44.44155300	-18.80368400
C	-8.91718200	47.14093100	-11.29065200
H	-8.38675000	47.96422900	-11.35924000
C	-12.76615600	44.64264600	-17.59899600
H	-13.51279700	48.92001200	-20.49376500
O	-6.94520700	44.13873100	-15.07530700
O	-6.51903800	46.20644000	-14.37359800
C	-6.28436600	44.96912600	-14.43515200
C	-5.07151700	44.46994300	-13.64902700
H	-4.98063400	43.49996500	-13.76861600
H	-5.19035000	44.67103600	-12.69934600
H	-4.26291300	44.91471300	-13.97789800
O	-6.17723800	48.61245800	-16.64755700
O	-6.17040000	48.19134600	-18.82303000
C	-5.63382500	48.60062900	-17.75551800
C	-4.23032000	49.13293400	-17.89269400
H	-3.90142200	49.42156200	-17.01511800
H	-4.22820400	49.89708800	-18.50822800
H	-3.64573000	48.42792600	-18.24442800
O	-7.09401800	43.32253000	-18.39039700
O	-6.62871300	45.01407700	-19.78502100
C	-6.40944700	43.88085800	-19.29787000
C	-5.24710600	43.11670500	-19.88174800
H	-4.81018900	43.66083900	-20.56938700
H	-5.57036500	42.28394300	-20.28272400
H	-4.60381500	42.90851500	-19.17300500
O	-10.03902300	42.68139800	-17.87862500
O	-10.32247300	42.73817700	-20.08399500
C	-10.04689500	42.14672700	-18.99889600

C	-9.73315900	40.66337000	-19.05869100
H	-9.54362500	40.33215800	-18.15473600
H	-8.95196400	40.51669100	-19.63201700
H	-10.50447100	40.18074700	-19.42625300
O	-9.15612700	47.53128800	-13.55054100
O	-10.22842400	45.76640100	-12.71693200
C	-9.51448400	46.81681600	-12.63955100
H	-7.79788754	41.61172320	-15.96535040
H	-10.08329199	43.14064796	-15.00873568
H	-16.97922372	45.38202610	-11.40109612
H	-10.27682016	51.21374247	-17.19458133
H	-6.62356702	49.16595786	-13.79780145
H	-8.89917175	49.87239348	-15.43774965
H	-11.65957392	46.96467958	-15.22406525
H	-11.23549626	44.57766485	-21.23344806
H	-10.11568972	46.84623471	-13.53625955
H	-12.13366693	44.89859482	-18.43616252

Table S1. Selected bond length of $\{\text{Mn}^{\text{II}}_3\text{Mn}^{\text{IV}}\text{Dy}^{\text{III}}_3\}$ and $\{\text{Mn}^{\text{II}}_3\text{Mn}^{\text{IV}}\text{Yb}^{\text{III}}_3\}$ complexes. Data for $\{\text{Mn}^{\text{II}}_3\text{Mn}^{\text{IV}}\text{Yb}^{\text{III}}_3\}$ complex has been taken from [35].

Bond	Distance in Å	Bond	Distance in Å
$\{\text{Mn}^{\text{II}}_3\text{Mn}^{\text{IV}}\text{Dy}^{\text{III}}_3\}$		$\{\text{Mn}^{\text{II}}_3\text{Mn}^{\text{IV}}\text{Yb}^{\text{III}}_3\}$	
$\text{Mn}^{\text{II}}\text{--N}_{\text{imine}}$	2.207(7)–2.269(5)	$\text{Mn}^{\text{II}}\text{--N}_{\text{imine}}$	2.229(4)–2.239(4)
$\text{Mn}^{\text{II}}\text{--O}_{\text{alkoxide}}$	2.099(6)–2.186(4)	$\text{Mn}^{\text{II}}\text{--O}_{\text{alkoxide}}$	2.143(3)–2.180(3)
$\text{Dy}^{\text{III}}\text{--O}_{\text{alkoxide}}$	2.289(5)–2.447(4)	$\text{Yb}^{\text{III}}\text{--O}_{\text{alkoxide}}$	2.295(3)–2.310(3)
$\text{Dy}^{\text{III}}\text{--O}_{\text{ether}}$	2.488(5)–2.667(6)	$\text{Yb}^{\text{III}}\text{--O}_{\text{ether}}$	2.493(3)–2.523(3)
$\text{Dy}^{\text{III}}\text{--O}_{\text{acetate}}$	2.221(5)–2.488(5)	$\text{Yb}^{\text{III}}\text{--O}_{\text{acetate}}$	2.261(3)–2.326(3)
$\text{Mn}^{\text{II}}\text{--O}_{\text{acetate}}$	2.067(4)–2.527(4)	$\text{Mn}^{\text{II}}\text{--O}_{\text{acetate}}$	2.112(3)–2.603(3)
$\text{Mn}^{\text{II}}\text{--}\mu_4\text{--O}$	2.067(4)–2.184(4)	$\text{Mn}^{\text{II}}\text{--}\mu_4\text{--O}$	2.102(3)–2.140(3)
$\text{Dy}^{\text{III}}\text{--O(H)}$	2.361(5)–2.458(5)	$\text{Yb}^{\text{III}}\text{--O(H)}$	2.325(3)–2.344(3)

Dy ^{III} ...Dy ^{III}	3.7661(7)–3.8606(7)	Yb ^{III} ...Yb ^{III}	3.6765(3)–3.7119(3)
Mn ^{II} ...Mn ^{II}	5.5129(18)–5.7492(20)	Mn ^{II} ...Mn ^{II}	5.4468(10)–5.5796(10)
Mn ^{II} ...Mn ^{IV}	3.1816(15)–3.3067(17)	Mn ^{II} ...Mn ^{IV}	3.1704(10)–3.2151(10)
Dy ^{III} ...Mn ^{IV}	3.0427(12)–3.2973(9)	Yb ^{III} ...Mn ^{IV}	3.1395(7)–3.1506(8)
Mn ^{IV} –O _{acetate}	1.955(4)–2.049(4)	Mn ^{IV} –O _{acetate}	1.986(3)–2.004(3)
Mn ^{IV} – μ_4 -O	1.791(4)–1.880(4)	Mn ^{IV} – μ_4 -O	1.816(3)–1.822(3)
Dy ^{III} – μ_4 -O	2.269(4)–2.411(5)	Yb ^{III} – μ_4 -O	2.277(3)–2.300(3)

S.2 X-ray spectroscopy measurements

All XAS were performed on powdered samples. For the XMCD experiment, {Mn^{II}₃Mn^{IV}Dy^{III}₃} and {Mn^{II}₃Mn^{IV}Yb^{III}₃} coordination complexes have been dissolved in an acetonitrile solution before being applied to a gold substrate. The gold substrate was prepared in a vacuum atmosphere by sputtering and its quality was controlled by the STM method. Drops of the sample in solution were deposited onto the gold surface and dried in air. The method ensured efficient adsorption of molecules on a gold substrate, which was confirmed by the stability of the XMCD signal during measurements.

EXAFS experiments at the P64 beamline of the PETRA-III synchrotron radiation facility in Hamburg (Germany) were conducted in the transmission mode using nitrogen filled ionization chambers for a detection of the intensities of incident and transmitted X-rays. The energy scan was performed with the use of the Si(111) double crystal monochromator. The DCM resolving power was between 1 and 2×10⁴, which corresponds to the experimental resolution of 1.5 eV at the Mn K-edge. The energy step size was set to 0.15 eV in the near-edge region, while for EXAFS signal acquisition, it was k-dependent with a value equal to 0.005 Å⁻¹. Calibration was performed using the Mn foil to the first inflection point in the Mn K-edge XANES spectrum (6550 eV); Mn EXAFS spectra were measured up to 1000 eV above the Mn K-edge at room temperature.

Mn L_{2,3} XAS spectra were collected at the BESSY synchrotron radiation facility in Berlin (Germany) using the U49-2 GM-1 and RGLB beamlines.

REXS spectra were acquired at the PEAXIS beamline at the BESSY synchrotron radiation facility with an incident angle on the sample of 65° and a scattering angle 2θ of 130°. To maximize signal intensity and reduce measurement time, the REXS spectrometer was operated in backscattering geometry.

The XAS/XMCD study was performed at the 4IDC beamline of the Advanced Photon Source located at Argonne National Laboratory (Chicago, IL, USA). The XMCD experiment was conducted at the sample temperatures of 6 and 25K. The X-ray incident angle is fixed at $\sim 20 \pm 2$ degrees with respect to the sample surface and XAS/XMCD spectra were collected in the total-electron-yield mode which was performed by measuring the drain current from an electrically isolated sample. At the same time, the X-ray fluorescence yield was measured with a Vortex detector mounted perpendicular to the X-ray beam. The TEY mode probes approximately the first 2 nm of the sample surface, while TFY is bulk sensitive. We must point out that the XAS TEY spectra of powder samples measured at low temperature contain low-frequency oscillations in the background due to charging effect of the isolating grains. This effect is energy and temperature dependent and is more pronounced at higher energies. Due to the grazing incidence geometry, the TFY signal is particularly susceptible to self-absorption, which distorts the spectra noticeably. Therefore, TEY spectra were used for subsequent analysis. The samples were mounted on a double-sided carbon tape and placed in a vacuum chamber with a split-coil superconducting magnet. The magnetic field was applied in a helicity-switching mode in the same direction as the propagation vector of the incident polarized X-rays. We switched the directions of the magnetic field to provide right and left circular X-ray configurations with fixed circular polarization of the incident X-ray beam. Magnetic fields up to ± 5 Tesla were applied during the measurements.

The incident photon flux and the overall energy resolution for the soft X-ray experiments are shown in Table S2.

Table S2. The incident photon flux and the overall energy resolution for the soft X-ray experiments.

