Supporting Information for

Methods for Computing Accurate Atomic Spin Moments for Collinear and Noncollinear Magnetism in Periodic and Nonperiodic Materials

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CONTENTS:

1. Computational algorithm and uniqueness proof for the least squares fitting (LSF) functional that computes ASM's

The LSF functional does not perform as well as the χ_{spin} functional that minimizes information distance. The theory and methods for the χ_{spin} functional are described in the main body of the paper. The theory and methods for the LSF functional are described below. Data for the LSF functional are labeled LSF in the main paper.

1.1 Form of the LSF Optimization Functional

First, we construct the least squared difference between $\vec{m}_A(\vec{r}_A)$ and its spherical average, $\vec{m}_A^{avg}(r_A)$, to obtain the non-negative distance measure

$$H_A = \oint \frac{\left|\vec{m}_A(\vec{r}_A) - \vec{m}_A^{avg}(r_A)\right|^2}{2\rho_A^{avg}(r_A)} d^3\vec{r}_A \,. \quad (1)$$

(Herein the symbols H_A, H, $\vec{\Lambda}_A(\vec{r}_A)$, and $\vec{L}_A(\vec{r}_A)$ have slightly different meanings than their counterparts for the information distance functional described in the main body of the paper.) The denominator $\rho_A^{avg}(r_A)$ in Eq. (1) insures H_A is a bone fide extensive property with units of charge, whereas omitting this denominator would give H_A units of charge-squared per meter cubed which is an ill-formed combination for an extensive property. In the denominator, $\rho_A^{avg}(r_A)$ is used instead of $\rho_A(\vec{r}_A)$ to give all points at the same r_A equal weight which allows Eq. (1) to be equivalently written as

$$H_A = \oint \frac{\left(m_A(\vec{r}_A)\right)^2 - \left(m_A^{avg}(r_A)\right)^2}{2\rho_A^{avg}(r_A)} d^3\vec{r}_A \,. \quad (2)$$

This means H_A also minimizes the difference in squared magnitudes between the local and spherically averaged spin moments of atom A. The factor of two in the denominator is a convenience to cancel the factor of two that arises during differentiation and does not affect the optimized distributions. This gives the following optimization functional

$$H = \sum_A H_A + \int_U \vec{\Lambda}(\vec{r}) \bullet \vec{\Delta}(\vec{r}) d^3\vec{r} - \sum_A \oint \nu_A(\vec{r}_A) \kappa_A(\vec{r}_A) d^3\vec{r}_A \,, \quad (3)$$

where the Lagrange multipliers $\nu(\vec{r}_A) \geq 0$ and $\vec{\Lambda}(\vec{r})$ are used to enforce the constraints

$$\kappa_A(\vec{r}_A) = \rho_A(\vec{r}_A) - m_A(\vec{r}_A) \geq 0 \quad (4)$$

$$\vec{\Delta}(\vec{r}) = \vec{m}(\vec{r}) - \sum_{k,A} \vec{m}_A(\vec{r}_A) = 0 \,. \quad (5)$$

Minimization occurs when

$$\delta H = \sum_A \oint \frac{\partial H}{\partial \vec{m}_A(\vec{r}_A)} \bullet \delta\vec{m}_A(\vec{r}_A) d^3\vec{r}_A = 0 \quad (6)$$

for arbitrary $\delta\vec{m}_A(\vec{r}_A)$, which is true when

$$\frac{\partial H}{\partial \vec{m}_A(\vec{r}_A)} = \frac{\vec{m}_A(\vec{r}_A) - \vec{m}_A^{avg}(r_A)}{\rho_A^{avg}(r_A)} - \vec{\Lambda}(\vec{r}) + \nu_A(\vec{r}_A)\hat{m}_A(\vec{r}_A) \quad (7)$$

equals zero. Defining

$$\vec{L}_A(\vec{r}_A) = \left(\nu_A(\vec{r}_A)\rho_A^{avg}(r_A) + m_A(\vec{r}_A)\right)\hat{m}_A(\vec{r}_A), \quad (8)$$

$$\vec{\Lambda}_A(\vec{r}_A) = \frac{\vec{L}_A(\vec{r}_A) - \vec{m}_A^{avg}(r_A)}{\rho_A^{avg}(r_A)}, \quad (9)$$

this solution takes the form

$$\vec{\Lambda}_A(\vec{r}_A) = \vec{\Lambda}(\vec{r}). \quad (10)$$

1.2 Uniqueness of Solution

To prove uniqueness, it is sufficient to show that H is everywhere convex, which is necessarily true if its second order variational derivative

$$\delta^2 H = \sum_A \sum_B \oint\oint \delta\vec{m}_A(\vec{r}_A) \bullet \frac{\partial^2 H}{\partial\vec{m}_A(\vec{r}_A)\partial\vec{m}_B(\vec{r}'_B)} \bullet \delta\vec{m}_B(\vec{r}'_B) d^3\vec{r}_A d^3\vec{r}'_B \quad (11)$$

is greater than or equal to zero for arbitrary $\{\delta\vec{m}_A(\vec{r}_A)\}$. Since the only non-zero second order derivatives of H with respect to the independent variables $\{\vec{m}_A(\vec{r}_A)\}$ are

