

Supplementary material for the article:

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## SUPPLEMENTARY INFORMATION

### **Origin of the zero-field splitting in mononuclear octahedral Mn<sup>IV</sup> complexes: A combined experimental and theoretical investigation.**

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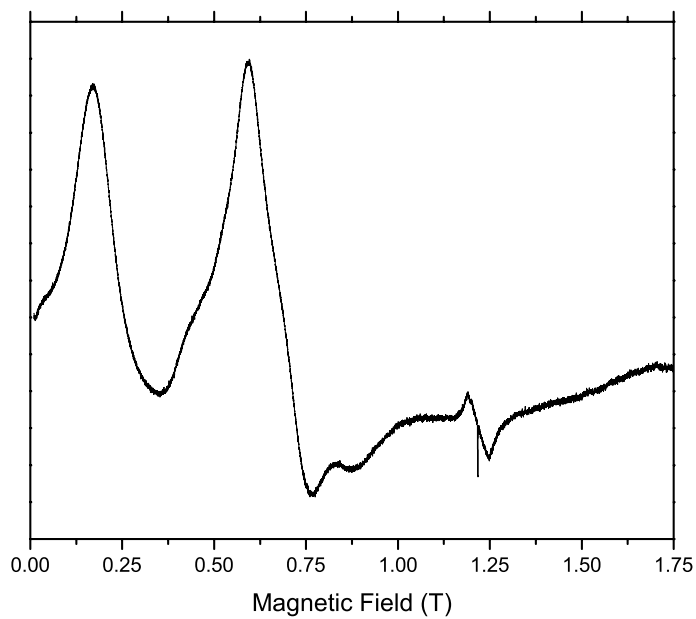
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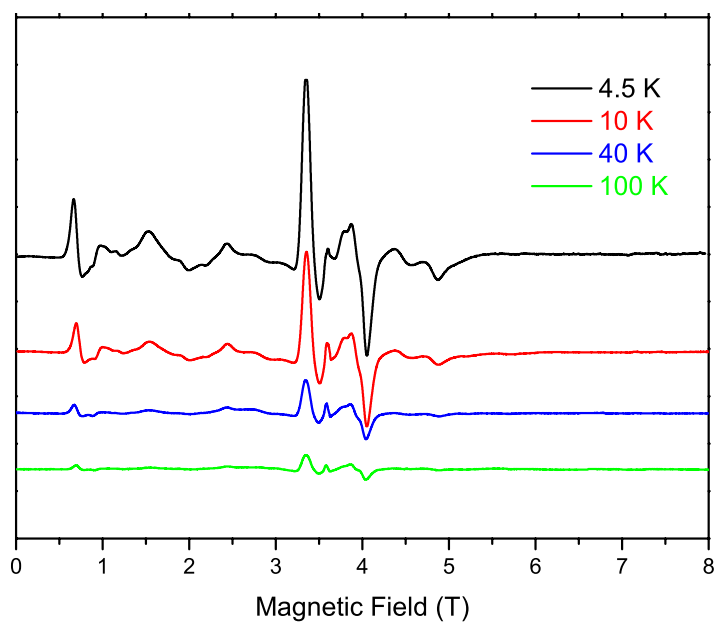
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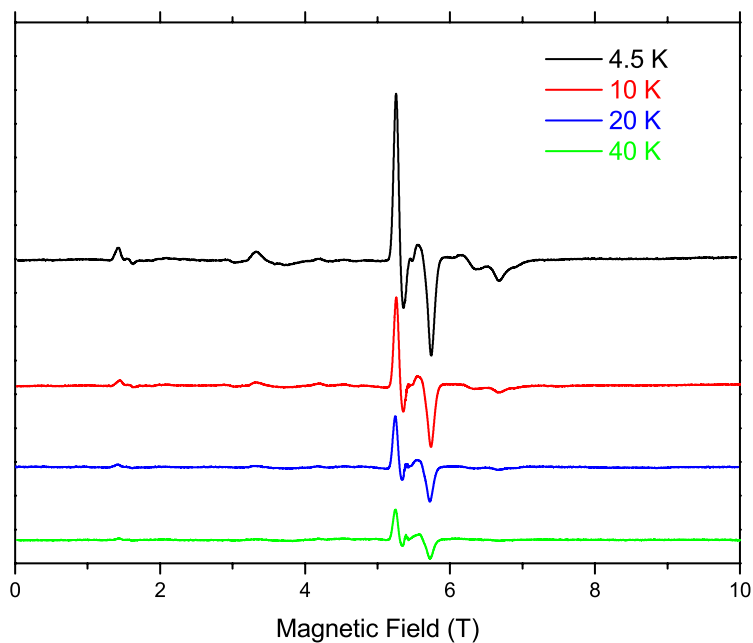
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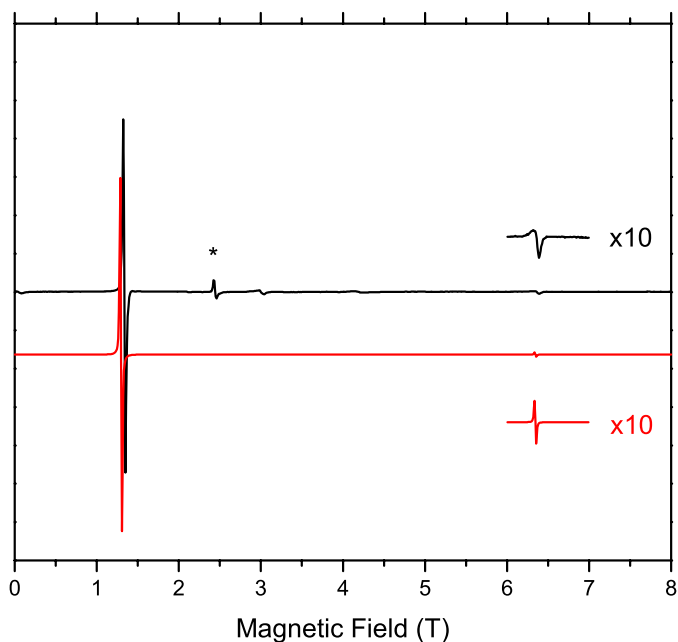
**Figure S1.** Experimental powder Q-band EPR spectra of  $\text{MnL}^{\text{trans-N}_2\text{O}_4}$  recorded at 5 K.