Beamline	Photon flux (phot/sec) at 600 eV	Energy resolution (eV) at 600 eV
RGBL, BESSY	1×10^9	0.12
PEAXIS, BESSY	1×10^{12}	0.085
4-ID-C, APS	2×10^{12}	0.343

Mn L_{2,3} XAS spectra of {Mn^{II}₃Mn^{IV}Dy^{III}₃} and {Mn^{II}₃Mn^{IV}Yb^{III}₃} coordination complexes measured at the different beamlines are shown in Figure S1.

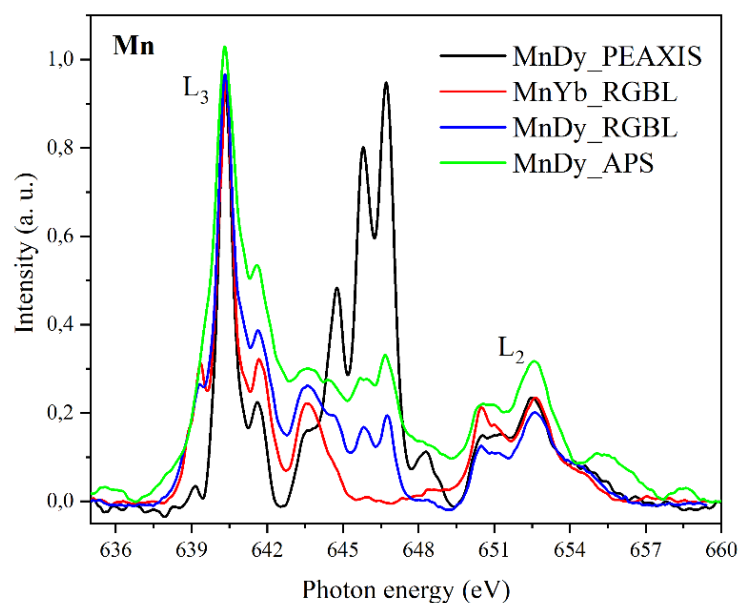


Figure S1. Mn L_{2,3} XAS spectra of {Mn^{II}₃Mn^{IV}Dy^{III}₃} and {Mn^{II}₃Mn^{IV}Yb^{III}₃} coordination complexes measured at the different beamlines.

Dy $M_{4,5}$ XAS spectra have been compared those of the reference Dy_2O_3 compound (from Alfa Aesar) and confirm the formal 3+ b valence state for the Dy atoms in the $\{Mn^{II}_3Mn^{IV}Dy^{III}_3\}$ coordination complex.

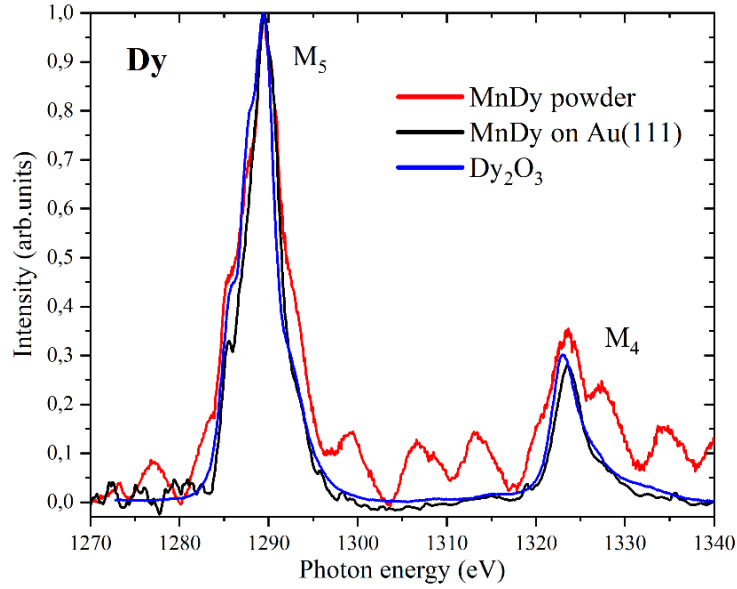


Figure S2. Dy $M_{4,5}$ XAS spectra of the Dy_2O_3 oxide and the $\{Mn^{II}_3Mn^{IV}Dy^{III}_3\}$ complex as powder and after deposition on Au(111) substrate.

S.3 XMCD sum rules analysis

Sum rules for the Mn single ion have been used to estimate spin and orbital components to the shell-specific magnetic moment, projected onto the axis of external magnetic field [S1]:

$$m_L = -\frac{4}{3} \frac{\int_{L_3+L_2} (\mu^+ - \mu^-) d\varepsilon}{\int_{L_3+L_2} (\mu^+ + \mu^-) d\varepsilon} N_{3d} = \frac{4q}{3r} N_{3d}, \quad (1)$$

$$m_S + \frac{7}{2} \langle T_Z \rangle = -\frac{6 \int_{L_3} (\mu^+ - \mu^-) d\varepsilon - 4 \int_{L_2} (\mu^+ - \mu^-) d\varepsilon}{\int_{L_3+L_2} (\mu^+ + \mu^-) d\varepsilon} N_{3d} = -\frac{(6p-4q)}{r} N_{3d}, \quad (2)$$

$$m_{tot} = m_L + m_S = -(\langle L_Z \rangle + 2\langle S_Z \rangle), \quad (3)$$

where $\langle T_Z \rangle$ is the magnetic-dipole operator, N_{3d} is the number of holes on the Mn 3d energy level, p is the integrated XMCD intensity at the Mn L_3 edge, q is the integrated XMCD intensity

at the Mn L₂ edge, r is the sum of the integrated intensities at Mn L₃ and L₂ edges. m_L , m_S and m_{tot} are the orbital, spin, and total magnetic moments, respectively.

The sum rules for the M_{4,5} edges of Dy, for the expectation values of the orbital angular momentum $\langle L_Z \rangle$ and the spin angular momentum $\langle S_Z \rangle$ can be written as [S2]:

$$m_L = \langle L_Z \rangle = -\frac{(q+p)N_{4f}}{r}, \quad (4)$$

$$\langle S_Z \rangle + \frac{7}{2}\langle T_Z \rangle = -\frac{(2p-3q)N_{4f}}{2r}, \quad (5)$$

where N_{4f} is the number of holes on the Dy 4f energy level, p is the integrated XMCD intensity at the Dy M₅ edge, q is the integrated XMCD intensity at the Dy M₄ edge, r is the sum of the integrated intensities at Dy M₅ and M₄ edges.

Figure S13 shows the application of the sum rule analysis to the Mn L_{2,3} and Dy M_{4,5} XMCD spectra of the {Mn^{II}₃Mn^{IV}Dy^{III}₃} complex.

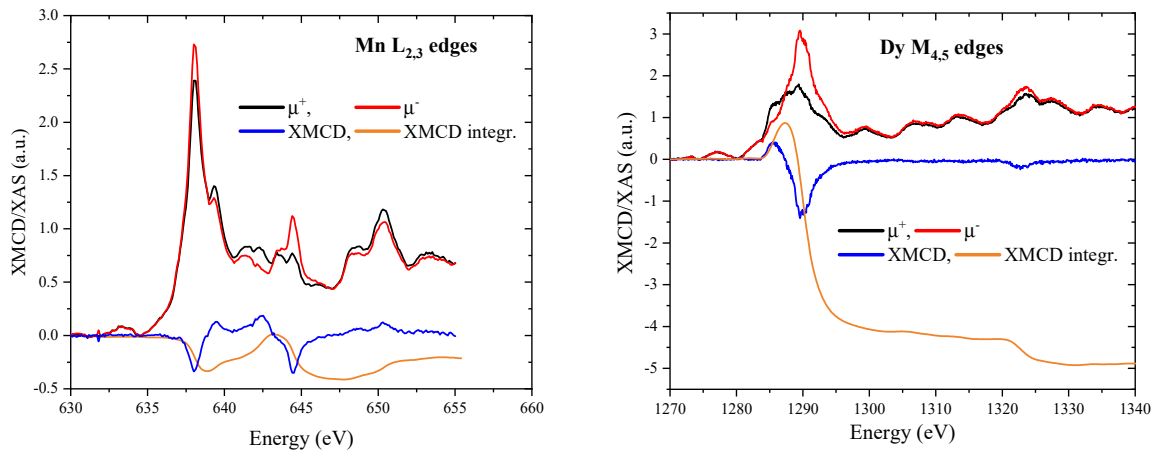


Figure S3. XAS spectra beyond the Mn L_{2,3} (left) and Dy M_{4,5} (right) edges of the {Mn^{II}₃Mn^{IV}Dy^{III}₃} complex in an external magnetic field of B = 5T and at a temperature of T = 6K, performed with right (RCP) and left (LCP) circular polarized photons leading to the dichroic spectra labelled μ^+ and μ^- . The corresponding XMCD signals and their integrals are also shown.

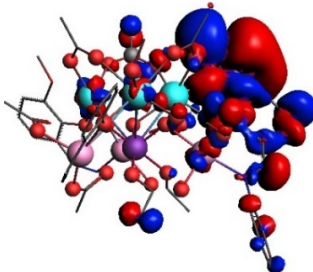
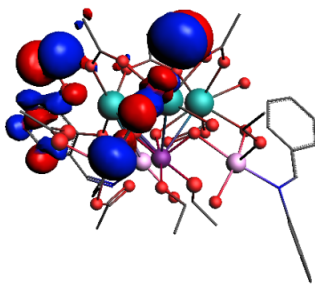
REFERENCES

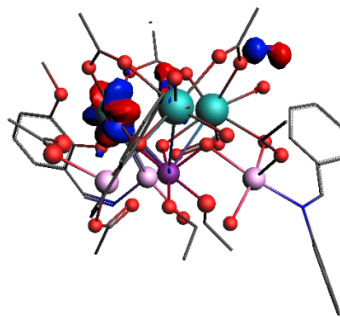
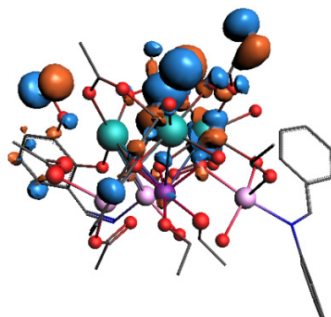
[S1] Crocombette, J.P., Thole, B.T., Jollet, F. The importance of the magnetic dipole term in magneto-circular x-ray absorption dichroism for 3d transition metal compounds. *J. Phys.: Condens. Matter* **1996**, 8, 4095.