$$\frac{\partial^2 H}{\partial\vec{m}_A(\vec{r}_A)\partial\vec{m}_A(\vec{r}'_A)} = \frac{\partial}{\partial\vec{m}_A(\vec{r}'_A)}\left(\frac{\vec{m}_A(\vec{r}_A) - \vec{m}_A^{avg}(r_A)}{\rho_A^{avg}(r_A)}\right) + \nu_A(\vec{r}_A)\frac{\partial\hat{m}_A(\vec{r}_A)}{\partial\vec{m}_A(\vec{r}'_A)}, \quad (12)$$

it follows from Eq. (11) that H is convex if

$$\oint\oint \vec{\varphi}(\vec{r}_A) \bullet \frac{\partial^2 H}{\partial\vec{m}_A(\vec{r}_A)\partial\vec{m}_A(\vec{r}'_A)} \bullet \vec{\varphi}(\vec{r}'_A) d^3\vec{r}_A d^3\vec{r}'_A \geq 0. \quad (13)$$

Expanding

$$\frac{\partial\hat{m}_A(\vec{r}_A)}{\partial\vec{m}_A(\vec{r}'_A)} = \frac{\hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z} - \hat{m}_A(\vec{r}_A)\hat{m}_A(\vec{r}_A)}{m_A(\vec{r}_A)}\delta^{dirac}(\vec{r}'_A - \vec{r}_A) \quad (14)$$

which gives

$$\oint\oint \vec{\varphi}(\vec{r}_A) \bullet \nu_A(\vec{r}_A)\frac{\partial\hat{m}_A(\vec{r}_A)}{\partial\vec{m}_A(\vec{r}'_A)} \bullet \vec{\varphi}(\vec{r}'_A) d^3\vec{r}_A d^3\vec{r}'_A = \oint \nu_A(\vec{r}_A)\frac{\left|\vec{\varphi}(\vec{r}_A)\right|^2 - \left|\vec{\varphi}(\vec{r}_A) \bullet \hat{m}_A(\vec{r}_A)\right|^2}{m_A(\vec{r}_A)} d^3\vec{r}_A \geq 0. \quad (15)$$

The inequality in Eq. (15) follows from the facts that $\nu_A(\vec{r}_A) \geq 0$ and the absolute value of the scalar projection of a vector onto any unit direction is less than or equal to the magnitude of that vector. Expanding

$$\frac{\partial}{\partial\vec{m}_A(\vec{r}'_A)}\left(\frac{\vec{m}_A(\vec{r}_A) - \vec{m}_A^{avg}(r_A)}{\rho_A^{avg}(r_A)}\right) = \frac{(\hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z})}{\rho_A^{avg}(r_A)}\left(\delta^{dirac}(\vec{r}'_A - \vec{r}_A) - \frac{\delta^{dirac}(r'_A - r_A)}{4\pi(r_A)^2}\right) \quad (16)$$

gives

$$\begin{aligned} &\oint\oint \vec{\varphi}(\vec{r}_A) \bullet \frac{\partial}{\partial\vec{m}_A(\vec{r}'_A)}\left(\frac{\vec{m}_A(\vec{r}_A) - \vec{m}_A^{avg}(r_A)}{\rho_A^{avg}(r_A)}\right) \bullet \vec{\varphi}(\vec{r}'_A) d^3\vec{r}_A d^3\vec{r}'_A \\ &= \oint \frac{\left|\vec{\varphi}(\vec{r}_A)\right|^2 - \left|\vec{\varphi}^{avg}(r_A)\right|^2}{\rho_A^{avg}(r_A)} d^3\vec{r}_A \geq 0 \end{aligned} \quad (17)$$

Combining Eqs. (11), (12), (15) and (17) gives $\delta^2 H \geq 0$, which proves H has a unique minimum.

1.3 Iterative Solution

We now describe an iterative algorithm that efficiently converges to H's unique minimum. Prior to the first iteration the following quantity is computed

$$\rho^{avg}(\vec{r}) = \sum_{k,A} \rho_A^{avg}(r_A). \quad (18)$$

Each iteration involves three loops. The first loop runs over $\{A, \vec{r}_A\}$, where all grid points having $r_A \leq r_{cutoff}$ are included. A cutoff of 4 Å was used. This loop generates an updated and unstored estimate of $\vec{m}_A(\vec{r}_A)$ that is used to accumulate sums stored for use in the second and third loops. In the first iteration, proportional partitioning is used:

$$\vec{m}_A(\vec{r}_A)\big|_1 = \vec{m}_A^0(\vec{r}_A) \quad (19)$$

$$\nu_A(\vec{r}_A)\big|_1 = 0. \quad (20)$$

In subsequent iterations, an estimate for $\vec{L}_A(\vec{r}_A)$ is computed by

$$\vec{L}_A(\vec{r}_A) = \rho_A^{avg}(r_A)\vec{\Lambda}(\vec{r}) + \vec{m}_A^{avg}(r_A) \quad (21)$$