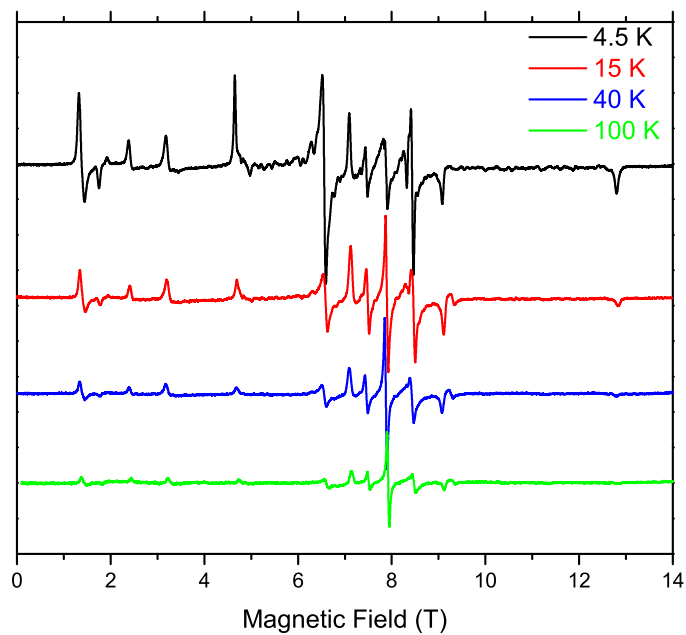
**Figure S2.** Experimental powder HFEPR spectra of  $\text{MnL}^{\text{trans-N}_2\text{O}_4}$  recorded at 100.8 GHz and different temperatures.