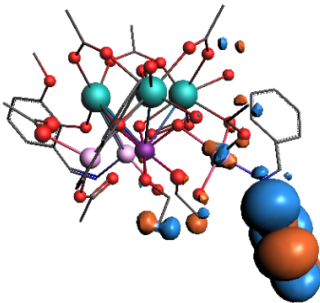
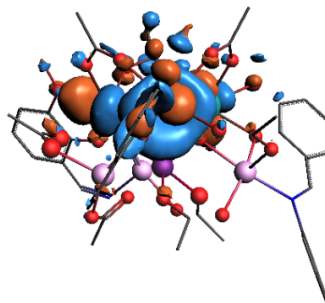
[S2] Krishnamurthy, V.V., Keavney, D.J., Haskel, D., Lang, J.C., Srajer, G., Sales, B.C., Mandrus, D.G., Robertson, J.L. Temperature dependence of Eu 4f and Eu 5d magnetizations in the filled skutterudite $\text{EuFe}_4\text{Sb}_{12}$. *Phys. Rev. B* **2009**, 79, 014426.

S4. DFT analysis of molecular orbitals

Table S3. A detailed composition of HOMO-1, HOMO, LUMO, and LUMO+1 molecular orbitals for the $\{\text{Mn}^{\text{II}}_3\text{Mn}^{\text{IV}}\text{Dy}^{\text{III}}_3\}$ complex.

Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
-6.418 (HOMO-1)	326 A	39.31%	1 P:y	39 C	-6.612	326 B	32.66%	1 P:z	86 C
		23.24%	1 P:z	39 C			25.91%	1 P:y	63 C
		8.75%	1 P:x	39 C			6.66%	1 P:z	63 C
		2.14%	1 P:y	13 O			3.49%	1 P:y	69 C
		1.84%	1 P:x	42 C			2.00%	1 P:z	54 C
		1.76%	1 F:z3	3 Dy			1.78%	1 P:x	54 C
		1.60%	2 S	42 C			1.70%	1 P:z	47 C
		1.41%	1 P:y	44 C			1.49%	1 P:x	43 C
		1.36%	1 F:z3	2 Dy			1.37%	1 P:y	68 C
		1.29%	1 F:z	3 Dy			1.25%	1 P:x	67 C
		1.07%	2 P:x	41 C			1.23%	1 P:x	69 C
Spin up					Spin down				

E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom		
-6.377 (HOMO)	327 A	49.43%	1 F:z3	3 Dy	-6.557	327 B	23.12%	1 F:z2x	1 Dy		
		31.18%	1 F:z	3 Dy			15.46%	1 P:x	11 O		
		2.65%	1 F:x	3 Dy			11.23%	1 F:z	1 Dy		
		2.56%	1 F:xyz	3 Dy			8.26%	1 P:z	86 C		
		1.97%	1 F:y	3 Dy			5.11%	1 P:y	63 C		
		1.57%	1 P:y	39 C			3.73%	1 F:z2y	1 Dy		
		1.28%	1 F:z3	2 Dy			3.34%	1 P:x	84 C		
		1.22%	1 P:x	11 O			2.57%	1 P:y	11 O		
							1.68%	1 P:z	63 C		
Spin up					Spin down						
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom		

-6.163	328 A	11.75	1 P:y	53 C	-6.374 (LUMO)	328 A	30.80	1 F:x	1 Dy
		10.26	2 S	53 C			15.83	1 F:z2x	1 Dy
		10.16	1 P:y	57 C			13.42	1 P:x	11 O
		7.51	2 S	59 C			9.32	1 F:z2y	1 Dy
		7.29	2 S	57 C			7.72	1 F:z3	1 Dy
		6.32	1 P:z	53 C			5.35	1 F:y	1 Dy
		5.87	2 S	55 C			2.05	1 P:y	51 C
		5.82	1 P:x	59 C			1.99	1 P:y	11 O
		5.31	2 S	56 C					
		5.28	1 P:z	57 C					
		4.26	1 P:x	55 C					
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
-6.059	329 A	64.99	1 F:xyz	2 Dy	-6.267 (LUMO+1)	329 A	53.63	1 F:xyz	1 Dy

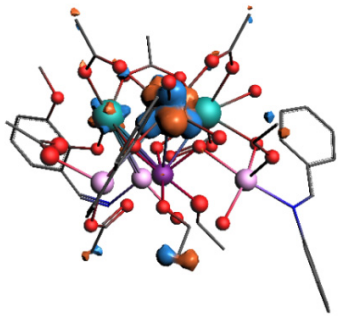
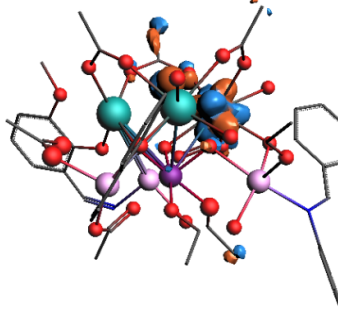
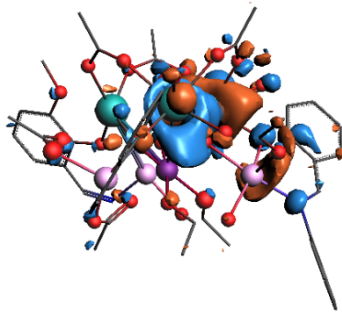
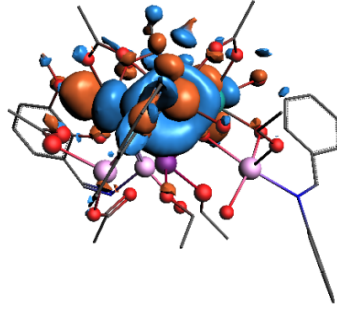
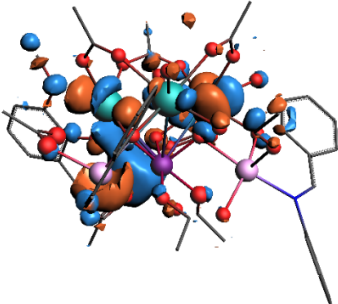
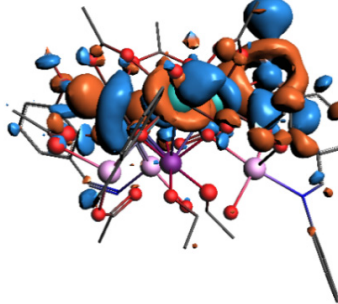
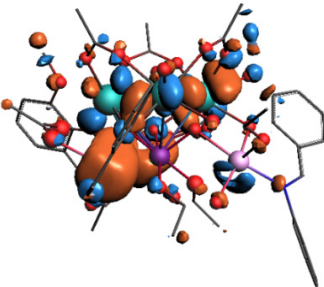
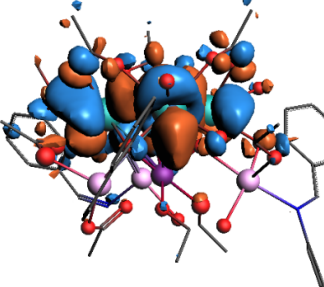
	13.79	1 F:z	2 Dy		25.72	1 F:z	1 Dy
	1.82	1 F:z2y	3 Dy		3.23	1 F:z2y	1 Dy
	1.73	1 F:z2x	2 Dy		2.70	1 F:z2x	1 Dy
	1.57	1 F:xyz	3 Dy		2.30	1 P:z	11 O
	1.47	1 F:y	2 Dy		1.13	1 P:x	65 C
	1.13	1 P:z	78 C		1.12	1 F:x	1 Dy
	1.05	1 F:y	3 Dy				

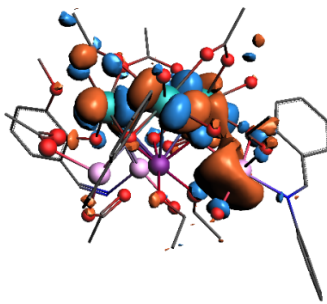
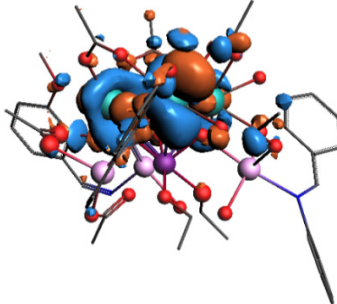
Table S4. A detailed composition of selected molecular orbitals in the energy range 0 – 3 eV above the Fermi level for the $\{\text{Mn}^{\text{II}}_3\text{Mn}^{\text{IV}}\text{Dy}^{\text{III}}_3\}$ complex.

