SUPPORTING INFORMATION

for

Experimental and Theoretical EPR Study of Jahn-Teller Active [HIPTN$_3$N]MoL Complexes (L = N$_2$, CO, NH$_3$)

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Additional Details for the PJTE in [Mo]L,

It was first speculated, and then suggested by DFT computations, that E(a) > E(e), giving rise to the ligand-field diagram of **Scheme 1**. In that case the low-spin d^3 Mo(III) ion would have an (e^3) configuration, as opposed to an (a^2e) configuration if the inequality were reversed, **Scheme 1**.

In either case the ligand-field ground state is orbitally doubly degenerate with an additional two-fold spin degeneracy, ^{2}E, and is susceptible to a Jahn-Teller (JT) distortion induced by vibronic coupling to a doubly-degenerate, e, vibration. If we consider only linear JT coupling to a single 'effective' mode (see below), with coupling parameter F, and take as basis functions the angular momentum eigenfunctions, [|+1>, |-1>], then the JT coupling Hamiltonian can be written in terms of the magnitude of the distortion, ρ, and its 'phase angle', ϕ

$$H_{\pm}JT = F\rho\, e^{i\phi}$$

If we consider a deformation mode of the 'in-plane' nitrogen triangle, as ϕ varies a distortion that puts ligand N_1 at the apex of an isosceles triangle transforms into one in which N_2 is at the apex, and then N_3 (psuedo-rotation). Symmetry lowering also is induced by a rhombic ligand field component,

Two-Orbital, $^2E_1$ Model.

In treating the PJT one first determines the adiabatic electronic wave functions written as a function of the nuclear coordinates, to obtain the ground and excited molecular potential surfaces, $W_{\pm}(\rho, \phi)$, then solves the Hamiltonian for the nuclear motions of the ground state, characterized by W_{+}. As the three interactions can be comparable, they must be treated

consistently, through diagonalization of the electronic Hamiltonian matrix which incorporates all three, rather than sequentially, with one dominant and the other(s) as perturbations, **eq SA1**, where F is the linear JT coupling, λ = 800cm-1 is the SOC param for Mo(III), and V is the rhombic ligand-field:

$$\begin{vmatrix} |+1,+\tfrac{1}{2}\rangle & |-1,-\tfrac{1}{2}\rangle & |-1,+\tfrac{1}{2}\rangle & |+1,-\tfrac{1}{2}\rangle \\ +\lambda/2 & 0 & \frac{\gamma}{2}e^{-i\alpha} & 0 \\ 0 & +\lambda/2 & 0 & \frac{\gamma}{2}e^{+i\alpha} \\ \frac{\gamma}{2}e^{+i\alpha} & 0 & -\lambda/2 & 0 \\ 0 & \frac{\gamma}{2}e^{-i\alpha} & 0 & -\lambda/2 \end{vmatrix} \qquad \text{(SA1)}$$

$$\frac{\gamma}{2} = \left[(F\rho_0 \sin\phi)^2 + \left(F\rho_0 \cos\phi + \frac{\mathbf{V}}{\mathbf{2}} \right)^2 \right]^{1/2} \qquad \tan\alpha(q) = \frac{F\rho_0 \sin\phi}{F\rho_0 \cos\phi + \frac{V}{2}}$$

Odd-electron/hole delocalization onto the ligands introduced by replacing λ with $k\lambda$ where k is the SOC orbital reduction factor, $k \leq 1$ see text. Inspection shows that this matrix can be rearranged to give two block-diagonal 2x2 submatrices.

For present purposes, the $[a^2e^1]$ configuration can be treated as a single electron in the [e] electronic level, while the e^3 configuration can be treated as a single hole in the [e] subshell. The result in either case is that the ground-state electronic energies and wavefunctions are determined by the ratio between the magnitude of the off-diagonal matrix element, γ, and SOC, coupling constant, λ,

$$\tan 2\theta \equiv \frac{\gamma}{\lambda} \equiv r \qquad \text{(SA2)}$$

further introducing the fictitious angle, θ, which is useful in writing the resulting eigenfunctions and their expectation values; the ratio, *r*, will be useful in discussing experimental results. The formulas for the energies of the resulting molecular energy surfaces are given in the text.The adiabatic wavefunctions for the ground states of the [a^2e] and [e^3] configurations can be obtained by solving the Hamiltonian (**eq SA1)** for fixed nuclear configuration, and can be written in terms of the basis functions and trigonometric functions of the angle θ (**eq SA3**). From the wavefunctions we can calculate the g-values as a function of θ:

$$\begin{cases} |\nu_{up}+> &= \cos\theta e^{+i\alpha/2} |+1+\frac{1}{2}> &+ \sin\theta e^{-i\alpha/2} |-1+\frac{1}{2}> \\ |\nu_{up}-> &= \cos\theta e^{-i\alpha/2} |-1-\frac{1}{2}> &+ \sin\theta e^{+i\alpha/2} |+1-\frac{1}{2}> \end{cases} \qquad \text{(SA3)}$$

With the inclusion of *k*, these wavefunctions yield the g-values of **eq 11**.