The magnitude $L_A(\vec{r}_A)$ was used to update the estimate for $m_A(\vec{r}_A)$ according to two cases. *Case 1:* If $L_A(\vec{r}_A) > \rho_A(r_A)$, then $m_A(\vec{r}_A) = \rho_A(\vec{r}_A)$ and $\nu_A(\vec{r}_A) = \left(L_A(\vec{r}_A) - \rho_A(\vec{r}_A)\right)/\rho_A^{avg}(\vec{r}_A)$. *Case 2:* If $L_A(\vec{r}_A) \leq \rho_A(r_A)$, then $\vec{m}_A(\vec{r}_A) = \vec{L}_A(\vec{r}_A)$ and $\nu_A(\vec{r}_A) = 0$. These two cases insure Eqs. (4) is satisfied for all iterations. The updated spin magnetization is given by

$$\vec{m}_A(\vec{r}_A) = m_A(\vec{r}_A)\hat{L}_A(\vec{r}_A). \quad (22)$$

During this loop the sum of valid grid points for each r_A is accumulated and stored, as well as the accumulated sum of $\vec{m}_A(\vec{r}_A)$ for each r_A value. Finally, the following sum is accumulated and stored:

$$\vec{\nu}(\vec{r}) = \sum_{k,B} \frac{\nu_B(\vec{r}_B)\hat{m}_B(\vec{r}_B)\rho_B^{avg}(r_B)}{\rho^{avg}(\vec{r})}. \quad (23)$$

The second loop runs over $\{A, r_A\}$. This loop computes and stores $\vec{m}_A^{avg}(r_A)$, $m_A^{avg}(r_A)$, and M_A from the sums accumulated in the first loop. The third loop runs over $\{A, \vec{r}_A\}$ like the first loop. This loop accumulates and stores

$$\vec{m}^{avg}(\vec{r}) = \sum_{k,A} \vec{m}_A^{avg}(r_A), \quad (24)$$

and uses it to subsequently compute

$$\vec{\Lambda}(\vec{r}) = \frac{\vec{m}(\vec{r}) - \vec{m}^{avg}(\vec{r})}{\rho^{avg}(\vec{r})} + \vec{\nu}(\vec{r}). \quad (25)$$

After the third loop, the program starts the next iteration by going back to the first loop. At least ten iterations were performed in all cases. Additional iterations were performed until all components in $\{\vec{M}_A\}$ changed by less than 5×10^{-5}.

We now show this iterator converges to H's global minimum. Upon convergence, summing Eq. (21) over $\{k_1, k_2, k_3, A\}$ and dividing by $\rho^{avg}(\vec{r})$ gives

$$\nu(\vec{r}) + \sum_{k,A} \frac{\vec{m}_A(\vec{r}_A)}{\rho^{avg}(\vec{r})} = \vec{\Lambda}(\vec{r}) + \frac{\vec{m}^{avg}(\vec{r})}{\rho^{avg}(\vec{r})} \ . \qquad (26)$$

Comparing Eqs. (25) and (26) shows that at convergence

$$\sum_{k,A} \vec{m}_A(\vec{r}_A) = \vec{m}(\vec{r}), \quad (27)$$

which proves constraint (5) is satisfied. Combining Eqs. (9) and (21) gives

$$\vec{\Lambda}_A(\vec{r}_A) = \vec{\Lambda}(\vec{r}), \qquad (28)$$

which is the required solution.

The above iterator minimizes overall memory requirements by only requiring functions of $\vec{r}_A$ to be stored for the current position, and this allows systems containing hundreds of atoms in the unit cell to be analyzed on a typical computer processor with a few gigabytes of memory. Since only complete functions of $\vec{r}$ and r_A need to be stored, the overall memory requirements scale linearly with the number of grid points (i.e. volume) in the unit cell. Furthermore, the use of a cutoff radius causes the overall computational time to scale linearly with the number of atoms in the unit cell. In summary, both the computational time and the memory requirements scale linearly with increasing system size, which makes the algorithm efficient for both small and large systems. For collinear magnetism, all $\vec{m}_A(\vec{r}_A)$ are parallel to a global spin quantization axis. In this case, vectors can be replaced with their scalar projection onto the global spin quantization axis; therefore, it is only necessary to compute one-third as many components as in the non-collinear case. For collinear magnetism, the program automatically avoids the computation and storage of all zero-valued spin components. Except for this simplification, all other details are the same for the collinear and non-collinear cases.

2. Grid for Computing Mean Absolute Error (MAE) of $\vec{B}^{spin}$

Computing $\vec{B}^{spin}(\vec{p})$ required integrating over $\{\vec{r}'\}$ inside the surface defined by 2.4× vdW radii, as shown in the following equation:

$$\vec{B}^{spin}(\vec{p}) = \frac{\mu_0}{4\pi}\left(\frac{g_e \mu_B}{2}\right)\oint\left(\frac{3(\vec{p}-\vec{r}')\left(\vec{m}(\vec{r}')\bullet(\vec{p}-\vec{r}')\right)}{|\vec{p}-\vec{r}'|^5} - \frac{\vec{m}(\vec{r}')}{|\vec{p}-\vec{r}'|^3}\right) d^3\vec{r}' \ . \quad (29)$$

To compute NACs and ASMs, electron and spin densities were output from GAUSSIAN or VASP on a grid of $N_1 \times N_2 \times N_3$ points defined by translation vectors $\vec{v}_1 / N_1$, $\vec{v}_2 / N_2$, and $\vec{v}_3 / N_3$. The subset of these grid points inside the surface defined by 2.4× vdW radii comprised the $\{\vec{r}'\}$ grid points used to compute the above integral.