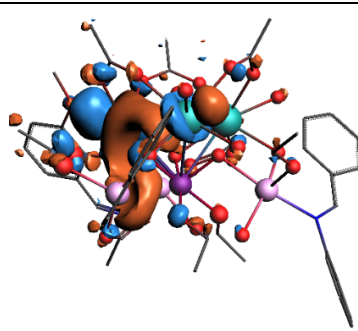
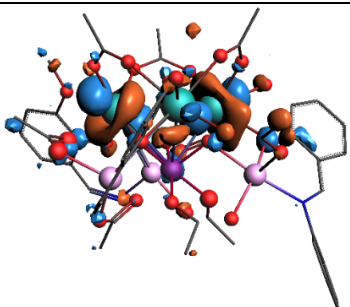
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
0.322	404 A	9.52	1 D:yz	1 D	0.323	404 A	15.90	1 D:yz	2 Dy

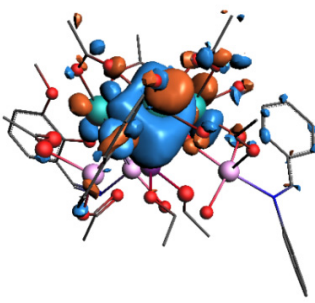
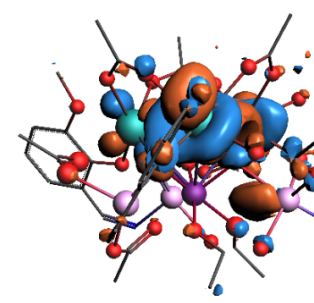
		9.16	1 D:x2-y2	1 Dy			15.3	1 D:yz	3 Dy
		9.16	2 S	3 Dy			8.98	1 D:x2-y2	1 Dy
		8.88	2 S	2 Dy			5.01	2 S	4 Mn
		8.39	1 D:z2	1 D			4.75	3 S	6 Mn
		4.71	2 S	7 Mn			2.16	1 P:y	66 C
		2.59	3 S	5 Mn					
		2.41	2 S	6 Mn					
		2.36	2 P:y	5 Mn					
		1.67	1 D:xy	1 D					
		1.57	2 P:x	2 Dy					
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
0.378	405 A	15.49	1 D:yz	1 Dy	0.373	405 A	9.60	1 D:yz	3 Dy

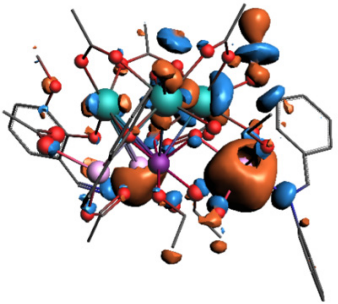
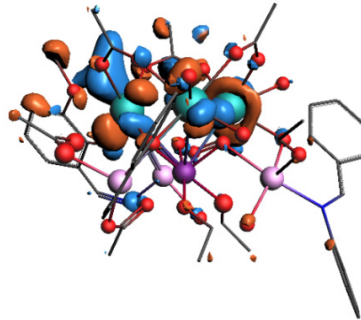
					12.23	2 S	2 Dy						8.48	1 P:x	39 C
					6.24	1 D:z2	3 Dy						7.43	1 D:z2	2 Dy
					6.08	2 S	1 Dy						5.99	3 S	5 Mn
					5.07	3 S	7 Mn						4.86	2 S	2 Dy
					4.95	2 S	6 Mn						4.77	1 D:x2-	1 Dy
					4.95	3 S	2 Dy						4.40	1 D:z2	1 Dy
					4.46	1 D:xz	3 Dy						3.89	2 S	6 Mn
					4.44	2 S	7 Mn						2.61	2 S	13 O
					4.24	3 S	5 Mn						2.46	3 S	13 O
					4.07	1 D:z2	2 Dy						1.99	1 P:y	49 C
					2.30	2 P:z	2 Dy						1.89	1 D:xz	3 Dy
					2.20	1 P:x	86 C						1.89	1 D:xz	2 Dy
					2.09	2 P:y	1 Dy								
Spin up					Spin down										
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom						
0.503	406 A	14.04	2 S	1 Dy	0.503	406 A	13.65	1 D:z2	1 Dy						

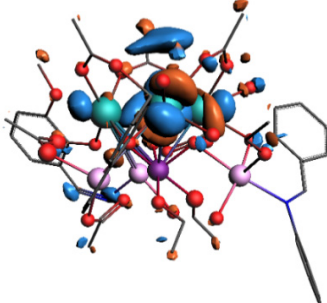
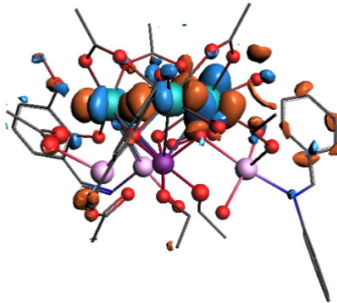
		8.82	1 D:yz	2 Dy			10.95	1 D:z2	3 Dy
		8.55	2 S	5 Mn			9.06	1 D:xz	3 Dy
		8.23	2 S	3 Dy			6.94	1 D:xy	2 Dy
		6.36	3 S	7 Mn			5.65	2 S	4 Mn
		5.51	2 S	6 Mn			5.20	1 D:xz	2 Dy
		3.67	1 D:xz	3 Dy			4.56	1 D:x2-y2	3 Dy
		3.58	3 S	6 Mn			4.43	1 D:xy	3 Dy
		3.51	1 D:z2	1 Dy			3.77	2 S	2 Dy
		2.84	1 D:xz	1 Dy			2.57	3 S	7 Mn
		2.60	3 S	3 Dy			2.46	1 D:yz	2 Dy
		2.58	1 D:xy	1 Dy					
		2.38	1 D:z2	3 Dy					
		2.08	2 S	4 Mn					
		2.06	2 P:y	1 Dy					
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
0.525	407 A	15.91	3 S	5 Mn	0.614	407 A	12.99	1 D:xz	2 Dy

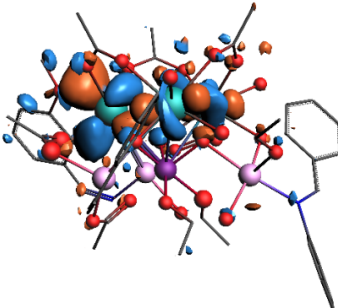
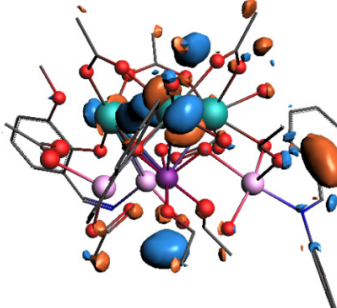
		12.38	1 D:xy	1 Dy			10.67	1 D:z2	2 Dy
		7.50	2 S	4 Mn			8.42	1 D:z2	3 Dy
		6.76	1 D:xy	2 Dy			6.27	2 S	6 Mn
		6.70	2 S	5 Mn			5.88	2 S	3 Dy
		5.09	2 S	3 Dy			5.86	1 D:x2-y2	1 Dy
		4.84	3 S	7 Mn			4.24	2 S	4 Mn
		4.75	1 D:yz	1 Dy			3.94	1 D:xy	2 Dy
		4.50	2 S	6 Mn			3.12	3 S	4 Mn
		3.84	1 D:x2-y2	3 Dy			3.12	3 S	7 Mn
		3.49	1 D:z2	3 Dy			2.89	2 S	1 Dy
		3.38	1 D:z2	2 Dy			2.27	2 D:xz	2 Dy
		3.03	3 S	1 Dy			1.94	2 P:y	3 Dy
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
0.646	408 A	24.71	1 D:yz	3 Dy	0.688	408 A	13.11	2 S	7 Mn

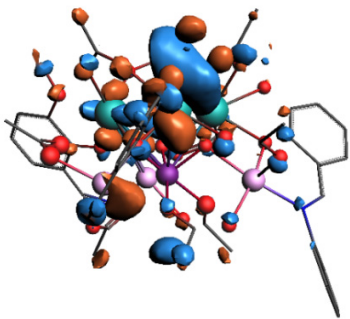
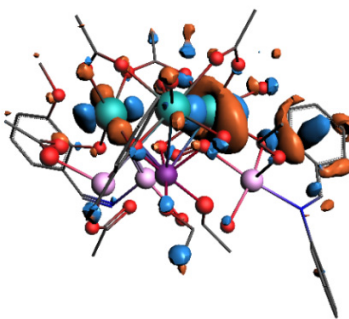
		15.38	3 S	6 Mn			6.71	2 S	1 Dy
		7.78	1 D:z2	2 Dy			6.54	1 D:xy	3 Dy
		6.98	2 S	6 Mn			6.50	3 S	2 Dy
		5.77	2 S	4 Mn			6.35	2 S	3 Dy
		4.60	2 S	7 Mn			6.21	1 D:z2	3 Dy
		4.48	2 S	3 Dy			5.95	2 S	2 Dy
		4.03	1 D:xy	3 Dy			4.78	1 D:yz	2 Dy
		3.69	1 D:yz	2 Dy			3.88	1 D:x2-y2	1 Dy
		3.21	2 S	2 Dy			3.52	2 P:z	2 Dy
		2.30	2 P:y	72 C			3.28	2 S	6 Mn
		2.25	1 D:xz	3 Dy			2.97	2 P:z	1 Dy
		2.03	3 S	4 Mn			2.25	1 D:z2	2 Dy
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
0.751	409 A	12.54	1 D:z2	2 Dy	0.718	409 A	13.97	1 D:yz	1 Dy

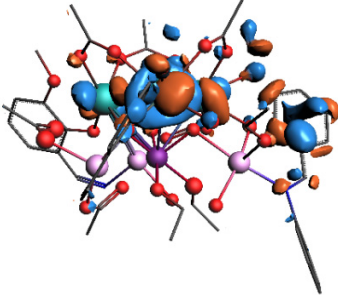
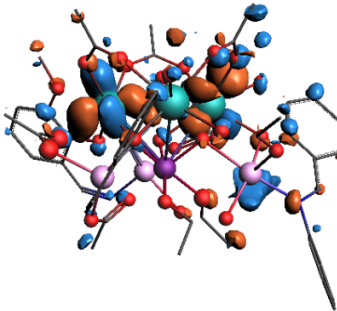
									
		7.01	1 D:xz	2 Dy			10.34	1 D:xy	2 Dy
		6.94	1 D:yz	2 Dy			8.21	1 D:z2	2 Dy
		5.89	1 D:x2-y2	1 Dy			7.06	2 S	6 Mn
		5.77	1 D:xy	1 Dy			4.07	1 D:xz	3 Dy
		5.16	2 S	2 Dy			3.78	2 S	2 Dy
		3.47	3 S	4 Mn			3.69	2 P:z	2 Dy
		3.34	1 D:xy	2 Dy			3.41	1 D:xz	2 Dy
		3.01	2 S	6 Mn			2.85	1 D:yz	2 Dy
		2.91	2 S	4 Mn			2.46	2 P:y	1 Dy
		2.04	1 D:xz	1 Dy			2.31	3 S	3 Dy
		1.96	1 D:xz	3 Dy			2.26	1 D:xy	1 Dy
		1.95	3 S	5 Mn			1.98	1 D:z2	3 Dy
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
0.802	410 A	12.67	3 S	5 Mn	0.786	410 A	18.87	2 S	3 Dy