Vibronic Interactions

1. Projection of Nuclear displacements onto eigenvectors of the molecular Hessian modes

Within the harmonic approximation the nuclear Hamiltonian is given by

$$\widehat{H}_N = \sum_i^{3N} \frac{p_{x,i}^2}{2m_i} + \frac{1}{2}\sum_i^{3N}\sum_j^{3N} V_{ij} x_i x_j \tag{1}$$

where $p_{x,i}^2$ is the momentum operator of nucleus i in the space representation, m_i the mass of nucleus i and $V_{ij} = \frac{\partial E}{\partial x_i \partial x_j}$ the second derivative of the electronic energy with respect to nuclear displacements along x_i and x_j. The matrix **V** is the so-called molecular Hessian. Introducing mass weighted coordinates this can be rewritten as

$$\widehat{H}_N = \sum_i^{3N} \frac{p_{xmw,i}}{2} + \frac{1}{2}\sum_i^{3N}\sum_j^{3N} U_{i,j} x_{mw,i} x_{mw,j} \tag{2}$$

with

$$\begin{aligned} x_{mw,i} &= \sqrt{m_i}\, x_i \\ \vec{p}_{mw,i} &= \frac{\vec{p}_i}{\sqrt{m_i}} \\ U_{ij} &= \frac{V_{ij}}{\sqrt{m_i m_j}} \end{aligned} \tag{3}$$

U is called the mass-weighted molecular Hessian. **V** and **U** are real and symmetric and thus can be diagonalized by unitary transformation matrices **T** and **L**:

$$\mathbf{P}_X = \mathbf{T}^T\mathbf{V}\mathbf{T} \text{ and } \mathbf{W} = \mathbf{L}^T\mathbf{U}\mathbf{L} \tag{4}$$

With

$$P_{X,ij} = k_i \delta_{ij} \text{ and } W_{Q,ij} = \omega_i^2 \delta_{ij} \tag{5}$$

Here k denotes the force constant of the respective internal mode i and ω_i the angular frequency of the respective normal mode i. Since six eigenvectors that correspond to molecular translation and rotation have vanishing eigenvalues the space spanned by these eigenvectors is projected out before the diagonalization-step. The transformation matrices **T** and **L** are now used to evaluate the projection of geometry differences onto internal or normal modes. The projection vectors $\mathbf{\Delta}_i$ on internal modes and $\mathbf{\Delta}_Q$ on normal modes respectively are given by

$$\begin{aligned} \mathbf{\Delta}_i &= \mathbf{T}^T \mathbf{D} \\ \mathbf{\Delta}_Q &= \mathbf{L}^T \mathbf{D}^{(m)} \end{aligned} \tag{6}$$

where **D** and $\mathbf{D}^{(m)}$ are the geometry differences in Cartesian and mass-weighted Cartesian coordinates, respectively.

Within this work the molecular Hessians are obtained from numerical frequency calculation which are stored in files with the suffix .hess. In addition to the Hessian file a file that contains the initial and final geometry is needed. A file geom.xyz which contains the initial and final geometry is needed:

```
2 30
0
        -0.046213     -0.004535      0.000244
         2.167050     -0.001097      0.000052
         0.320376      2.091981     -0.040210
         0.326238     -1.086728     -1.795461
         0.325803     -1.019456      1.834401
         2.593038      1.344047     -0.450925

                    .
                    .
                    .

   2.593038      1.344047     -0.450925


1
        -0.018013      0.003432      0.125081
         2.193271     -0.020634      0.062594
         0.352643      2.024334     -0.485244
         0.224571     -0.860366     -1.785776
         0.373467     -1.042261      1.903194

.
                    .
                    .

   1.807578     -1.913741     -2.730711
```

The projection on dimensionless normal modes is invoked by

```
>orca_vib myfile.hess ddnc geom.xyz
```

Projection on internal modes is invoked by

```
>orca_vib myfile.hess dcic geom.xyz
```

The orca_vib program generates a file named geom.ddnc or geom.dcic which contains the projections vector **Δ**. In order to perform a multidimensional scan along either an internal or normal mode one has to add the keyword “mtr” to the command line of the ORCA input file and define the nature and number of the mode(s), the hessian file, number of steps and stepsize for each mode in the %mtr-block:

```
! TZVP TZV/J TightSCF   ZORA mtr


%mtr    HessName "your_hess.hess"
        modetype normal
        mlist   10, 11
        rsteps  8, 8
        lsteps  8, 8
        dxyz  0.195792, 0.195792
        end




* xyz 0 4
  Mo     -0.046213     -0.004535      0.000244
  N       2.167050     -0.001097      0.000052
  N       0.320376      2.091981     -0.040210
  N       0.326238     -1.086728     -1.795461
  N       0.325803     -1.019456      1.834401
  C       2.593038      1.344047     -0.450925
                    .
                    .
                    .
*
```

1. **Performing a direct scan between two geometries**

The procedure for performing a direct scan between two geometries is very similar to that for performing a scan along internal or normal modes. The basic idea behind it is that one adds a so-called quadratic perturbation to the nuclear Hamiltonian:

$$\widehat{H}_N = \sum_i^{3N} \frac{p_{x,i}^2}{2m_i} + \frac{1}{2}\sum_i^{3N}\sum_j^{3N} V_{ij} x_i x_j + U\mathbf{D}^2 \tag{7}$$

where ***D*** is the geometry difference vector in Cartesian coordinates. This quadratic perturbation adds some terms that depend on the size of U and the direction of **D** to the molecular Hessian. Thus for obtaining a Hessian of the form of equation (5) the new matrix **G** which is defined by

$$G_{ij} = V_{ij} + UD_iD_j \tag{8}$$

has to be diagonalized. If the value of U is chosen very high the quadratic perturbation dominates the molecular Hessian and thus one eigenvector of **G** has the same direction as **D**. In order to obtain the new internal modes that arise from the diagonalization of **G**, one has to proceed the following steps: First a geom.xyz file shown above has to be provided with an additional factor U in the first line:

```
2 30 10000000000
0
        -0.046213     -0.004535      0.000244
         2.167050     -0.001097      0.000052
         0.320376      2.091981     -0.040210
         0.326238     -1.086728     -1.795461
         0.325803     -1.019456      1.834401
         2.593038      1.344047     -0.450925

                    .
                    .
                    .

   2.593038      1.344047     -0.450925


1
        -0.018013      0.003432      0.125081
         2.193271     -0.020634      0.062594
         0.352643      2.024334     -0.485244
         0.224571     -0.860366     -1.785776
         0.373467     -1.042261      1.903194

                    .
                    .
                    .

   1.807578     -1.913741     -2.730711
```