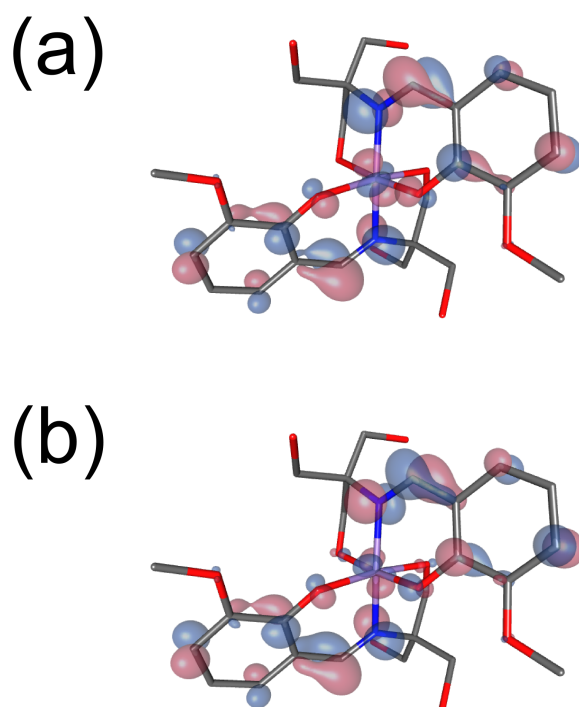
**Figure S3.** Experimental powder HFEPR spectra of  $\text{MnL}^{\text{trans-N}_2\text{O}_4}$  recorded at 151.2 GHz and at different temperatures.



**Figure S4.** An HFEPR spectrum of a loose (unconstrained powder) sample of  $\text{MnL}^{\text{O}_4\text{S}_2}$  recorded at 84 GHz and 4.2 K (black line) and simulated single-crystal spectrum (red line) using the following parameters:  $D = + 2.29 \text{ cm}^{-1}$ ,  $|E| = 0.33 \text{ cm}^{-1}$ ,  $g_{\text{iso}} = 1.99$ . The crystal was assumed to be oriented with  $B_0 \parallel y$ . The asterisk marks a  $\text{Mn}^{\text{II}}$  impurity.



**Figure S5.** Experimental HFEPR spectra of  $\text{MnL}^{\text{O4S2}}$  at 220.8 GHz and different temperatures.



**Figure S6.** Graphical representation of the two empty low-energy mainly-ligand orbitals in  $\text{MnL}^{\text{trans-N2O4}}$  [(a) lowest, (b) higher] that appear below the empty  $e_g^*$  orbitals and that influence its  $D$ -value.

**Coordinates of reoriented structures**

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**MnL-N303**

Mn	-0.057200	-0.056000	-0.060300
N	0.052000	0.143600	2.046300
N	2.048700	0.043100	0.156400
N	0.139500	2.043300	0.046300
O	0.127000	-1.842200	0.010700
O	-1.834700	0.013500	0.132700
O	0.009200	0.125000	-1.858000
C	-0.962400	-2.805300	-0.005000
C	1.482100	0.088800	2.520800
C	2.320500	-0.568200	1.497400
C	2.541800	1.459600	0.104500
C	1.469600	2.339900	-0.615700
C	0.063300	2.514000	1.474700
C	-0.573900	1.471400	2.345100
C	-2.793500	-0.117700	-0.878900
C	-0.123200	-0.928400	-2.770700
C	-0.849900	2.717300	-0.754000
C	2.680700	-0.764900	-0.854200
C	-0.743900	-0.865900	2.695100
H	-1.461300	1.511700	2.041900
H	-0.555800	-3.814200	0.048800
H	-1.613800	-2.630500	0.849900
H	-1.533300	-2.692700	-0.925500
H	-3.789900	-0.029900	-0.448300
H	-2.648300	0.666400	-1.620600
H	-2.688200	-1.091500	-1.354800
H	-0.044400	-0.541400	-3.785600
H	0.665700	-1.659100	-2.598600
H	-1.093800	-1.403900	-2.637900
H	3.762200	-0.710600	-0.738500
H	2.355700	-1.798800	-0.748000
H	2.402100	-0.396300	-1.840300
H	-0.712300	3.794300	-0.670300
H	-0.740500	2.417200	-1.795100
H	-1.845100	2.450000	-0.401900
H	-0.673600	-0.745100	3.775100
H	-1.782900	-0.763700	2.385300
H	-0.377100	-1.852500	2.415600
H	-0.554400	3.407100	1.392600
H	-0.565100	1.371500	3.429500
H	1.086100	2.800900	1.714800
H	1.903000	1.093100	2.521800
H	2.072500	-0.552900	3.173200
H	2.846000	-1.410600	1.944700
H	2.981200	0.296900	1.466600
H	2.041300	3.218200	-0.319600