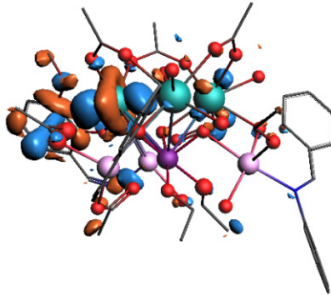
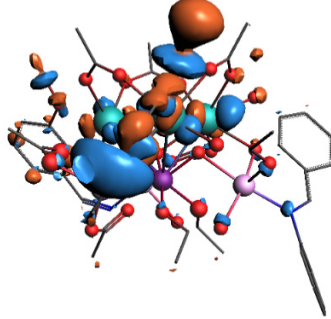
					6.90	2 S	7 Mn						12.03	1 D:xz	3 Dy
					6.00	1 P:x	39 C						8.18	2 S	2 Dy
					5.16	2 S	6 Mn						6.44	2 S	7 Mn
					4.87	2 S	2 Dy						5.72	3 S	5 Mn
					3.90	2 S	4 Mn						5.31	1 D:x2-y2	1 Dy
					3.80	1 D:z2	1 Dy						3.81	2 S	5 Mn
					2.64	2 S	5 Mn						3.43	3 S	3 Dy
					2.42	1 D:xy	1 Dy						3.06	3 S	43 C
													2.89	2 P:x	60 C
										2.35	1 D:xy	2 Dy			
										2.21	3 S	6 Mn			
										2.06	1 D:yz	1 Dy			
Spin up					Spin down										
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom						
0.861	411 A	17.89	2 S	1 Dy	0.828	411 A	15.19	2 S	1 Dy						

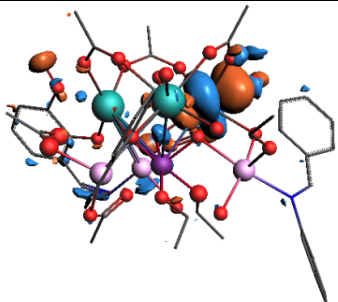
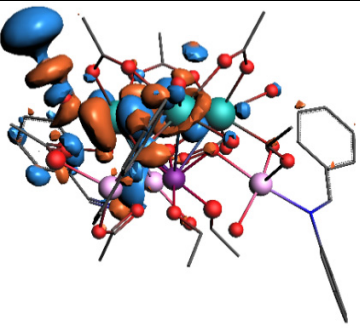
		10.11	3 S	4 Mn			9.21	2 S	6 Mn
		9.35	2 S	4 Mn			8.16	2 S	3 Dy
		8.72	3 S	7 Mn			8.16	1 D:z2	3 Dy
		5.43	3 S	1 Dy			5.17	3 S	6 Mn
		4.79	2 P:x	3 Dy			4.43	1 D:yz	1 Dy
		3.95	1 D:xz	2 Dy			3.67	2 S	2 Dy
		3.40	2 P:x	70 C			3.63	1 D:x2-y2	1 Dy
		3.12	1 D:yz	1 Dy			3.25	3 S	3 Dy
		2.87	1 D:xy	2 Dy			3.14	1 D:yz	2 Dy
		2.82	2 S	3 Dy			2.53	2 P:y	41 C
		2.81	2 S	7 Mn			2.40	3 S	1 Dy
		2.47	1 D:yz	2 Dy			2.38	2 P:y	48 C
		2.46	2 P:x	1 Dy			2.35	1 D:z2	1 Dy
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
0.894	412 A	26.38	1 D:xz	3 Dy	0.862	412 A	29.69	2 S	4 Mn

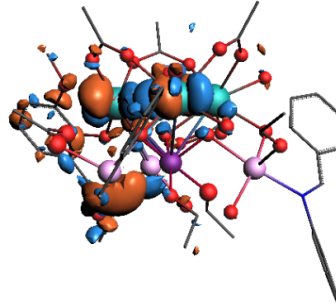
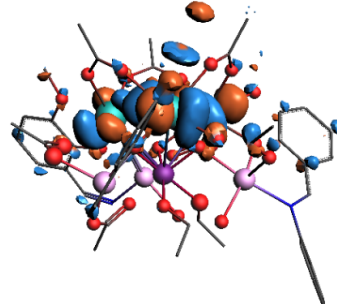
		11.87	2 S	1 Dy			20.78	3 S	4 Mn
		5.92	3 S	6 Mn			17.32	2 S	1 Dy
		3.94	1 D:z2	2 Dy			8.40	2 S	3 Dy
		3.42	2 S	3 Dy			8.09	3 S	5 Mn
		2.75	3 S	7 Mn			6.97	2 S	5 Mn
		2.27	1 D:yz	1 Dy			6.58	2 S	6 Mn
		2.20	2 P:y	7 Mn			4.26	2 S	2 Dy
		2.09	2 D:yz	1 Dy			3.85	3 S	6 Mn
		1.94	2 P:x	3 Dy			3.66	2 P:x	83 C
		1.91	2 S	5 Mn			3.58	2 P:x	3 Dy
							3.39	2 P:z	3 Dy
							3.32	2 P:x	1 Dy
							3.28	2 D:z2	3 Dy
							3.09	1 D:z2	2 Dy
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
0.902	413 A	9.44	2 S	5 Mn	0.989	413 A	7.91	1 D:x2-y2	1 Dy

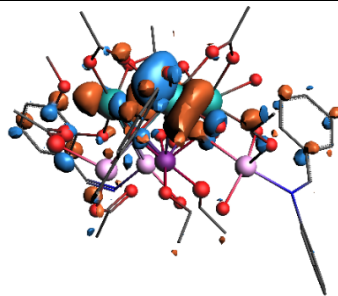
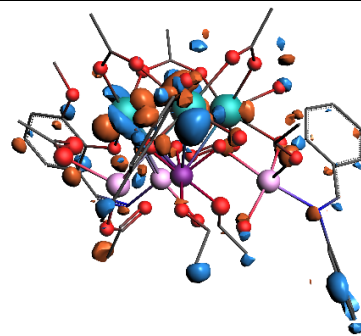
		8.64	2 P:x	2 Dy			6.98	2 P:x	2 Dy
		7.00	2 S	6 Mn			6.92	1 D:z2	1 Dy
		5.86	1 D:yz	2 Dy			5.65	2 S	6 Mn
		5.74	1 D:xz	2 Dy			5.43	1 D:yz	1 Dy
		5.28	3 S	4 Mn			4.20	2 P:y	3 Dy
		4.44	2 S	2 Dy			3.94	1 D:xz	3 Dy
		4.32	1 D:xy	2 Dy			3.27	1 D:xy	1 Dy
		4.03	2 P:x	72 C			3.26	2 S	3 Dy
		3.87	2 S	4 Mn			2.76	1 P:y	49 C
		3.83	2 P:y	3 Dy			2.71	3 S	44 C
		2.31	1 D:z2	2 Dy			2.50	3 S	7 Mn
		2.31	1 D:xy	1 Dy			2.45	3 S	5 Mn
		2.30	3 S	5 Mn			2.18	1 D:yz	2 Dy
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
0.973	414 A	15.71	1 D:yz	2 Dy	0.997	414 A	11.81	1 D:xy	1 Dy

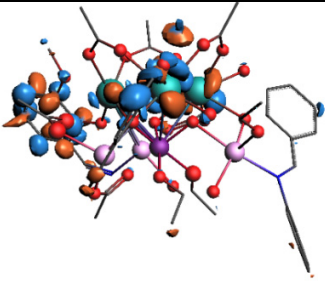
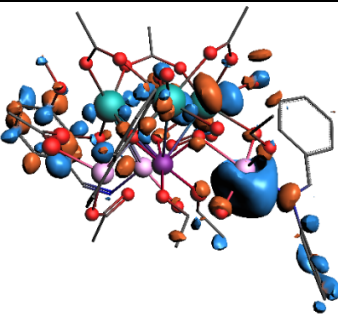
		13.77	2 S	2 Dy			10.53	1 D:yz	3 Dy
		8.25	2 S	5 Mn			7.09	2 P:x	49 C
		6.35	1 D:yz	1 Dy			5.01	2 P:z	2 Dy
		6.26	3 S	5 Mn			4.34	2 P:x	1 Dy
		5.03	3 S	2 Dy			4.02	1 D:xy	2 Dy
		4.38	1 D:x2-y2	1 Dy			3.95	2 P:x	3 Dy
		4.21	1 D:z2	2 Dy			3.30	1 D:xz	1 Dy
		2.98	3 S	44 C			2.98	1 D:yz	2 Dy
		2.65	2 S	4 Mn			2.34	2 P:y	79 C
		2.25	2 P:z	49 C			2.08	2 P:x	60 C
		2.22	3 S	4 Mn			1.99	1 D:z2	2 Dy
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
1.022	415 A	13.64	1 D:z2	3 Dy	1.240	415 A	9.58	2 S	5 Mn