The storage of the new internal coordinates and projection of the geometry difference onto them is achieved by the command

```
>orca_vib myfile.hess dcic geom.xyz -nm
```

The command –nm invokes the storage of the new internal modes in the myfile.hess file. As described above the orca_vib program will generate a geom.dcic file that contains the projections onto the new internal modes. Of course all projections are zero except for one. The last step is to perform a scan along the internal mode with the non-zero projection with an input file similar to that shown above.

2. Geometries

2.1 Model 1

[**Mo**]N_2

```
C      -0.387099     -0.735053     -7.257754
C      -0.433861     -1.957981     -6.515671
C       0.102565     -3.154540     -7.081538
C       0.685874     -3.112582     -8.365801
C       0.739767     -1.921344     -9.096336
C       0.203082     -0.753017     -8.541387
C      -1.006805     -2.021684     -5.120007
C      -0.155680     -1.863790     -4.002947
C      -0.654742     -1.917629     -2.681429
C      -2.035841     -2.125382     -2.493371
C      -2.919201     -2.270043     -3.590514
C      -2.385288     -2.240017     -4.898646
N      -4.329400     -2.364695     -3.363925
Mo     -5.659585     -3.800572     -3.872439
N      -4.334168     -5.025223     -4.762716
C       0.250157     -1.721451     -1.492620
C       1.060976     -2.795479     -1.019935
C       1.869867     -2.590597      0.117311
C       1.893091     -1.356817      0.780332
C       1.103971     -0.301602      0.305257
C       0.278683     -0.458717     -0.827889
C       1.039941     -4.178140     -1.676026
C       2.453039     -4.709376     -1.993826
C      -0.551495      0.736354     -1.306692
C      -1.659667      1.101231     -0.294848
C       0.094410     -4.488085     -6.328659
C       1.513191     -4.857048     -5.842474
C      -0.906356      0.632789     -6.779583
C      -0.135510      1.209261     -5.572842
C      -4.881583     -1.122180     -2.780417
C      -6.220922     -1.402375     -2.105923
N      -7.053988     -2.287301     -2.972826
C      -7.669263     -1.536234     -4.104399
C      -7.986522     -2.490220     -5.250754
N      -6.855083     -3.411606     -5.459422
C      -6.842192     -4.010469     -6.758012
C      -6.714300     -3.206503     -7.916927
C      -6.803189     -3.763275     -9.207969
C      -7.021962     -5.155119     -9.331336
C      -7.141739     -5.986565     -8.195875
C      -7.036021     -5.401226     -6.914430
C      -6.675734     -2.883969    -10.425079
C      -5.410054     -2.736818    -11.065294
```

C	-5.309865	-1.886745	-12.186333
C	-6.426232	-1.195986	-12.676162
C	-7.668260	-1.350387	-12.046995
C	-7.817338	-2.189286	-10.922658
C	-7.368324	-7.470685	-8.352909
C	-6.225792	-8.314964	-8.499797
C	-6.409188	-9.704311	-8.663035
C	-7.689249	-10.267219	-8.677519
C	-8.805954	-9.435177	-8.529526
C	-8.682359	-8.037102	-8.368216
C	-4.153032	-3.429138	-10.533382
C	-3.268968	-2.427039	-9.759113
C	-9.196324	-2.318098	-10.269253
C	-10.277370	-2.781189	-11.268725
C	-4.799085	-7.758875	-8.522465
C	-4.230428	-7.773032	-9.959107
C	-10.004369	-7.256718	-8.259833
C	-10.289936	-6.364257	-9.486686
C	-8.057078	-3.070659	-2.200171
C	-7.359636	-4.186763	-1.432184
N	-6.435348	-4.917159	-2.317955
C	-5.995726	-6.156102	-1.789082
C	-6.010303	-6.422894	-0.392952
C	-5.644041	-7.681513	0.126322
C	-5.266676	-8.706046	-0.765974
C	-5.241739	-8.478455	-2.163545
C	-5.590390	-7.206300	-2.655179
C	-5.665032	-7.906750	1.616783
C	-4.510879	-7.600523	2.396390
C	-4.558946	-7.797133	3.792467
C	-5.714072	-8.285164	4.417483
C	-6.845009	-8.584033	3.646549
C	-6.843588	-8.402982	2.247522
C	-3.235303	-7.034698	1.766680
C	-1.980835	-7.857561	2.127053
C	-8.113213	-8.724290	1.455040
C	-9.253424	-7.739005	1.792656
C	-4.820448	-9.586778	-3.098533
C	-5.771911	-10.416267	-3.773038
C	-5.287835	-11.442465	-4.614814
C	-3.918360	-11.671866	-4.795830
C	-2.995554	-10.861052	-4.127882
C	-3.422462	-9.816102	-3.281678
C	-7.302084	-10.329053	-3.637560
C	-7.938823	-9.035017	-4.188764
C	-2.355116	-8.975654	-2.574108
C	-1.608857	-9.805793	-1.506498
C	-0.517327	-5.633086	-7.162131
C	-2.433390	0.706288	-6.562600
C	0.249831	-5.182227	-0.808563
C	0.328923	1.962129	-1.631586
C	-3.855952	-8.493169	-7.547838
C	-10.210864	-6.483966	-6.939329
C	-3.347040	-4.146336	-11.635681
C	-9.613010	-1.006565	-9.568004
C	-7.810761	-10.649774	-2.216605
C	-1.366526	-8.331884	-3.568689
C	-8.565153	-10.187851	1.642638
C	-3.049041	-5.546261	2.135986
H	-6.768781	-0.458658	-1.865692
H	-6.039874	-1.947779	-1.157279
H	-4.190148	-0.690146	-2.019904
H	-4.984980	-0.337343	-3.573764