H	1.856400	1.955900	-1.558400
H	2.762500	0.958400	-0.836800
H	3.421000	2.089100	-0.024500

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**MnL-tN204**

Mn	-0.015200	-0.015200	0.000000
N	0.103800	0.146500	1.981500
N	0.146500	0.103800	-1.981500
O	1.853100	-0.077600	0.085100
O	-1.949700	-0.060300	0.125900
O	-0.060300	-1.949700	-0.125900
O	-0.077600	1.853100	-0.085100
C	-2.662300	0.569700	1.042400
C	-2.193400	0.851300	2.334600
C	-3.054700	1.442200	3.278700
H	-2.736700	1.599400	4.160500
C	-4.336200	1.796100	2.958600
H	-4.902000	2.196700	3.609100
C	-4.802600	1.559700	1.661100
H	-5.684700	1.821800	1.422800
C	-3.991400	0.949300	0.718900
O	-4.360700	0.659700	-0.559600
C	-5.698700	0.947700	-0.942600
H	-6.318600	0.482000	-0.342700
H	-5.847600	0.647300	-1.863900
H	-5.854300	1.913600	-0.886500
C	-0.834000	0.557300	2.740700
H	-0.621800	0.682700	3.658100
C	1.509100	-0.000800	2.467800
C	2.356300	0.450500	1.261100
H	2.355200	1.437600	1.206700
H	3.292200	0.151800	1.384000
C	1.822600	0.823000	3.685700
H	1.307800	0.474900	4.456400
H	2.785900	0.737400	3.899200
O	1.509800	2.179400	3.496900
H	1.369000	2.541200	4.242000
C	1.768300	-1.498500	2.688400
H	1.562200	-1.993500	1.856300
H	2.724700	-1.639900	2.902000
O	0.952000	-2.013200	3.770600
H	0.140300	-1.960700	3.558700
C	0.569700	-2.662300	-1.042400
C	0.851300	-2.193400	-2.334600
C	1.442200	-3.054700	-3.278700
H	1.599400	-2.736700	-4.160500
C	1.796100	-4.336200	-2.958600
H	2.196700	-4.902000	-3.609100

C	1.559700	-4.802600	-1.661100
H	1.821800	-5.684700	-1.422800
C	0.949300	-3.991400	-0.718900
O	0.659700	-4.360700	0.559600
C	0.947700	-5.698700	0.942600
H	0.482000	-6.318600	0.342700
H	0.647300	-5.847600	1.863900
H	1.913600	-5.854300	0.886500
C	0.557300	-0.834000	-2.740700
H	0.682700	-0.621800	-3.658100
C	-0.000800	1.509100	-2.467800
C	0.450500	2.356300	-1.261100
H	1.437600	2.355200	-1.206700
H	0.151800	3.292200	-1.384000
C	0.823000	1.822600	-3.685700
H	0.474900	1.307800	-4.456400
H	0.737400	2.785900	-3.899200
O	2.179400	1.509800	-3.496900
H	2.541200	1.369000	-4.242000
C	-1.498500	1.768300	-2.688400
H	-1.993500	1.562200	-1.856300
H	-1.639900	2.724700	-2.902000
O	-2.013200	0.952000	-3.770600
H	-1.960700	0.140300	-3.558700

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**MnL-cisN2O4**

Mn	-0.035100	-0.035700	0.002600
N	0.029200	2.022900	0.032100
N	2.038500	0.041400	-0.023600
O	-1.888800	0.026900	-0.184400
O	-0.006800	-1.875400	0.187600
O	-0.003300	0.192200	1.851400
O	0.210200	-0.027400	-1.871100
C	2.299400	-2.358400	0.586900
C	2.531100	-0.240200	-1.408600
C	1.801900	-5.020600	0.137000
C	-5.012500	1.856400	-0.303500
C	3.341400	-3.282100	0.589300
C	-1.546000	-4.236800	1.169700
C	-4.369900	-1.627100	-0.717200
C	4.958800	-5.625600	1.694600
C	0.715900	-4.133800	0.115200
C	3.114400	-4.629500	0.340100
C	-0.899000	2.609300	-0.974400
C	-3.267300	3.343700	-0.832800
C	-4.136600	0.798100	-0.086400
C	-5.641700	4.257500	-0.942100
C	-0.289800	2.513500	1.411400