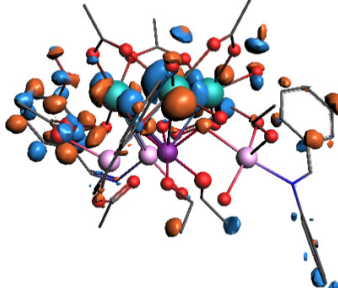
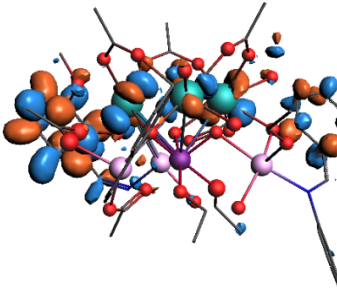
		10.03	1 D:yz	3 Dy			8.02	1 P:x	63 C
		6.57	3 S	6 Mn			4.14	2 P:y	66 C
		5.45	3 S	3 Dy			3.97	3 S	68 C
		4.73	1 D:xy	1 Dy			3.58	1 P:x	21 O
		3.69	3 S	47 C			3.25	1 P:z	63 C
		3.42	2 P:z	2 Dy			3.15	2 P:y	71 C
		3.32	1 P:z	40 C			2.97	1 D:z2	1 Dy
		3.31	2 P:x	1 Dy			2.95	3 S	6 Mn
		3.23	2 P:z	1 Dy			2.91	3 S	69 C
		3.10	2 D:z2	3 Dy			2.89	1 D:yz	1 Dy
		2.64	2 S	3 Dy			2.83	2 S	4 Mn
		2.41	2 P:y	72 C			2.54	2 P:y	67 C
		2.35	2 P:z	43 C			2.45	1 P:x	86 C
		2.29	2 P:y	2 Dy			2.34	1 D:yz	3 Dy
		2.24	2 P:z	40 C			2.23	2 P:x	21 O
		2.19	2 P:x	49 C			2.05	2 S	7 Mn
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom

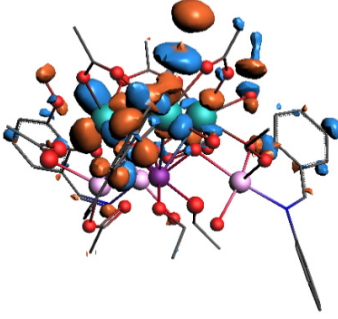
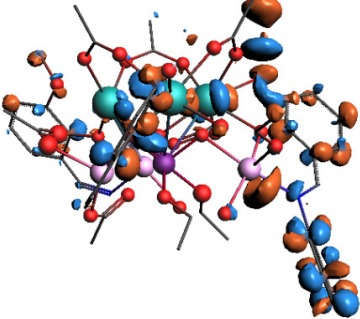
1.227	416 A	16.11	1 D:yz	1 Dy	1.294	416 A	10.75	1 P:x	86 C
		11.71	2 S	3 Dy			10.17	1 D:z2	3 Dy
		10.39	3 S	5 Mn			4.96	2 P:x	86 C
		9.60	3 S	7 Mn			4.72	1 D:x2-y2	3 Dy
		7.37	1 D:xy	1 Dy			4.21	3 S	7 Mn
		2.81	2 S	7 Mn			3.84	1 D:yz	3 Dy
		2.79	2 S	5 Mn			3.31	1 P:x	34 O
		2.20	1 D:z2	3 Dy			2.99	1 D:xy	2 Dy
							2.84	1 D:yz	1 Dy
							2.39	2 D:z2	3 Dy
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
1.345	417 A	10.94	3 S	6 Mn	1.299	417 A	16.00	1 D:yz	1 Dy

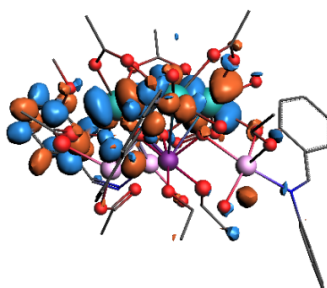
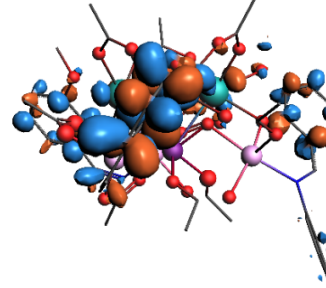
		9.41	1 D:z2	3 Dy			11.33	1 D:z2	2 Dy
		6.18	3 S	7 Mn			6.67	1 D:x2-y2	2 Dy
		5.47	2 S	2 Dy			6.10	1 D:yz	3 Dy
		3.23	2 P:x	58 C			3.54	1 D:xz	2 Dy
		3.00	2 P:x	61 C			2.72	1 P:x	63 C
		2.77	1 D:z2	2 Dy			2.37	1 D:xz	3 Dy
		2.42	1 D:yz	2 Dy			2.25	2 P:z	60 C
		2.06	2 S	1 Dy			2.22	2 P:x	63 C
		2.00	2 S	6 Mn			2.11	2 P:z	58 C
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
1.408	418 A	17.65	1 D:z2	2 Dy	1.370	418 A	7.03	2 P:x	52 C

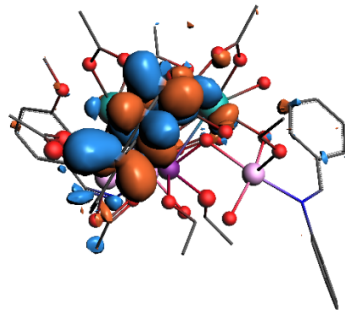
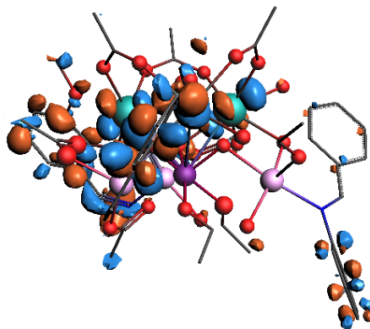
	7.84	1 D:xy	2 Dy		5.06	2 P:x	50 C		
	6.49	1 D:yz	3 Dy		3.72	1 P:x	52 C		
	6.42	1 D:xz	2 Dy		3.68	3 S	5 Mn		
	4.59	3 S	5 Mn		3.20	2 P:x	53 C		
	3.72	2 S	5 Mn		3.11	2 S	2 Dy		
	3.02	2 S	4 Mn		2.83	2 P:x	77 C		
	2.56	3 S	4 Mn		2.70	2 P:z	1 Dy		
	2.46	1 D:yz	1 Dy		2.69	2 S	5 Mn		
	2.12	2 P:x	52 C		1.00	2 P:y	3 Dy		
2.03	2 P:z	48 C							
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
1.449	419 A	3.58	2 P:x	73 C	1.425	419 A	7.05	3 S	5 Mn

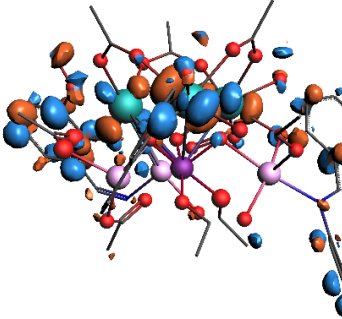
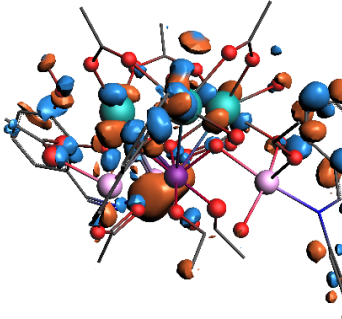
									
	3.49	1 P:y	58 C			5.28	2 P:x	52 C	
	3.41	3 S	68 C			4.83	1 D:yz	1 Dy	
	2.80	1 D:xz	2 Dy			4.00	1 P:x	52 C	
	2.69	1 P:y	40 C			3.34	2 P:x	50 C	
	2.66	1 P:y	43 C			3.27	2 P:x	53 C	
	2.49	2 P:x	71 C			3.20	2 P:y	58 C	
	2.43	2 P:z	40 C			3.16	1 P:y	58 C	
	2.31	2 S	3 Dy			2.90	2 P:x	82 C	
	2.20	2 P:y	50 C			2.68	1 P:y	60 C	
	2.20	1 D:yz	3 Dy			2.26	2 P:y	50 C	
	1.99	1 D:yz	2 Dy			2.10	2 P:x	61 C	
	1.90	1 D:xy	1 Dy			2.04	1 P:y	43 C	
	1.53	3 S	6 Mn						
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
1.485	420 A	4.02	1 D:z2	3 Dy	1.441	420 A	7.78	1 P:y	58 C

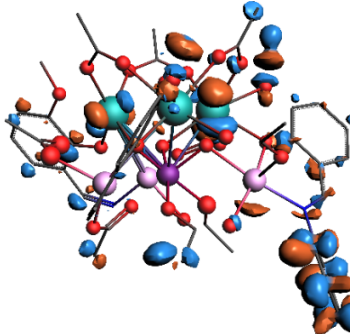
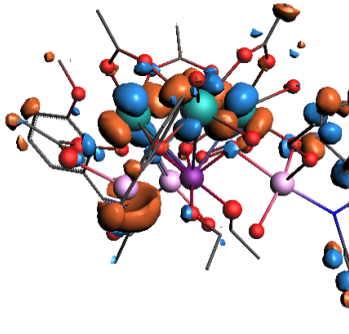
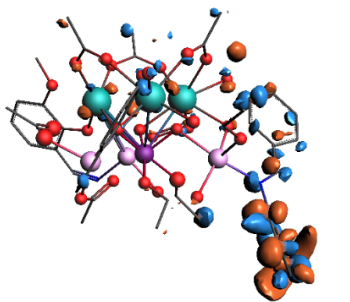
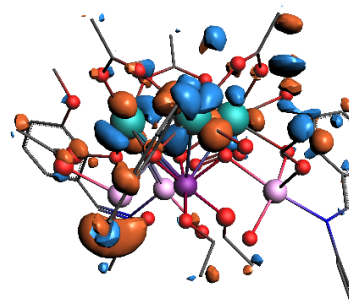
		3.03	3 S	7 Mn			7.39	1 P:y	40 C
		2.84	2 P:x	52 C			6.79	1 P:y	54 C
		2.73	2 P:x	48 C			6.57	1 P:y	60 C
		2.63	2 P:x	50 C			6.26	1 P:y	47 C
		2.45	1 P:y	54 C			5.50	1 P:y	43 C
		2.29	3 S	44 C			4.32	2 P:y	58 C
		2.18	1 D:xy	2 Dy			3.99	1 D:xy	3 Dy
		2.14	1 P:y	58 C			3.61	1 D:xy	1 Dy
							2.69	1 P:y	61 C
			2.65	1 P:z			48 C		
			2.47	1 D:xz	1 Dy				
			2.18	2 S	7 Mn				
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
1.497	421 A	4.94	1 D:xz	3 Dy	1.504	421 A	6.77	2 P:y	50 C