H	-8.636616	-2.406985	-1.511955
H	-8.761588	-3.514069	-2.933170
H	-6.919844	-0.794036	-4.448569
H	-8.577243	-0.983785	-3.759626
H	-8.191891	-1.887731	-6.165980
H	-8.924899	-3.068170	-5.050294
H	-6.831965	-3.760855	-0.541800
H	-8.136338	-4.877342	-1.024929
H	-6.298059	-5.638604	0.322520
H	-4.996224	-9.699249	-0.372151
H	-5.590556	-7.024365	-3.740003
H	-2.439956	-2.173228	-1.468180
H	0.919347	-1.682048	-4.166185
H	-3.069322	-2.358336	-5.754485
H	-6.537378	-2.123439	-7.807237
H	-7.104338	-5.598854	-10.337027
H	-7.142030	-6.025814	-6.012785
H	1.108271	-4.033958	-8.800321
H	1.198834	-1.900479	-10.099268
H	0.244117	0.187746	-9.117665
H	2.493243	-3.417691	0.496418
H	2.531457	-1.216263	1.669146
H	1.132664	0.670256	0.826719
H	-5.528637	-10.357342	-8.778943
H	-7.819914	-11.355335	-8.804371
H	-9.816920	-9.878661	-8.542705
H	-4.334913	-1.758916	-12.685542
H	-6.327955	-0.535277	-13.554347
H	-8.543762	-0.806572	-12.440591
H	-6.017869	-12.084221	-5.137717
H	-3.573033	-12.485167	-5.456487
H	-1.916271	-11.041136	-4.266616
H	-7.752279	-8.966152	4.144756
H	-5.732847	-8.433190	5.510726
H	-3.672810	-7.561294	4.405693
H	-0.544824	-4.367574	-5.428471
H	-0.613430	-6.551063	-6.541296
H	-1.533630	-5.368439	-7.525534
H	0.111373	-5.889873	-8.045028
H	1.495375	-5.809117	-5.265164
H	2.212172	-4.992833	-6.699317
H	1.936917	-4.065787	-5.185806
H	-0.693139	1.321024	-7.628950
H	-0.432168	2.269283	-5.401428
H	-0.343025	0.643713	-4.639354
H	0.962744	1.188038	-5.749218
H	-2.746780	1.768384	-6.438866
H	-2.984935	0.287693	-7.433532
H	-2.751828	0.151798	-5.654316
H	-4.842014	-6.698085	-8.195119
H	-3.207908	-7.332677	-9.981839
H	-4.161921	-8.812320	-10.354518
H	-4.870558	-7.189510	-10.657039
H	-2.869213	-7.980950	-7.511569
H	-4.265232	-8.509271	-6.514844
H	-3.673745	-9.547425	-7.855587
H	0.499459	-4.085491	-2.642221
H	2.389048	-5.664690	-2.561207
H	3.031064	-3.984960	-2.609023
H	3.041259	-4.913496	-1.070650
H	0.196438	-6.177235	-1.306192
H	0.731166	-5.322618	0.186167
H	-0.791270	-4.831523	-0.635332