The $\{\vec{p}\}$ grid points between surfaces defined by 3.0× and 4.0× vdW radii were chosen as following. First, a sphere whose radius was γ^{vdW} times an atom's vdW radius (R^{vdW}) was drawn such that the atom's nucleus coincided with the sphere's center. This process was repeated for each atom in the system. Next, 60 points forming a truncated icosahedron were placed on each of these spheres. Then, a point was discarded if a small zero tolerance (e.g., 0.01 bohr) plus its distance to an atom was less than or equal to γ^{vdW} times that atom's vdW radius for at least one atom in the system. This forced the set of valid grid points to lie on the surface defined by γ^{vdW} × vdW radii. This entire process was repeated using γ^{vdW} = 19/6, 21/6, and 23/6 to produce valid grid points residing on the surfaces defined by 19/6×, 21/6×, and 23/6× vdW radii. The finite element volume, $u(\vec{p})$, for each grid point was

$$u(\vec{p}) = \frac{4\pi R^2}{N_{pts}} \Delta R = \frac{4\pi\left(R^{vdW}\gamma^{vdW}\right)^2}{60}\left(\frac{R^{vdW}}{3}\right) \quad (30)$$

where $N_{pts} = 60$ is the number of points originally placed on each sphere (before discarding invalid points), $R = R^{vdW}\gamma^{vdW}$, and $\Delta R = R^{vdW}\Delta\gamma^{vdW} = \frac{R^{vdW}}{3}$. For computing $u(\vec{p})$, the γ^{vdW} and R^{vdW} values in Eq. (30) are the multiplier and vdW radius, respectively, that generated the truncated icosahedron on which $\vec{p}$ resides.

3. Sample Input Files for Coupled Cluster and SAC-CI Calculations

CCSD and SAC-CI calculations were performed in GAUSSIAN 09. For all CCSD calculations, all electrons were correlated (Gaussian keyword: Full). Calculations performed with guess = mix removed the molecular symmetry in the initial guess, and calculations performed without guess=mix preserved the molecular symmetry in the initial guess. For ozone SAC-CI calculations, all electrons except the 1s electrons were correlated. Example input files are given below:

Ozone cation CCSD calculation

```
%chk=ozone+1_CCSD.chk
%mem=8000MB
%nproc=4
# opt CCSD(full,SaveAmplitudes)/aug-cc-pVTZ geom=connectivity scf=(fermi,maxcycle=400)
# density=current guess=mix

Title Card Required

1 2
 O
 O            1          B1
 O            1          B2    2          A1

  B1         1.21000000
  B2         1.21000000
  A1       134.00000000

 1 2 1.0 3 1.0
 2
 3
```

Ozone preliminary SAC-CI calculation to determine the symmetries and relative energies of different singlet, triplet, and cation doublet states

```
%chk=ozone_defaultlevel.chk
%mem=8000MB
%nproc=4
# SAC-CI(Singlet=(NState=3,Density,SpinDensity), Triplet=(NState=3,Density,SpinDensity),
CationDoublet=(NState=3,Density,SpinDensity),MaxR2Op=200000)/aug-cc-pVTZ geom=connectivity

Title Card Required
```

```
0 1
 O
 O            1          B1
 O            1          B2    2          A1

  B1          1.23900000
  B2          1.23900000
  A1        117.75770000

 1 2 1.0 3 1.0
 2
 3
```

Ozone SAC-CI geometry optimization of singlet state

```
%chk=ozone_singlet.chk
%mem=8000MB
%nproc=4
# SAC-CI(SacOnly,TargetState=(SpinState=Singlet,Symmetry=1,Root=0))/aug-cc-pVTZ
# geom=connectivity opt density=current

Title Card Required

0 1
 O
 O            1          B1
 O            1          B2    2          A1

  B1          1.24000000
  B2          1.24000000
  A1        117.80000000

 1 2 1.0 3 1.0
 2
 3
```

Ozone SAC-CI geometry optimization of triplet state with A2 symmetry

```
%chk=triplet_a.chk
%mem=8000MB
%nproc=4
# SAC-CI(Triplet=(NState=(0,1,0,0)), TargetState=(SpinState=Triplet,Symmetry=2,Root=1))/aug-cc-
pVTZ geom=connectivity opt
# density=current

Title Card Required

0 1
 O
```

```
O          1          B1
O          1          B2    2          A1

 B1         1.32000000
 B2         1.32000000
 A1        97.50000000

1 2 1.0 3 1.0
2
3
```

---

4. Optimized Geometry, NACs, and ASMs for $Cu_3(BTC)_2$

computational details: DFT optimized geometry, PW91 functional, Gaussian smearing, smearing parameter = 0.05 eV, no Vosko-Wilk-Nusair interpolation

optimized lattice vectors (Å):
(-0.0001, 13.2548, 13.2547), (13.2548, -0.0001, 13.2547), (13.2548, 13.2548, -0.0001)