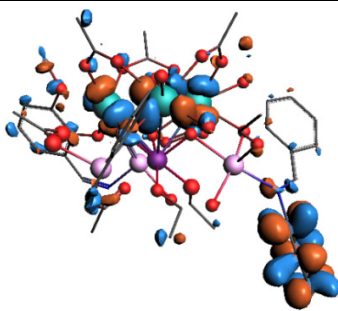
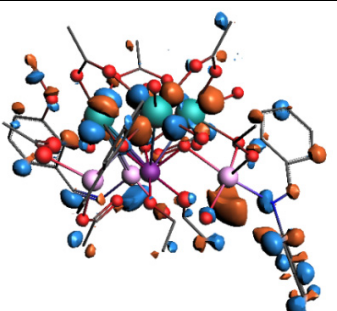
		4.58	1 D:xz	1 Dy			6.53	2 S	5 Mn
		4.43	1 P:x	63 C			5.67	1 P:x	39 C
		4.35	2 P:x	61 C			3.30	2 P:x	39 C
		3.99	1 D:xz	2 Dy			3.10	2 S	4 Mn
		3.39	1 P:x	39 C			2.58	2 P:y	48 C
		3.36	1 D:yz	3 Dy			2.36	1 P:z	55 C
		2.58	2 P:y	41 C			2.28	2 P:z	73 C
		2.55	2 P:x	58 C			2.24	1 P:y	50 C
		2.42	2 P:y	48 C			2.17	1 P:z	48 C
		2.38	3 S	63 C			2.06	1 D:z2	3 Dy
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
1.594	422 A	8.09	1 D:xz	1 Dy	1.536	422 A	4.85	1 P:z	66 C

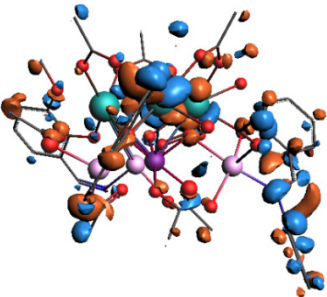
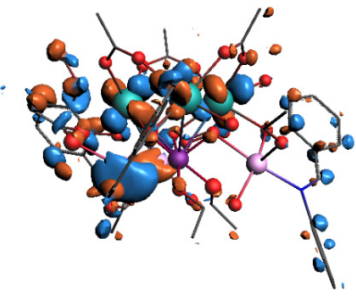
					5.45	1 D:z2	3 Dy						4.84	1 P:z	71 C
					4.49	1 P:y	58 C						4.75	1 P:x	72 C
					4.23	1 P:y	54 C						4.16	1 P:x	71 C
					4.04	1 P:y	43 C						4.01	1 P:x	69 C
					3.61	1 P:y	40 C						3.53	1 P:z	72 C
					3.33	1 P:y	60 C						3.29	1 P:x	67 C
					3.21	2 P:y	58 C						3.20	1 D:yz	1 Dy
					2.92	1 P:y	47 C						3.06	1 P:x	68 C
					2.66	2 P:x	5 Mn						2.88	1 P:z	69 C
					2.41	1 D:yz	3 Dy						2.85	1 P:z	68 C
					2.32	1 P:y	11 O						2.53	1 P:z	67 C
					2.30	1 D:x2-y2	3 Dy						2.44	1 D:z2	2 Dy
					2.11	1 D:xz	3 Dy						2.34	2 P:z	71 C
Spin up					Spin down										
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom						
1.633	423 A	5.12	1 P:z	66 C	1.563	423 A	5.83	2 P:x	61 C						

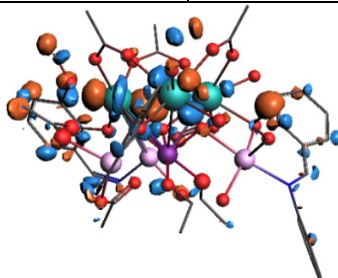
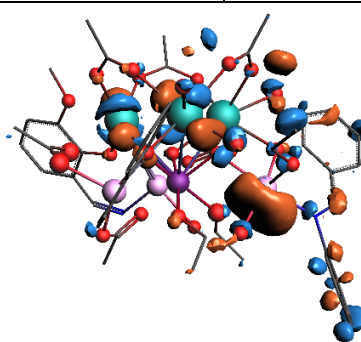
					4.97	1 P:x	72 C						5.67	2 P:x	58 C
					4.59	1 P:x	69 C						3.60	3 S	7 Mn
					4.25	1 P:z	71 C						3.07	1 P:x	58 C
					3.93	2 P:x	58 C						2.70	2 P:x	60 C
					3.92	2 P:x	61 C						2.51	3 S	61 C
					3.44	1 P:x	67 C						2.39	1 P:z	66 C
					3.37	1 P:z	69 C						2.31	1 P:y	54 C
					3.34	1 P:z	67 C						2.16	1 D:z2	3 Dy
					3.28	1 P:x	71 C						2.15	1 D:yz	1 Dy
					2.99	1 D:z2	2 Dy						2.13	3 S	47 C
					2.09	2 P:x	6 Mn								
					2.06	1 D:xy	1 Dy								
Spin up								Spin down							
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom						
1.644	424 A	3.62	1 D:z2	2 Dy	1.624	424 A	3.73	1 P:z	49 C						

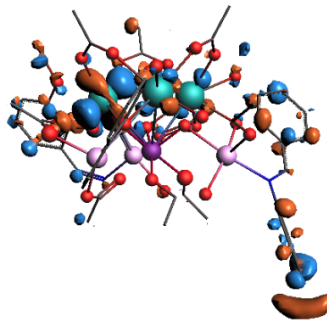
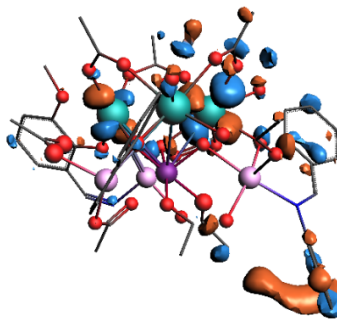
		3.37	2 P:x	52 C			3.52	2 S	4 Mn
		3.05	1 D:yz	1 Dy			3.26	2 P:z	50 C
		3.04	1 P:y	54 C			2.96	2 S	7 Mn
		2.94	2 P:z	48 C			2.88	3 S	7 Mn
		2.48	1 D:xy	3 Dy			2.82	2 S	1 Dy
		2.40	3 S	68 C			2.74	1 P:x	48 C
		2.19	1 D:xy	2 Dy			2.67	2 P:z	2 Dy
		2.18	1 P:y	40 C			2.41	1 P:y	66 C
		2.18	2 P:x	53 C			2.21	1 D:xy	3 Dy
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
1.814	427 A	4.35	1 D:xz	1 Dy	1.735	427 A	8.91	1 D:xz	1 Dy

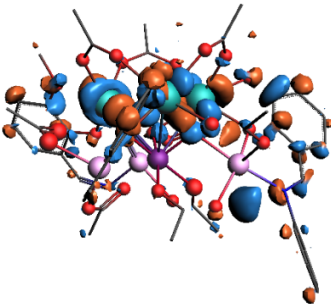
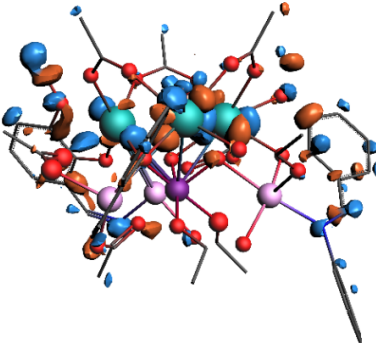
		3.81	2 P:x	58 C			6.16	1 D:xy	2 Dy
		3.69	1 P:z	52 C			5.08	1 D:xy	3 Dy
		3.45	2 S	1 Dy			3.20	2 P:y	72 C
		3.33	2 P:x	61 C			3.11	3 S	6 Mn
		3.03	2 P:x	60 C			2.96	1 P:z	48 C
		2.87	1 P:x	39 C			2.86	3 S	73 C
		2.69	1 P:z	55 C			2.75	2 P:z	40 C
		2.08	2 P:x	5 Mn			2.03	2 S	6 Mn
Spin up					Spin down				
E(eV)	MO	Occupation, %	SFO (first member)	Atom	E(eV)	MO	Occupation, %	SFO (first member)	Atom
2.004	431 A	8.61	2 P:x	48 C	1.966	431 A	4.94	2 P:z	66 C
		7.87	2 P:x	49 C			3.78	2 P:y	46 C
		5.23	2 P:x	50 C			3.58	1 P:x	39 C
		3.35	3 S	55 C			3.32	1 D:xz	2 Dy
		3.35	2 P:x	53 C			2.92	2 S	6 Mn
		3.08	2 P:y	59 C			2.82	2 P:z	67 C
		3.06	2 P:y	56 C			2.56	2 S	3 Dy
		2.90	1 P:z	53 C			2.55	2 P:y	72 C