H	-1.054531	0.438365	-2.251223
H	-2.284660	1.939673	-0.678966
H	-2.328631	0.234223	-0.096545
H	-1.231364	1.420992	0.682355
H	-0.290394	2.786974	-2.051331
H	0.841005	2.358000	-0.725513
H	1.112642	1.708872	-2.378766
H	-10.791607	-8.044617	-8.269661
H	-11.328343	-5.963743	-9.437344
H	-9.594992	-5.498572	-9.536152
H	-10.191017	-6.938438	-10.434414
H	-11.272904	-6.156938	-6.857333
H	-9.981599	-7.122242	-6.057343
H	-9.573299	-5.576456	-6.880565
H	-4.478722	-4.207181	-9.809750
H	-2.504269	-4.717123	-11.185841
H	-3.981204	-4.861974	-12.204247
H	-2.905005	-3.430650	-12.365252
H	-2.374922	-2.929542	-9.326344
H	-2.909319	-1.610643	-10.425674
H	-3.833177	-1.955247	-8.924456
H	-9.122515	-3.100370	-9.483637
H	-10.596726	-1.125490	-9.058762
H	-8.863652	-0.700597	-8.804204
H	-9.708429	-0.168780	-10.295802
H	-11.246298	-2.947566	-10.745856
H	-10.456022	-2.026342	-12.067589
H	-9.988030	-3.734163	-11.763558
H	-7.876165	-8.591352	0.378092
H	-9.444216	-10.410985	0.996743
H	-7.753506	-10.898243	1.371589
H	-8.861879	-10.399245	2.695023
H	-10.154551	-7.951680	1.173204
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H -4.63352833  -5.02526733  -6.63116825
C -4.21148338  -4.66661934  -3.96405490
C  2.00457653  -4.79748611   4.46738755
H  3.89117661  -6.50687596   3.75559091
H  6.12287521  -6.13236862   2.69782033
H  6.82990331  -3.81390912   2.08661027
C  5.48781602  -1.48199583   2.40015295
C  0.63851825  -0.56628274   7.53101285
H  1.25511916   1.15064930   9.55680663
H  2.91557055   3.01324719   9.58327715
H  4.28829773   3.49106000   7.55575652
C  4.24869432   2.24631432   5.12648689
C  4.87532965  -1.79635607  -3.38256269
C  6.53249951   0.07063283  -3.87167048
H  4.59703943   0.29606942  -2.96029713
H  5.36604023  -1.99802801  -2.40350023
H  3.80162769  -2.07646848  -3.29728811
H  5.33690205  -2.47826899  -4.13215077
H  7.05318684  -0.13198728  -2.90843456
H  7.05469095  -0.51042451  -4.66532684
H  6.65687697   1.15003655  -4.10776360
H  1.23669904   2.23984977  -7.65694999
C  0.15091691   2.01481883  -5.83636633
C  1.92857692   3.77348140  -6.34428274
H  1.13845923   4.47695730  -6.69303321
H  2.12172845   3.98444813  -5.27080603
H  2.85913003   3.99946404  -6.91071458
H -0.65704146   2.67245024  -6.23133873
H -0.16548292   0.95907289  -5.98911396
H  0.22975669   2.19728050  -4.74374372
C  3.65568827  -4.73030683  -0.68252915
C  3.15528849  -6.30485768  -2.61980367
H  1.92646046  -4.66612299  -1.96715856
H  3.77339735  -5.67617776  -3.30018872
H  3.81067674  -7.11134630  -2.21943297
```

```
H  2.35977483  -6.78822401  -3.22850480
H  4.25926398  -4.07182929  -1.34746349
H  3.22917104  -4.10792933   0.13541089
H  4.35548069  -5.44944157  -0.20185927
C  6.04818761   3.11409854   0.53511022
H  5.43813616   2.58434431  -1.46023332
C  7.49577494   3.20511346  -1.55842460
H  7.87687519   2.17604507  -1.37078765
H  7.51588037   3.38244834  -2.65638233
H  8.21517976   3.91401315  -1.08961599
H  6.45614951   2.10541424   0.77486916
H  6.66329882   3.86610158   1.07974423
H  5.01266788   3.16997408   0.93725387
C  2.39571574   7.16147121  -4.20262398
H  1.91313032   5.31860676  -3.20629945
C  1.23297831   6.92757053  -1.94927508
H  0.24209628   7.01603816  -2.45054109
H  1.10492694   6.29594610  -1.04221206
H  1.53043479   7.94527268  -1.60794021
H  1.41318473   7.21043901  -4.72435399
H  2.71368027   8.20793229  -3.99321453
H  3.13460544   6.71828600  -4.90581571
H -2.34174558  -7.50500892   1.31895490
C -2.61665435  -5.40208314   1.10358008
C -2.87621480  -7.16626920  -0.72059486
H -3.96412696  -7.24295211  -0.49361254
H -2.75238610  -6.42963778  -1.54333289
H -2.53470368  -8.15776476  -1.09228996
H -3.68377370  -5.51058868   1.40506566
H -2.03978114  -5.08728075   2.00120770
H -2.55928915  -4.58348638   0.35552025
C  1.57784409  -5.03556195  -6.27771498
C  0.96619796  -2.56585590  -6.13292254
H  0.80947842  -4.01574521  -4.54865796
H  2.63550497  -4.81095872  -6.01279235
H  1.34542687  -6.06327970  -5.92057207
H  1.51125592  -5.04117568  -7.38920892
H  2.02666146  -2.30279564  -5.91918031
H  0.81025294  -2.46767024  -7.23118198
H  0.31913023  -1.81030902  -5.63474591
C -5.17726809  -3.46367400  -4.03722804
C -4.98686595  -6.00120228  -3.95577905
H -3.67290955  -4.59633794  -2.99480560
H -5.90734937  -3.49108291  -3.19627878
H -4.62580737  -2.49871400  -3.98293149
H -5.75665661  -3.46475728  -4.98861927
H -5.67659107  -6.04541409  -3.08271187
H -5.60427762  -6.12992287  -4.87351528
H -4.29541128  -6.86971860  -3.88949475
C  0.89214429  -1.57017840   8.67533280
C -0.79881791  -0.00456734   7.59004517
H  0.73042931  -1.12750370   6.57677392
H  0.17142239  -2.41706544   8.61817752
H  1.91983131  -1.99205297   8.62158682
H  0.77229556  -1.09828294   9.67696026
H -1.54634931  -0.83009960   7.56222981
H -0.97188310   0.57724431   8.52415174
H -1.00207315   0.67193766   6.73038260
C  3.72952061   3.54019404   4.46088161
C  5.75717261   2.34635465   5.43421190
H  4.11813205   1.42372846   4.39076528
H  4.30555888   3.76768071   3.53496951
H  2.65674422   3.44611770   4.18246933
```