C	4.291800	-5.608700	0.322000
C	-4.637200	-0.586400	0.373300
C	3.846700	-7.032800	-0.013100
C	-6.038400	4.191800	-2.410100
C	-0.794100	-6.170000	-0.183600
C	-4.620900	3.141700	-0.666800
C	-6.140300	-0.584700	0.657100
C	1.361800	-0.732600	-2.251300
C	5.296100	-5.171100	-0.746300
C	-0.719800	-4.640300	-0.057100
C	-0.696900	1.332700	2.262000
C	-2.338300	2.326300	-0.676500
C	-1.350200	-4.045200	-1.326000
C	-2.757800	1.038700	-0.307900
C	0.996200	-2.763000	0.294000
C	1.427400	2.373100	-0.334200
C	2.583400	-0.931500	0.967700
C	2.374800	1.434300	0.379100
C	-3.926900	-0.997300	1.668300
C	-5.057700	5.618600	-0.640200
C	-6.898300	4.112900	-0.098200
H	2.902300	0.566300	-1.797800
H	3.226200	-0.914500	-1.381300
H	1.630100	-5.925600	0.007800
H	-5.920900	1.693800	-0.198700
H	4.208400	-2.990900	0.760100
H	-1.527800	-3.282200	1.267200
H	-2.454000	-4.528800	1.054300
H	-1.174300	-4.647100	1.953500
H	-3.428800	-1.662600	-0.901200
H	-4.669800	-2.488200	-0.418000
H	-4.842400	-1.383000	-1.515400
H	4.316200	-5.880700	2.359700
H	5.683200	-6.256900	1.690800
H	5.298500	-4.751400	1.897200
H	-0.766300	3.569900	-1.005300
H	-0.681300	2.251900	-1.849500
H	-2.965900	4.195000	-1.058200
H	0.486600	2.947600	1.796600
H	-1.012500	3.159200	1.374400
H	3.441800	-7.044500	-0.883600
H	4.609600	-7.616100	-0.007900
H	3.209400	-7.330700	0.639100
H	-6.410800	3.327900	-2.602000
H	-6.690700	4.870400	-2.595500
H	-5.263400	4.335200	-2.956400
H	-0.418700	-6.574500	0.602300
H	-1.710700	-6.439200	-0.276300
H	-0.298600	-6.452300	-0.954500

H	-6.618800	-0.387600	-0.150600
H	-6.405300	-1.448200	0.982700
H	-6.339900	0.081100	1.318500
H	1.229900	-1.683000	-2.112100
H	1.546000	-0.583800	-3.192400
H	5.639000	-4.300900	-0.527100
H	6.020300	-5.799700	-0.780400
H	4.861400	-5.137500	-1.600800
H	-1.651200	1.183100	2.177700
H	-0.498900	1.517100	3.193500
H	-0.873300	-4.358400	-2.098100
H	-2.268200	-4.318300	-1.385200
H	-1.301800	-3.087700	-1.288100
H	1.545900	2.296600	-1.293300
H	1.616500	3.290100	-0.077300
H	3.542000	-0.807300	1.041600
H	2.193600	-0.751200	1.836400
H	2.281900	1.534500	1.338700
H	3.292100	1.638300	0.136100
H	-4.104300	-0.346900	2.351300
H	-4.248700	-1.856100	1.952000
H	-2.980900	-1.045200	1.513400
H	-4.337400	5.800300	-1.248600
H	-5.738100	6.289200	-0.742400
H	-4.727500	5.632600	0.261000
H	-6.662500	4.116500	0.831700
H	-7.492300	4.846100	-0.280100
H	-7.336800	3.286500	-0.315000