Atom	X_A	Y_A	Z_A	NAC		Atomic Spin Moments (ASM)				
				Bader	DDEC	Bader	χ_{spin}=1	χ_{spin}=3/14	χ_{spin}=1/2	LSF
C	7.863	15.092	18.636	1.545	0.675	0.000	0.000	0.000	0.000	0.000
C	7.863	18.636	15.092	1.545	0.675	0.000	0.000	0.000	0.000	0.000
C	11.407	18.636	18.636	1.535	0.679	0.000	0.000	0.000	0.000	0.000
C	9.668	16.831	18.545	-0.057	-0.006	-0.002	-0.001	-0.001	-0.001	-0.001
C	9.668	18.545	16.831	-0.057	-0.006	0.000	0.000	0.000	0.000	0.000
C	7.954	16.831	16.831	-0.066	-0.006	0.002	0.001	0.001	0.001	0.001
C	8.525	16.262	17.974	0.006	-0.135	0.000	0.000	0.000	0.000	0.000
C	10.237	17.974	17.974	0.068	-0.135	-0.001	-0.001	-0.001	-0.001	-0.003
C	8.525	17.974	16.262	0.007	-0.135	0.001	0.001	0.001	0.001	0.003
C	7.863	11.407	18.636	1.528	0.677	0.000	0.000	0.000	0.000	0.001
C	7.862	18.636	11.407	1.528	0.677	0.000	0.000	0.000	0.000	0.001
C	15.092	18.636	18.636	1.539	0.677	0.000	0.000	0.000	0.000	0.000
C	8.525	10.237	17.974	0.005	-0.134	-0.001	-0.001	-0.001	-0.001	-0.003
C	16.262	17.974	17.974	-0.033	-0.136	-0.001	-0.001	-0.001	-0.001	-0.003
C	8.525	17.974	10.237	0.005	-0.134	-0.001	-0.001	-0.001	-0.001	-0.003
C	9.668	9.668	18.545	-0.056	-0.008	-0.002	-0.001	-0.001	-0.001	-0.001
C	16.831	16.830	18.545	0.011	-0.004	-0.002	-0.001	-0.001	-0.001	-0.001
C	16.831	18.544	16.831	0.012	-0.004	0.000	0.000	0.000	0.000	0.000
C	9.668	18.545	9.668	-0.057	-0.008	-0.002	-0.001	-0.001	-0.001	-0.001
C	7.955	9.668	16.831	-0.016	-0.006	0.000	0.000	0.000	0.000	0.000
C	7.954	16.831	9.668	-0.018	-0.006	0.000	0.000	0.000	0.000	0.000
C	10.237	8.525	17.975	0.005	-0.134	0.000	0.000	0.000	0.000	0.000
C	17.974	16.261	17.974	-0.032	-0.136	0.000	0.000	0.000	0.000	0.000
C	8.525	8.525	16.262	-0.035	-0.135	0.001	0.001	0.001	0.001	0.003
C	17.974	17.974	16.262	-0.033	-0.136	0.001	0.001	0.001	0.001	0.003
C	8.525	16.261	8.524	-0.035	-0.135	0.001	0.001	0.001	0.001	0.003
C	10.237	17.974	8.525	0.005	-0.134	0.000	0.000	0.000	0.000	0.000
C	18.637	15.090	18.637	1.544	0.677	0.000	0.000	0.000	0.000	0.000
C	7.863	7.863	15.092	1.528	0.675	0.000	0.000	0.000	0.000	0.000
C	18.636	18.636	15.092	1.538	0.677	0.000	0.000	0.000	0.000	-0.001
C	7.862	15.090	7.861	1.531	0.675	0.000	0.000	0.000	0.000	0.000
C	11.407	7.863	18.636	1.528	0.677	0.000	0.000	0.000	0.000	0.000
C	11.407	18.636	7.863	1.528	0.677	0.000	0.000	0.000	0.000	0.000
C	9.668	7.954	16.831	-0.017	-0.006	0.002	0.001	0.001	0.001	0.001