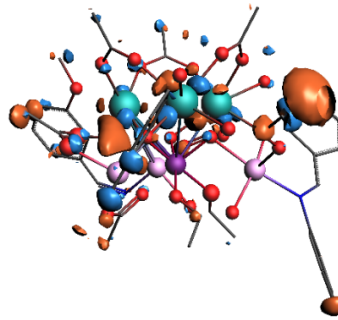
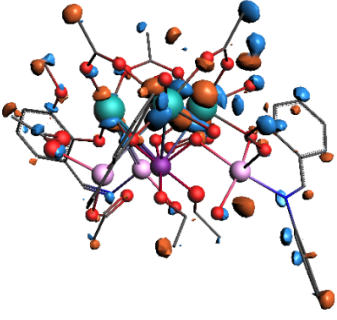
		2.81	2 P:x	52 C			2.51	3 S	67 C
		2.81	2 P:x	44 C			2.37	3 S	44 C
		2.78	2 P:y	50 C			2.36	2 P:y	48 C
		2.75	1 P:y	56 C			2.35	2 P:x	6 Mn
		2.58	1 D:xy	3 Dy			2.19	1 D:xy	2 Dy
Spin up					Spin down				
E(eV)	MO	Occupation,%	SFO (first member)	Atom	E(eV)	MO	Occupation,%	SFO (first member)	Atom
2.011	432 A	5.80	1 P:z	59 C	1.981	432 A	4.14	2 P:x	60 C
		4.26	1 P:y	52 C			3.47	2 S	5 Mn
		3.46	1 P:z	57 C			2.77	1 D:xz	2 Dy
		3.32	1 P:z	56 C			2.54	2 P:x	58 C
		3.22	1 D:xz	1 Dy			2.29	3 S	61 C
		3.08	1 P:z	53 C			2.22	2 P:x	48 C
		2.96	1 D:xy	3 Dy			2.20	2 P:x	47 C
		2.57	1 P:y	55 C			2.13	2 P:z	81 C
		2.57	2 P:x	73 C			2.00	2 P:x	5 Mn
		2.54	2 P:x	6 Mn					

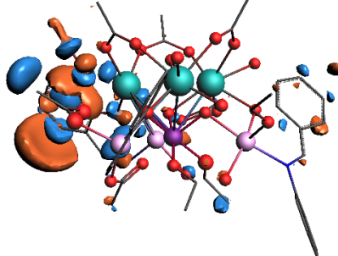
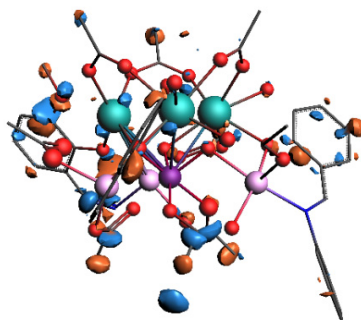
		2.04	1 D:xz	2 Dy					
Spin up					Spin down				
E(eV)	MO	Occupation,%	SFO (first member)	Atom	E(eV)	MO	Occupation,%	SFO (first member)	Atom
2.126	433 A	3.58	2 P:x	72 C	2.051	433 A	6.48	2 P:x	60 C
		3.38	2 P:z	85 C			4.77	3 S	6 Mn
		3.37	2 P:z	1 Dy			4.04	3 S	7 Mn
		3.27	2 P:x	49 C			3.39	1 P:x	40 C
		3.22	2 P:y	3 Dy			3.25	2 P:z	80 C
		2.80	2 P:z	75 C			3.22	2 P:x	40 C
		2.70	2 P:x	6 Mn			3.04	3 S	43 C
		2.52	2 D:xz	1 Dy			2.75	2 S	2 Dy
		2.49	1 P:x	66 C			2.66	2 D:xz	3 Dy
		2.41	2 P:x	53 C			2.38	2 S	7 Mn
		2.28	2 P:x	48 C			2.37	1 D:yz	1 Dy
		2.18	2 S	2 Dy			2.24	2 P:y	3 Dy
Spin up					Spin down				

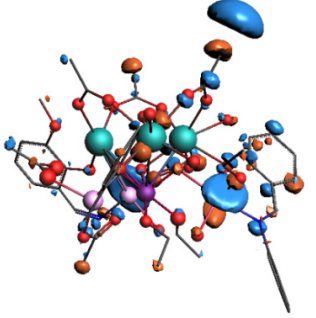
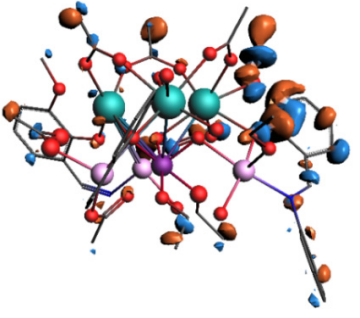
E(eV)	MO	Occupation,%	SFO (first member)	Atom	E(eV)	MO	Occupation,%	SFO (first member)	Atom
2.161	434 A	6.58	2 P:x	60 C	2.104	434 A	5.06	3 S	5 Mn
		4.88	1 D:xz	2 Dy			4.39	2 P:x	53 C
		3.51	3 S	75 C			3.81	2 P:y	2 Dy
		3.20	2 P:x	40 C			3.35	1 D:xz	2 Dy
		3.01	1 P:x	40 C			3.22	2 P:y	42 C
		2.94	2 D:yz	3 Dy			2.89	2 P:y	46 C
		2.85	2 P:x	7 Mn			2.83	2 S	5 Mn
		2.49	2 P:z	74 C			2.78	2 P:x	52 C
		2.45	2 P:y	40 C			2.65	2 P:y	36 N
		2.25	2 D:z2	2 Dy			2.41	1 D:xy	3 Dy
		2.02	2 S	4 Mn			2.24	3 S	6 Mn
1.97	2 D:yz	1 Dy	1.95	1 D:xz	3 Dy				
Spin up					Spin down				
E(eV)	MO	Occupation,%	SFO (first member)	Atom	E(eV)	MO	Occupation,%	SFO (first member)	Atom
2.193	435 A	8.60	1 D:xy	3 Dy	2.136	435 A	10.13	1 D:xz	1 Dy

					6.14	2 P:x	53 C						4.75	2 P:x	82 C
					4.55	2 P:x	55 C						4.69	2 P:x	53 C
					4.19	3 S	55 C						3.53	1 D:xy	3 Dy
					3.70	2 P:x	52 C						3.32	3 S	55 C
					2.59	2 P:x	60 C						3.04	2 P:x	49 C
					2.53	2 P:x	56 C						2.91	2 P:x	52 C
					2.50	2 S	1 Dy						2.19	2 D:xy	1 Dy
					2.47	1 D:x2-y2	3 Dy						2.00	2 P:x	65 C
					2.29	2 P:x	57 C						1.99	2 P:y	56 C
					2.24	1 D:yz	3 Dy						1.97	3 S	7 Mn
					1.47	1 D:x2-y2	1 Dy	1.38	1 D:xy	1 Dy					
Spin up					Spin down										
E(eV)	MO	Occupation,%	SFO (first member)	Atom	E(eV)	MO	Occupation,%	SFO (first member)	Atom						
2.244	436 A	5.35	2 P:x	5 Mn	2.209	436 A	7.57	2 P:x	61 C						

					4.36	2 S	4 Mn						3.30	2 P:z	67 C				
					3.86	2 S	2 Dy						3.12	2 P:x	58 C				
					3.78	1 D:xy	2 Dy						3.01	1 P:x	61 C				
					3.57	3 S	6 Mn						2.83	2 P:x	40 C				
					3.49	2 S	3 Dy						2.51	2 P:z	66 C				
					2.75	2 D:yz	1 Dy						2.49	2 P:z	43 C				
					2.56	1 D:xz	2 Dy						2.33	2 P:z	50 C				
					2.15	1 D:xz	3 Dy						2.29	2 P:y	41 C				
					2.09	2 S	1 Dy						2.19	2 P:y	42 C				
					2.05	2 P:x	77 C						2.17	3 S	38 N				
					2.02	2 P:z	40 C						2.16	2 P:z	83 C				
													2.01	1 P:x	86 C				
Spin up					Spin down														
E(eV)	MO	Occupation,%	SFO (first member)	Atom	E(eV)	MO	Occupation,%	SFO (first member)	Atom										
2.591	442 A	6.55	2 P:z	75 C	2.519	442 A	3.01	2 S	4 Mn										

					4.57	2 P:y	65 C						2.90	2 P:y	86 C
					4.46	2 P:x	6 Mn						2.90	2 P:x	5 Mn
					3.62	2 P:z	62 C						2.83	2 P:x	74 C
					3.47	3 S	75 C						2.50	2 P:x	70 C
					3.04	2 P:y	71 C						2.48	2 D:xy	2 Dy
					2.97	1 P:z	85 C						2.34	2 P:x	7 Mn
					2.92	2 P:z	85 C								
					2.75	2 P:z	74 C								
					2.67	2 P:z	2 Dy								
					2.01	2 S	6 Mn								
Spin up								Spin down							
E(eV)	MO	Occupation,%	SFO (first member)	Atom	E(eV)	MO	Occupation,%	SFO (first member)	Atom						
3.030	452 A	7.96	2 P:z	54 C	3.014	452 A	5.23	2 P:y	78 C						

					7.91	2 P:x	47 C						3.17	2 P:x	60 C
					7.84	3 S	54 C						3.13	1 P:x	40 C
					5.79	1 P:x	40 C						2.94	2 P:z	44 C
					4.26	2 P:z	61 C						2.86	2 P:z	7 Mn
					4.22	2 P:z	58 C						2.60	2 P:z	46 C
					3.66	1 P:z	40 C						2.13	2 P:z	42 C
					3.56	2 P:x	40 C						2.07	2 D:xy	2 Dy
					3.54	2 P:z	7 Mn						2.00	2 P:x	81 C
					3.34	2 P:x	43 C								
					3.34	1 P:x	34 O								
3.25	2 P:x	54 C													
Spin up					Spin down										
E(eV)	MO	Occupation,%	SFO (first member)	Atom	E(eV)	MO	Occupation,%	SFO (first member)	Atom						
3.081	453 A	8.57	2 P:x	84 C	3.066	453 A	4.47	2 P:y	51 C						

	6.11	2 P:x	76 C		4.08	1 P:x	39 C
	5.31	2 P:y	7 Mn		3.96	1 P:x	13 O
	5.00	2 S	4 Mn		3.65	2 P:y	76 C
	4.38	2 P:z	5 Mn		3.32	3 S	46 C
	3.48	3 S	84 C		3.01	2 P:y	82 C
	3.37	2 P:x	83 C		2.82	2 P:y	50 C
	3.02	1 P:x	83 C		2.76	3 S	76 C
	2.77	2 P:x	44 C		2.74	2 P:y	70 C
	2.52	3 S	7 Mn		2.64	2 P:x	13 O
2.45		2 P:x	70 C		2.24	2 S	1 Dy
					2.01	2 P:y	7 Mn