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**MnL-O4S2**

Mn	0.000300	0.000300	0.000000
S	-0.150900	2.353800	0.025600
S	2.353800	-0.150900	-0.025600
O	-1.838900	0.014000	-0.057200
O	0.159000	0.135200	1.874800
O	0.014000	-1.838900	0.057200
O	0.135200	0.159000	-1.874800
C	-2.538600	1.131400	-0.315700
C	-3.918000	1.061700	-0.613200
C	-4.571300	2.279000	-0.784600
H	-5.501600	2.253300	-0.979800
C	-3.960600	3.539900	-0.691500
C	-2.594600	3.564800	-0.467000
H	-2.128900	4.391500	-0.441000
C	-1.913700	2.373400	-0.281600
C	-4.609300	-0.303100	-0.737800
C	-6.091400	-0.161400	-1.090500
H	-6.496700	-1.051100	-1.161000

H	-6.179900	0.306400	-1.946400
H	-6.547400	0.350200	-0.389500
C	-4.513800	-1.081600	0.587900
H	-3.572700	-1.185400	0.838300
H	-4.922500	-1.965100	0.479100
H	-4.985400	-0.587200	1.291100
C	-3.934100	-1.099800	-1.865600
H	-2.979900	-1.204200	-1.666600
H	-4.038400	-0.618600	-2.713700
H	-4.351700	-1.982200	-1.938700
C	-4.795700	4.822600	-0.862300
C	-5.272600	4.917500	-2.314900
H	-4.497600	4.929100	-2.912500
H	-5.791800	5.740100	-2.435100
H	-5.835600	4.142600	-2.524000
C	-3.958000	6.071400	-0.524600
H	-3.650600	6.016800	0.404200
H	-4.510100	6.873900	-0.638600
H	-3.185800	6.118600	-1.124000
C	-6.010700	4.803500	0.073100
H	-5.705900	4.743800	1.002600
H	-6.573300	4.030600	-0.138100
H	-6.528100	5.626900	-0.048500
C	0.238700	1.326600	2.496800
C	0.018300	2.509800	1.784000
C	0.011200	3.766000	2.374600
H	-0.139200	4.540800	1.846000
C	0.221700	3.884600	3.730500
C	0.505400	2.695500	4.436100
H	0.692400	2.771400	5.364400
C	0.531700	1.427500	3.882100
C	0.869200	0.174400	4.701800
C	-0.337900	-0.768200	4.736100
H	-0.591800	-1.007500	3.820800
H	-1.089000	-0.320600	5.178100
H	-0.104600	-1.580700	5.234700
C	2.083800	-0.547100	4.080800
H	2.851700	0.063400	4.062200
H	1.866100	-0.825100	3.166900
H	2.306800	-1.334100	4.617300
C	1.235800	0.526100	6.150000
H	2.007300	1.130400	6.154800
H	1.458900	-0.293900	6.637800
H	0.474600	0.966100	6.581200
C	0.178800	5.237600	4.446900
C	-0.042900	6.397600	3.479400
H	-0.063800	7.240400	3.980100
H	-0.895600	6.274000	3.011800
H	0.687700	6.423100	2.826700



C	-0.967000	5.215000	5.467200
H	-0.832900	4.473900	6.093400
H	-1.819100	5.098400	4.997500
H	-0.980000	6.062700	5.962000
C	1.511500	5.478000	5.179200
H	1.676100	4.744400	5.807400
H	1.466600	6.324600	5.669500
H	2.240500	5.517700	4.524900
C	1.131400	-2.538600	0.315800
C	1.061700	-3.918000	0.613100
C	2.278900	-4.571300	0.784700
H	2.253300	-5.501700	0.979800
C	3.539900	-3.960600	0.691600
C	3.564800	-2.594600	0.467100
H	4.391500	-2.128900	0.441000
C	2.373500	-1.913700	0.281600
C	-0.303100	-4.609300	0.737700
C	-0.161400	-6.091400	1.090600
H	-1.051100	-6.496700	1.161000
H	0.306300	-6.179900	1.946500
H	0.350200	-6.547400	0.389600
C	-1.081600	-4.513700	-0.587800
H	-1.185400	-3.572700	-0.838400
H	-1.965200	-4.922500	-0.479000
H	-0.587200	-4.985400	-1.291100
C	-1.099800	-3.934100	1.865600
H	-1.204200	-2.979900	1.666500
H	-0.618600	-4.038400	2.713800
H	-1.982200	-4.351600	1.938800
C	4.822600	-4.795800	0.862300
C	4.917500	-5.272600	2.314900
H	4.929100	-4.497600	2.912500
H	5.740100	-5.791800	2.435100
H	4.142600	-5.835600	2.524000
C	6.071400	-3.958000	0.524600
H	6.016800	-3.650600	-0.404200
H	6.873800	-4.510200	0.638600
H	6.118600	-3.185800	1.123900
C	4.803400	-6.010800	-0.073100
H	4.743800	-5.705900	-1.002600
H	4.030500	-6.573300	0.138100
H	5.626900	-6.528200	0.048400
C	1.326600	0.238600	-2.496900
C	2.509800	0.018200	-1.784100
C	3.766000	0.011100	-2.374800
H	4.540800	-0.139200	-1.846100
C	3.884600	0.221600	-3.730600
C	2.695400	0.505300	-4.436100
H	2.771400	0.692300	-5.364500