C	9.668	16.831	7.954	-0.016	-0.006	0.002	0.001	0.001	0.001	0.001
C	18.545	16.830	16.831	0.012	-0.004	0.002	0.001	0.001	0.001	0.001
C	16.831	9.669	18.545	-0.056	-0.006	-0.002	-0.001	-0.001	-0.001	-0.001
C	16.831	18.545	9.668	-0.056	-0.006	-0.002	-0.001	-0.001	-0.001	-0.001
C	7.955	9.669	9.668	-0.008	-0.009	-0.002	-0.001	-0.001	-0.001	-0.001
C	18.638	11.409	18.638	1.537	0.678	0.000	0.000	0.000	0.000	0.001
C	7.863	7.863	11.407	1.549	0.675	0.000	0.000	0.000	0.000	0.001
C	18.636	18.636	11.407	1.535	0.679	0.000	0.000	0.000	0.000	0.001
C	7.862	11.409	7.862	1.550	0.676	0.000	0.000	0.000	0.000	0.000
C	15.092	7.863	18.636	1.547	0.675	0.000	0.000	0.000	0.000	0.000
C	15.092	18.636	7.863	1.545	0.675	0.000	0.000	0.000	0.000	0.000
C	16.262	8.525	17.974	0.006	-0.135	0.000	0.000	0.000	0.000	0.000
C	16.262	17.974	8.525	0.006	-0.135	0.000	0.000	0.000	0.000	0.000
C	17.975	10.238	17.974	0.030	-0.135	-0.001	-0.001	-0.001	-0.001	-0.003
C	8.525	8.526	10.237	-0.029	-0.132	-0.001	-0.001	-0.001	-0.001	-0.003
C	17.974	17.974	10.237	0.068	-0.135	-0.001	-0.001	-0.001	-0.001	-0.003
C	8.525	10.239	8.525	-0.021	-0.133	0.000	0.000	0.000	0.000	0.000
C	16.831	7.955	16.831	-0.065	-0.006	0.002	0.001	0.001	0.001	0.001
C	9.668	7.955	9.668	-0.002	-0.009	0.000	0.000	0.000	0.000	0.000
C	9.668	9.669	7.954	-0.007	-0.009	0.002	0.001	0.001	0.001	0.001
C	16.831	16.831	7.954	-0.066	-0.006	0.002	0.001	0.001	0.001	0.001
C	18.545	9.668	16.831	-0.019	-0.006	0.000	0.000	0.000	0.000	0.000
C	18.545	16.831	9.668	-0.057	-0.006	0.000	0.000	0.000	0.000	0.000
C	10.238	8.526	8.525	-0.029	-0.132	0.001	0.001	0.001	0.001	0.003
C	17.974	8.525	16.262	0.006	-0.135	0.001	0.001	0.001	0.001	0.003
C	17.974	16.262	8.525	0.007	-0.135	0.001	0.001	0.001	0.001	0.003
C	18.636	7.863	15.092	1.547	0.675	0.000	0.000	0.000	0.000	0.000
C	18.636	15.092	7.863	1.545	0.675	0.000	0.000	0.000	0.000	0.000
C	11.407	7.863	7.863	1.549	0.675	0.000	0.000	0.000	0.000	0.000
C	16.262	8.525	8.525	-0.034	-0.135	0.001	0.001	0.001	0.001	0.003
C	17.975	8.525	10.237	0.005	-0.134	-0.001	-0.001	-0.001	-0.001	-0.003
C	17.975	10.237	8.525	0.005	-0.134	0.000	0.000	0.000	0.000	0.000
C	16.831	7.954	9.668	-0.016	-0.006	0.000	0.000	0.000	0.000	0.000
C	16.831	9.668	7.954	-0.016	-0.006	0.002	0.001	0.001	0.001	0.001
C	18.545	9.668	9.668	-0.056	-0.008	-0.002	-0.001	-0.001	-0.001	-0.001
C	18.636	7.863	11.407	1.528	0.677	0.000	0.000	0.000	0.000	0.001
C	18.636	11.407	7.863	1.527	0.677	0.000	0.000	0.000	0.000	0.000
C	15.092	7.863	7.863	1.528	0.675	0.000	0.000	0.000	0.000	0.000
Cu	19.008	20.746	13.249	1.042	0.887	0.492	0.489	0.482	0.486	0.468
Cu	26.504	20.746	20.746	1.041	0.887	0.492	0.489	0.482	0.487	0.470
Cu	19.002	13.249	20.751	1.060	0.885	0.490	0.487	0.479	0.484	0.467
Cu	13.249	19.008	20.746	1.042	0.887	0.492	0.489	0.482	0.486	0.468
Cu	20.746	26.504	20.746	1.040	0.887	0.492	0.489	0.482	0.486	0.469
Cu	20.746	20.746	26.504	1.041	0.887	0.492	0.489	0.482	0.486	0.468
Cu	20.746	19.008	13.249	1.061	0.887	-0.492	-0.489	-0.482	-0.486	-0.468
Cu	26.504	19.007	19.007	1.043	0.886	-0.492	-0.489	-0.482	-0.487	-0.470
Cu	20.750	13.249	19.004	1.043	0.886	-0.490	-0.487	-0.479	-0.484	-0.467
Cu	13.250	20.746	19.008	1.061	0.887	-0.492	-0.489	-0.482	-0.486	-0.468
Cu	19.007	26.504	19.007	1.044	0.886	-0.492	-0.489	-0.482	-0.487	-0.469
Cu	19.007	19.007	26.504	1.043	0.886	-0.492	-0.489	-0.482	-0.486	-0.468
H	7.054	16.401	16.401	0.140	0.135	-0.001	-0.001	-0.002	-0.001	-0.003
H	10.098	16.401	19.445	0.140	0.136	0.001	0.001	0.002	0.001	0.002
H	10.098	19.445	16.401	0.140	0.136	0.000	0.000	0.000	0.000	0.000
H	7.054	10.099	16.401	0.170	0.135	0.000	0.000	0.000	0.000	0.000
H	7.054	16.401	10.099	0.170	0.135	0.000	0.000	0.000	0.000	0.000
H	10.099	10.099	19.445	0.151	0.136	0.001	0.001	0.002	0.001	0.002
H	16.401	16.401	19.445	0.144	0.135	0.001	0.001	0.002	0.001	0.002
H	16.401	19.445	16.401	0.145	0.135	0.000	0.000	0.000	0.000	0.000
H	10.098	19.445	10.098	0.152	0.136	0.001	0.001	0.002	0.001	0.002