```
H   3.82588019    4.41369703    5.14565860
H   6.33436196    2.50914597    4.49609259
H   5.99045072    3.19604665    6.11514999
H   6.13614550    1.41636860    5.91260217
H   2.04656237   -5.90726953    4.54977672
C   1.93689347   -4.26704667    5.91568597
C   0.70617373   -4.49054856    3.69193488
H   1.05535587   -4.70041308    6.44122021
H   2.84765706   -4.54585346    6.49082123
H   1.83998118   -3.16032468    5.94298796
H  -0.15193220   -5.00333666    4.18363364
H   0.47963181   -3.40375279    3.66730571
H   0.76384892   -4.86225082    2.64495655
C   5.84372239   -1.38275229    0.90184547
H   4.66214016   -0.76373835    2.59034474
C   6.68002987   -1.04685542    3.27961257
H   7.00110545   -0.01129284    3.02489991
H   6.41060477   -1.06478343    4.35821533
H   7.55772517   -1.71818347    3.13958731
H   6.11525974   -0.33695935    0.63214085
H   6.70819944   -2.03140618    0.63417627
H   4.98893862   -1.69353109    0.25983120
```

2.2 Model 1'

2.2.1 symmetric structures

[**Mo**]N_2

```
C       0.007181     -0.001261      0.000839
C       1.537155      0.003634      0.003003
N       2.012056      1.372491      0.010377
Mo      0.791099      2.744477      0.833260
N       2.166088      4.558610      0.723008
N      -0.543438      0.992547      0.944307
C      -0.497392      0.531817      2.346655
C      -0.420112      1.705202      3.325449
N       0.525491      2.683457      2.827236
N      -0.726526      3.439578     -0.290942
C      -1.801627      2.510453     -0.574202
C      -1.882343      1.472793      0.547212
H      -0.385694     -0.992514      0.220785
H      -0.329787      0.276813     -0.987490
H       1.859366     -0.538259     -0.885368
H       1.909550     -0.567499      0.855457
H       2.970456      1.440252     -0.253383
H      -2.518666      0.635243      0.266304
H      -2.321110      1.946038      1.413924
H      -0.796699      4.273268     -0.832002
H       0.399584     -0.060342      2.458215
H      -1.349875     -0.109474      2.564204
H      -0.119535      1.297263      4.289763
H      -1.414206      2.130492      3.475264
H       0.812344      3.324244      3.534215
H      -1.672418      2.009710     -1.535503
H      -2.770800      3.005579     -0.621354
N       2.804151      5.413464      0.679144
```

[**Mo**]CO

```
Mo  0.00000000   0.00000000   0.00000000
N -0.00000000  -0.00000000   2.23582633
N -1.61000515  -1.14589591   0.33630993
N -0.18758777   1.96722856   0.33622866
N  1.79744083  -0.82125100   0.33617763
C -0.00353477   0.00132972  -2.12912268
O -0.01088652   0.00328505  -3.23893308
C  1.04614059  -0.95760352   2.64281198
C -1.35234280  -0.42714732   2.64293697
C -1.90434035  -1.50439651   1.70931346
C -0.35073984   2.40140878   1.70924021
C  0.30628488   1.38476806   2.64282657
C  2.25506265  -0.89694941   1.70917469
H  1.33663676  -0.78763666   3.67808456
H  0.61771699  -1.94746818   2.57743814
H  2.84828132  -1.79162761   1.89121416
H  2.89200420  -0.05250608   1.97700457
H  2.51340297  -1.05865090  -0.31384278
H -1.35031616  -0.76372588   3.67820190
H -1.99537242   0.43882051   2.57762667
H -2.17369136  -1.64718264  -0.31366409
H  1.37774222   1.50866267   2.57739877
H  0.01389552   1.55135357   3.67811417
H  0.12749145   3.36248666   1.89122078
H -1.40050316   2.53081243   1.97711173
H -0.34004315   2.70599617  -0.31375175
H -1.49150688  -2.47824016   1.97708412
H -2.97576066  -1.57079000   1.89136083
```

[**Mo**]NH_3

```
  Mo      0.000000      0.000000      0.000000
  N       0.000000      0.000000      2.374180
  N      -0.001940     -0.000248     -2.222232
  N      -2.002522     -0.002985     -0.318078
  N       1.003231     -1.732504     -0.320754
  N       0.998116      1.735388     -0.321116
  C      -1.352886     -0.433537     -2.624261
  C      -2.433773      0.125017     -1.695084
  C       1.048162     -0.953311     -2.626446
  C       1.106204     -2.169235     -1.698108
  C       0.297790      1.385941     -2.626069
  C       1.322995      2.043693     -1.698740
  H      -1.548942     -0.162520     -3.661248
  H      -1.375312     -1.511829     -2.555295
  H      -3.345680     -0.437382     -1.897583
  H      -2.654543      1.159849     -1.966576
  H      -2.760125      0.116747      0.318769
  H       0.909958     -1.257917     -3.663437
  H       1.993316     -0.433657     -2.558501
  H       1.279796     -2.448522      0.315397
  H      -0.624757      1.944559     -2.556603
  H       0.629331      1.419152     -3.663472
  H       1.291587      3.114443     -1.902159
  H       2.329292      1.717302     -1.971077
```

```
H       1.481448      2.332016      0.314726
H      -0.903349     -0.230565      2.739006
H       0.650575     -0.666623      2.741116
H       0.251239      0.897154      2.740624
H       0.320087     -2.877748     -1.968950
H       2.048974     -2.677592     -1.902117
```

2.2.2 distorted structures

[**Mo**]N_2