C	1.427400	0.531600	-3.882100
C	0.174400	0.869100	-4.701900
C	-0.768300	-0.338000	-4.736000
H	-1.007500	-0.591900	-3.820800
H	-0.320700	-1.089100	-5.178100
H	-1.580700	-0.104700	-5.234700
C	-0.547100	2.083700	-4.080800
H	0.063400	2.851700	-4.062300
H	-0.825100	1.866100	-3.166900
H	-1.334100	2.306800	-4.617300
C	0.526100	1.235700	-6.150100
H	1.130300	2.007200	-6.154900
H	-0.294000	1.458800	-6.637800
H	0.966100	0.474500	-6.581200
C	5.237500	0.178700	-4.446900
C	6.397600	-0.043000	-3.479600
H	7.240400	-0.063900	-3.980200
H	6.274000	-0.895600	-3.011900
H	6.423100	0.687600	-2.826800
C	5.214900	-0.967100	-5.467300
H	4.473800	-0.833000	-6.093400
H	5.098300	-1.819200	-4.997600
H	6.062600	-0.980100	-5.962100
C	5.478000	1.511400	-5.179300
H	4.744300	1.676000	-5.807500
H	6.324600	1.466500	-5.669600
H	5.517700	2.240500	-4.525000

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**MnL-N6**

Mn	-0.018100	-0.000100	-0.057700
N	0.068100	2.160600	0.329100
N	2.124300	0.632600	-0.151100
N	-2.115600	0.745800	-0.006000
N	-0.160800	-0.558400	2.125600
N	0.181300	-2.168300	0.097000
N	-0.017300	-0.797800	-2.131000
C	3.137800	-0.188000	-0.434200
C	2.422500	1.907700	0.175800
C	3.734200	2.353000	0.247000
C	4.791900	1.475900	-0.017900
C	4.451900	0.176800	-0.376000
C	1.246500	2.772600	0.463800
C	-1.070400	2.822600	0.595000
C	-1.056400	4.138900	0.996300
C	0.154900	4.818400	1.147800
C	1.319700	4.102700	0.869500
C	-2.312500	2.010300	0.436700
C	-3.183600	-0.042700	-0.129900