H	19.446	16.401	16.400	0.143	0.135	-0.001	-0.001	-0.002	-0.001	-0.003
H	10.099	7.054	16.401	0.170	0.135	-0.001	-0.001	-0.002	-0.001	-0.002
H	10.099	16.401	7.054	0.170	0.135	-0.001	-0.001	-0.002	-0.001	-0.002
H	7.054	10.099	10.099	0.139	0.136	0.001	0.001	0.002	0.001	0.002
H	16.400	10.098	19.445	0.139	0.136	0.001	0.001	0.002	0.001	0.002
H	16.401	19.445	10.098	0.140	0.136	0.001	0.001	0.002	0.001	0.002
H	19.446	10.098	16.400	0.139	0.136	0.000	0.000	0.000	0.000	0.000
H	19.445	16.401	10.098	0.140	0.136	0.000	0.000	0.000	0.000	0.000
H	16.401	7.054	16.401	0.139	0.135	-0.001	-0.001	-0.002	-0.001	-0.002
H	10.099	7.055	10.099	0.140	0.136	0.000	0.000	0.000	0.000	0.000
H	10.099	10.099	7.054	0.139	0.136	-0.001	-0.001	-0.002	-0.001	-0.002
H	16.401	16.401	7.054	0.140	0.135	-0.001	-0.001	-0.002	-0.001	-0.002
H	19.445	10.099	10.098	0.152	0.136	0.001	0.001	0.002	0.001	0.003
H	16.401	7.054	10.099	0.170	0.135	0.000	0.000	0.000	0.000	0.000
H	16.401	10.099	7.054	0.170	0.135	-0.001	-0.001	-0.002	-0.001	-0.002
O	11.847	18.094	19.706	-1.087	-0.559	0.091	0.087	0.092	0.090	0.096
O	8.405	14.651	19.706	-1.087	-0.557	0.091	0.087	0.092	0.090	0.096
O	11.847	19.707	18.094	-1.087	-0.559	-0.091	-0.087	-0.093	-0.090	-0.097
O	8.405	19.706	14.651	-1.087	-0.557	0.091	0.087	0.092	0.090	0.097
O	6.793	14.652	18.093	-1.082	-0.556	-0.091	-0.087	-0.092	-0.090	-0.096
O	6.793	18.094	14.652	-1.082	-0.556	-0.091	-0.087	-0.092	-0.090	-0.096
O	8.405	11.847	19.706	-1.088	-0.558	0.091	0.087	0.092	0.090	0.096
O	14.652	18.093	19.706	-1.094	-0.557	0.091	0.087	0.092	0.090	0.096
O	14.652	19.706	18.094	-1.094	-0.557	-0.091	-0.087	-0.093	-0.090	-0.097
O	8.405	19.706	11.847	-1.087	-0.558	0.091	0.087	0.092	0.090	0.096
O	6.792	11.847	18.094	-1.088	-0.557	-0.091	-0.087	-0.093	-0.090	-0.097
O	6.792	18.093	11.847	-1.088	-0.557	-0.091	-0.087	-0.093	-0.090	-0.097
O	11.847	8.405	19.706	-1.088	-0.558	0.091	0.087	0.092	0.090	0.096
O	18.093	14.653	19.707	-1.094	-0.556	0.090	0.087	0.092	0.090	0.095
O	18.094	19.706	14.652	-1.094	-0.557	0.091	0.087	0.093	0.090	0.097
O	11.847	19.706	8.405	-1.088	-0.558	0.091	0.088	0.093	0.090	0.096
O	6.793	8.405	14.651	-1.088	-0.557	0.090	0.087	0.092	0.090	0.097
O	6.792	14.653	8.405	-1.089	-0.556	0.090	0.087	0.092	0.090	0.096
O	18.093	11.845	19.707	-1.089	-0.558	0.090	0.087	0.092	0.089	0.095
O	14.651	8.405	19.706	-1.087	-0.557	0.091	0.087	0.093	0.090	0.096
O	18.094	19.707	11.847	-1.087	-0.560	0.091	0.087	0.092	0.090	0.096
O	14.651	19.706	8.405	-1.087	-0.557	0.091	0.087	0.092	0.090	0.096
O	6.792	8.405	11.847	-1.090	-0.557	0.091	0.087	0.092	0.090	0.096
O	6.792	11.846	8.406	-1.091	-0.556	0.090	0.087	0.092	0.090	0.095
O	8.405	6.792	14.652	-1.088	-0.557	-0.090	-0.087	-0.092	-0.090	-0.096
O	8.405	14.653	6.791	-1.089	-0.555	-0.090	-0.087	-0.092	-0.089	-0.095
O	11.847	6.792	18.094	-1.088	-0.557	-0.091	-0.087	-0.092	-0.090	-0.096
O	11.847	18.094	6.792	-1.088	-0.557	-0.091	-0.088	-0.093	-0.090	-0.096
O	19.707	14.653	18.094	-1.096	-0.556	-0.090	-0.087	-0.092	-0.090	-0.095
O	19.706	18.094	14.652	-1.093	-0.557	-0.091	-0.087	-0.092	-0.090	-0.096
O	8.405	6.793	11.846	-1.089	-0.557	-0.091	-0.087	-0.093	-0.090	-0.097
O	8.405	11.846	6.792	-1.091	-0.556	-0.090	-0.087	-0.092	-0.090	-0.095
O	14.652	6.793	18.094	-1.082	-0.556	-0.091	-0.087	-0.092	-0.090	-0.096
O	14.652	18.094	6.793	-1.082	-0.556	-0.091	-0.087	-0.092	-0.090	-0.096
O	19.708	11.846	18.094	-1.088	-0.558	-0.090	-0.087	-0.092	-0.090	-0.096
O	19.706	18.094	11.847	-1.087	-0.560	-0.091	-0.087	-0.093	-0.090	-0.097
O	18.094	6.793	14.652	-1.082	-0.556	-0.091	-0.087	-0.092	-0.090	-0.096
O	18.094	14.652	6.792	-1.082	-0.556	-0.091	-0.087	-0.092	-0.090	-0.096
O	11.847	6.793	8.405	-1.089	-0.557	0.091	0.087	0.093	0.090	0.097
O	11.847	8.405	6.792	-1.090	-0.557	-0.091	-0.087	-0.092	-0.090	-0.096
O	19.706	8.405	14.651	-1.087	-0.557	0.091	0.087	0.093	0.090	0.097
O	19.706	14.651	8.405	-1.087	-0.557	0.091	0.087	0.093	0.090	0.097
O	18.094	6.792	11.847	-1.088	-0.557	-0.091	-0.087	-0.093	-0.090	-0.097
O	18.094	11.847	6.792	-1.088	-0.557	-0.091	-0.087	-0.092	-0.090	-0.096