```
C       0.009596     -0.001549     -0.008509
C       1.539067     -0.010663      0.012595
N       2.025135      1.354462      0.029294
Mo      0.793201      2.744022      0.802878
N       2.166239      4.554532      0.698419
N      -0.540953      0.991303      0.933917
C      -0.493715      0.535345      2.338158
C      -0.410637      1.714414      3.309263
N       0.527832      2.691979      2.796913
N      -0.752497      3.456239     -0.271333
C      -1.814218      2.516903     -0.568852
C      -1.884007      1.465284      0.540182
H      -0.392598     -0.991525      0.200700
H      -0.313755      0.285952     -0.998791
H       1.868746     -0.551260     -0.873744
H       1.896228     -0.586793      0.867727
H       3.004745      1.406758     -0.147326
H      -2.511173      0.624142      0.250115
H      -2.328085      1.924381      1.411600
H      -0.858595      4.321457     -0.752933
H       0.401687     -0.058915      2.451084
H      -1.347358     -0.103164      2.559581
H      -0.102615      1.312035      4.273963
H      -1.405515      2.137301      3.465196
H       0.826062      3.325800      3.505810
H      -1.674597      2.030255     -1.535513
H      -2.789175      3.000120     -0.612722
N       2.805251      5.409262      0.660704
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[**Mo**]CO

```
Mo  0.00000000   0.00000000   0.00000000
N -0.00000000  -0.00000000   2.26277528
N -1.63450601  -1.06145642   0.38621089
N -0.20435990   1.94715884   0.35684154
N  1.81628686  -0.71428861   0.39123240
C -0.01625116   0.05293626  -2.08004705
O -0.03094890   0.10323538  -3.19784820
C  1.04242107  -0.95753715   2.67129010
C -1.34222921  -0.42732193   2.70078923
C -1.90870815  -1.47691150   1.74816310
C -0.35967276   2.39172566   1.72641160
C  0.30808186   1.38625682   2.66228386
C  2.26211604  -0.86120972   1.76206904
H  1.31487344  -0.80981615   3.71470007
H  0.62220775  -1.94868725   2.57688073
```

```
H  2.85345496  -1.76435602   1.90228141
H  2.89741368  -0.03001212   2.06892333
H  2.58498476  -0.69915241  -0.24518815
H -1.31131937  -0.78621326   3.72806259
H -1.98639779   0.43933524   2.67038082
H -2.36357746  -1.30363306  -0.24789637
H  1.37824932   1.51434961   2.58864358
H  0.02222943   1.55723245   3.69865433
H  0.11433659   3.35711008   1.89600994
H -1.40866361   2.51818437   1.99959352
H -0.34141438   2.68662582  -0.29580097
H -1.48682191  -2.45706033   1.96734802
H -2.97677636  -1.55700739   1.93396681
```

[**Mo**]NH_3

```
Mo  0.00000000   0.00000000   0.00000000
N -0.00000000  -0.00000000   2.37306753
N -0.01507861  -0.00534362  -2.22383176
N  2.00146649  -0.02974873  -0.32871554
N -1.06221823   1.69892981  -0.31660977
N -1.02218009  -1.71812894  -0.32273690
C  1.33411549   0.43134218  -2.62412111
C  2.41830799  -0.14649272  -1.71143787
C -1.06593442   0.94713854  -2.63105889
C -1.14700204   2.15139011  -1.68950879
C -0.31737348  -1.39058498  -2.62827071
C -1.34394694  -2.04117955  -1.69783532
H  1.52705340   0.17712629  -3.66603104
H  1.35872962   1.50826222  -2.53655709
H  3.33333014   0.41041496  -1.91470172
H  2.62711873  -1.17988756  -1.99541049
H  2.74122771  -0.25694738   0.30015804
H -0.91353013   1.26283809  -3.66261345
H -2.00881273   0.42139129  -2.58360306
H -1.43911065   2.36446811   0.32193025
H  0.60349179  -1.95193663  -2.55792342
H -0.64876487  -1.42466904  -3.66582671
H -1.31183348  -3.11401171  -1.89179830
H -2.35028531  -1.71872393  -1.97694614
H -1.51533957  -2.30803627   0.31289318
H  0.87908791   0.30695622   2.74115803
H -0.69770667   0.63243280   2.71383411
H -0.19491832  -0.90161089   2.76129810
H -0.36139984   2.86822403  -1.93837599
H -2.08971030   2.65564245  -1.90245896
```

2.3 model 1’’

[**Mo**]N_2

```
  Mo     -2.385288     -2.240016     -4.898649
  N      -3.145512     -2.282771     -3.036033
  N      -3.657229     -2.312676     -2.019790
  N      -1.711023     -2.133512     -7.038195
```