C	-4.449500	0.373600	0.178200	H	-0.539300	1.215000	2.863300
C	-4.695200	1.665400	0.617400	H	1.831800	-0.468900	-6.638500
C	-3.580500	2.481000	0.747800	H	2.159300	-1.857500	-7.405300
C	-6.099400	2.121200	0.981800	H	2.888800	-1.469700	-6.145700
C	-6.180200	3.645000	1.146100	H	-0.618000	-1.353800	-7.005000
C	0.237100	6.266000	1.644200	H	-1.054000	-2.796500	-6.574900
C	1.122300	7.070000	0.715800	H	-0.139100	-2.596600	-7.829900
C	6.239100	1.954000	0.116300	H	1.999500	-3.862200	-5.527700
C	7.240000	0.850100	-0.224900	H	1.599400	-4.190100	-6.951100
C	-6.486500	1.422000	2.283800	H	0.666700	-4.509600	-5.652000
C	-7.064600	1.699200	-0.148500	H	1.578200	-7.935300	-0.889900
C	-1.140200	6.918800	1.737100	H	1.870600	-6.558400	-1.579300
C	0.852300	6.242300	3.048800	H	0.391100	-7.032500	-1.375300
C	6.451700	3.150300	-0.813700	H	0.639300	-8.102400	1.367900
C	6.476100	2.412000	1.560000	H	-0.613700	-6.911100	1.057400
C	0.003200	-1.863800	2.456000	H	0.297800	-6.767200	2.148600
C	-0.090700	-2.284700	3.768500	H	3.142600	-6.021500	0.294100
C	-0.378500	-1.381900	4.796400	H	2.622500	-6.050200	2.102100
C	-0.558700	-0.066100	4.424600	H	3.018600	-7.128800	1.032700
C	-0.441400	0.303300	3.114900	H	-1.365900	-3.376700	7.249500
C	0.266800	-2.772100	1.295900	H	-1.106100	-3.706200	5.739000
C	0.386800	-2.883300	-1.025300	H	-2.287500	-2.757200	6.142900
C	0.685700	-4.229000	-0.962400	H	1.554400	-1.612100	6.548900
C	0.815800	-4.879400	0.247700	H	1.171300	-3.079100	6.148300
C	0.585300	-4.121200	1.397100	H	0.902700	-2.568700	7.605200
C	0.303200	-2.099900	-2.289100	H	-1.709100	-0.373700	6.900300
C	-0.072100	-0.035700	-3.235900	H	-0.199700	-0.050900	7.161500
C	0.200600	-0.525800	-4.478700	H	-0.949900	-1.083100	8.072900
C	0.547800	-1.848200	-4.668300	H	-2.876900	-0.889600	-0.427500
C	0.576300	-2.638000	-3.527200	H	-5.079100	-0.134900	0.071600
C	0.898700	-2.381000	-6.064100	H	-3.633800	3.451400	1.022100
C	1.323500	-3.852500	-6.036400	H	-1.860500	4.461900	1.175500
C	1.240300	-6.346000	0.360600	H	2.193400	4.520300	0.989600
C	2.649100	-6.346700	0.985800	H	3.858900	3.253800	0.460500
C	-0.475400	-1.840400	6.256500	H	5.059000	-0.549600	-0.590900
C	-0.869500	-0.739500	7.179400	H	2.912200	-0.976900	-0.615800
C	2.037100	-1.529200	-6.632200	H	-6.383200	0.232400	2.162000
C	-0.344400	-2.273300	-6.951600	H	-5.794100	1.642000	2.901700
C	1.271800	-7.030500	-0.996100	H	-7.206800	1.609700	2.403000
C	0.296200	-7.089400	1.284000	H	-7.216200	0.745800	-0.123500
C	-1.390600	-3.027500	6.357700	H	-6.763400	2.175700	-1.137000
C	0.919300	-2.320900	6.679500	H	-7.953000	1.919700	-0.029800
H	-0.221300	0.881300	-3.082200	H	-7.019400	3.913700	1.294500
H	0.191400	-0.060200	-5.072300	H	-5.729000	3.990700	1.944600
H	0.768300	-3.551100	-3.521200	H	-5.867100	4.132000	0.244400
H	0.858600	-4.582300	-1.629100	H	-1.049900	7.931200	1.876800
H	0.624000	-4.555100	2.206000	H	-1.396500	7.025800	0.689800
H	0.012600	-3.228700	3.950700	H	-1.589400	6.515400	2.402100
H	-0.817800	0.518000	4.993900	H	0.369400	5.731300	3.724300

H	0.813200	7.135900	3.251300	H	7.382400	2.631600	1.729000
H	1.845800	5.822400	2.945800	H	5.730000	3.227700	1.889900
H	1.142000	7.923200	0.970800	H	6.315500	1.760200	2.191700
H	0.585400	7.037800	0.007100	H	7.144400	0.123900	0.396800
H	2.082500	6.811800	0.762700	H	8.133500	1.198100	-0.172100
H	6.256000	2.892500	-1.717700	H	7.073700	0.530500	-1.114000
H	7.364200	3.441800	-0.757100				
H	5.869400	3.868000	-0.554300				