N	-2.227123	-0.235603	-5.135995
N	-3.955460	-3.140281	-5.800758
N	-0.646447	-3.347355	-4.775235
C	-2.019992	-0.757965	-7.523512
C	-1.720267	0.259776	-6.428414
C	-2.484526	-3.171959	-7.781121
C	-3.924383	-3.209241	-7.278430
C	-0.248517	-2.411737	-7.015708
C	0.043120	-3.562197	-6.060039
H	-2.004673	-4.150168	-7.573718
H	-2.435124	-2.986507	-8.881862
H	-4.526862	-2.371358	-7.715500
H	-4.400800	-4.146328	-7.649932
H	-3.104541	-0.730341	-7.755741
H	-1.454703	-0.537904	-8.461870
H	-2.197072	1.228607	-6.705601
H	-0.622234	0.470166	-6.358981
H	0.253988	-1.493467	-6.648965
H	0.130635	-2.633837	-8.043757
H	1.146728	-3.624043	-5.904322
H	-0.253712	-4.531874	-6.533571
C	-2.579193	0.826379	-4.190219
C	-0.340953	-4.356455	-3.762420
C	-5.251926	-3.546297	-5.251473
C	-3.908620	1.535372	-4.493257
C	-5.447713	-5.069362	-5.189192
C	1.024473	-4.152145	-3.085974
H	1.193868	-4.925369	-2.320521
H	1.852691	-4.213720	-3.807728
H	1.065954	-3.166748	-2.600654
H	-6.437581	-5.315661	-4.774379
H	-5.380678	-5.534212	-6.184659
H	-4.680934	-5.526395	-4.547614
H	-4.100826	2.329864	-3.755286
H	-3.907422	2.003335	-5.489698
H	-4.742098	0.819476	-4.454722
H	-1.125466	-4.316300	-2.991855
H	-0.385056	-5.375069	-4.203807
H	-5.341265	-3.134231	-4.237363
H	-6.071910	-3.095570	-5.848899
H	-2.624294	0.386001	-3.184695
H	-1.760916	1.575126	-4.162280

[**Mo**]CO

Mo	-0.370094	-0.776126	-7.259094
C	-0.445836	-2.467765	-6.227502
O	-0.456108	-3.508368	-5.672691
N	-2.180829	-0.867649	-8.155345
N	-0.302104	1.068364	-8.619048
N	-0.066366	0.713795	-5.856742
N	1.233382	-1.229416	-8.408901
C	1.564807	-0.287469	-9.502231
C	1.079196	1.120577	-9.171035
C	-1.326343	0.860461	-9.676380
C	-2.571029	0.218642	-9.072832
C	0.112274	2.070331	-6.405053
C	-0.621931	2.216351	-7.732252
H	1.733679	1.550703	-8.385508

H	1.125179	1.790721	-10.064693
H	-1.565909	1.823290	-10.191684
H	-0.368838	3.188274	-8.224595
H	-1.715761	2.195605	-7.549031
H	1.194643	2.317918	-6.543871
H	-0.285893	2.832225	-5.693149
H	-3.196798	0.974341	-8.532703
H	-3.210188	-0.165969	-9.901071
H	-0.889436	0.166583	-10.423969
H	1.121737	-0.649923	-10.465600
H	2.664989	-0.245081	-9.676875
C	0.576381	0.518587	-4.557763
C	-0.239170	1.091334	-3.386666
C	-3.158590	-1.961053	-8.102525
C	-3.126009	-2.902478	-9.315936
C	2.024039	-2.462181	-8.488605
C	3.443193	-2.321435	-7.917134
H	0.275987	0.903136	-2.432019
H	-0.379532	2.178609	-3.480401
H	-1.230896	0.619323	-3.346724
H	-3.898642	-3.681420	-9.221612
H	-3.311083	-2.365962	-10.259371
H	-2.146204	-3.395318	-9.390874
H	3.993728	-3.270505	-8.010697
H	4.024484	-1.547955	-8.442070
H	3.398853	-2.050946	-6.852516
H	0.707683	-0.562504	-4.400651
H	1.490733	-3.245140	-7.934325
H	2.085382	-2.802222	-9.543570
H	-2.973558	-2.538341	-7.187235
H	-4.175144	-1.529798	-7.997592
H	1.592216	0.967781	-4.555934

[**Mo**]NH_3

Mo	0.000000	0.000000	0.000000
N	0.000000	-0.000000	2.216533
N	-0.285171	0.004718	-2.279534
N	2.004311	0.474895	0.316334
N	-0.518640	-1.927117	0.328953
N	-1.436837	1.399372	0.350965
C	2.970024	0.928749	-0.594152
C	-0.581237	-2.365423	1.743326
C	-0.830393	-1.164002	2.652054
C	-0.582721	1.300275	2.658544
C	-1.760506	1.681705	1.765676
C	-2.297164	2.076237	-0.555955
C	-1.863288	3.517436	-0.893714
C	2.318314	0.721784	1.731216
C	1.427336	-0.143035	2.619678
C	-0.748254	-2.988987	-0.591353
C	-2.225153	-3.401980	-0.777574
C	4.230037	0.039526	-0.716681
H	3.306753	1.968583	-0.362264
H	-0.884911	1.257688	3.734853
H	0.214347	2.063803	2.551589
H	-1.987450	2.762476	1.926932
H	-2.688755	1.130205	2.070077
H	1.560266	0.116824	3.699429
H	1.702564	-1.208656	2.481159

H	-1.891664	-0.853055	2.556872
H	-0.634431	-1.411885	3.724765
H	-1.396483	-3.106776	1.917960
H	0.368415	-2.890826	2.024018
H	-1.174880	0.491053	-2.522161
H	0.462152	0.518729	-2.788176
H	-0.336996	-0.936202	-2.722830
H	2.201169	1.801001	2.006636
H	3.382951	0.463776	1.952892
H	2.515735	0.996716	-1.600586
H	-3.345231	2.108265	-0.176930
H	-2.372707	1.512731	-1.505640
H	-0.168591	-3.895865	-0.302868
H	-0.343914	-2.702078	-1.579029
H	-2.820366	-2.544804	-1.127277
H	-2.321620	-4.218722	-1.511452
H	-2.669196	-3.751571	0.166806
H	-1.822879	4.142017	0.011595
H	-0.857324	3.512842	-1.339810
H	-2.563100	3.993966	-1.599621
H	4.935889	0.454691	-1.454255
H	4.763546	-0.040601	0.242620
H	3.947836	-0.976362	-1.030904