O	14.652	6.793	8.405	-1.088	-0.557	0.090	0.087	0.092	0.090	0.097
O	14.652	8.405	6.793	-1.088	-0.556	-0.090	-0.087	-0.092	-0.090	-0.096
O	19.706	8.405	11.847	-1.088	-0.558	0.091	0.087	0.092	0.090	0.096
O	19.706	11.847	8.405	-1.088	-0.558	0.091	0.087	0.092	0.090	0.096

5. Optimized Geometries, NACs, and ASMs for Cu_2 Organometallic Complex

5.1 DFT Optimized Triple Geometry, NACs, and ASMs

Atom	X_A	Y_A	Z_A	net atomic charge (NAC)			
				MBS	Bader	DDEC	NPA
Cu	1.572	-0.007	-0.011	0.502	1.191	1.038	1.023
N	0.000	1.240	-0.193	-0.328	-0.545	-0.917	-0.671
Cu	-1.571	-0.008	-0.010	0.502	1.189	1.038	1.023
N	0.000	2.450	-0.520	0.153	-0.222	0.609	0.209
N	0.001	-2.464	0.500	0.153	-0.220	0.608	0.209
N	0.001	-1.254	0.175	-0.328	-0.534	-0.922	-0.670
N	-0.001	3.585	-0.815	-0.091	0.133	-0.275	-0.034
N	0.002	-3.599	0.793	-0.091	0.143	-0.275	-0.035
N	-2.953	1.456	-0.007	-0.263	-1.043	-0.449	-0.598
C	-2.931	2.431	0.952	0.014	0.265	0.128	0.071
C	-3.914	1.520	-0.971	0.026	0.301	0.152	0.095
C	-3.860	3.471	0.971	-0.103	-0.007	-0.241	-0.223
H	-2.153	2.362	1.705	0.147	0.094	0.120	0.226
C	-4.864	2.547	-1.009	-0.112	0.093	-0.255	-0.234
H	-3.918	0.732	-1.716	0.149	0.123	0.117	0.227
C	-4.867	3.565	-0.025	0.063	-0.063	0.170	0.061
H	-3.789	4.209	1.764	0.151	0.129	0.176	0.248
H	-5.595	2.543	-1.808	0.157	0.108	0.179	0.252
N	-2.951	-1.473	-0.020	-0.263	-1.034	-0.445	-0.598
C	-2.926	-2.443	-0.979	0.018	0.342	0.140	0.080
C	-3.918	-1.539	0.942	0.021	0.269	0.143	0.085
C	-3.856	-3.488	-1.008	-0.111	-0.027	-0.254	-0.232
H	-2.144	-2.373	-1.729	0.147	0.097	0.119	0.226
C	-4.864	-2.565	0.972	-0.103	-0.002	-0.245	-0.224
H	-3.924	-0.753	1.689	0.149	0.097	0.119	0.227
C	-4.864	-3.583	-0.018	0.063	0.030	0.171	0.061
H	-3.782	-4.221	-1.801	0.157	0.108	0.178	0.252
H	-5.599	-2.563	1.769	0.152	0.116	0.176	0.248
N	2.951	-1.473	-0.025	-0.263	-1.035	-0.446	-0.598
C	3.919	-1.542	0.937	0.021	0.269	0.144	0.085
C	2.926	-2.440	-0.986	0.018	0.298	0.141	0.080
C	4.864	-2.568	0.964	-0.103	0.015	-0.248	-0.224
H	3.925	-0.758	1.686	0.149	0.104	0.118	0.227
C	3.856	-3.486	-1.018	-0.111	-0.042	-0.253	-0.232
H	2.144	-2.369	-1.736	0.147	0.139	0.119	0.226
C	4.863	-3.584	-0.028	0.063	0.030	0.171	0.061
H	5.600	-2.569	1.761	0.152	0.116	0.177	0.248
H	3.781	-4.217	-1.813	0.157	0.109	0.178	0.252

N	2.953	1.456	-0.004	-0.263	-1.040	-0.448	-0.598
C	3.917	1.521	-0.965	0.026	0.301	0.151	0.095
C	2.929	2.430	0.955	0.014	0.255	0.126	0.071
C	4.867	2.549	-1.000	-0.112	-0.054	-0.253	-0.234
H	3.924	0.734	-1.711	0.149	0.128	0.118	0.227
C	3.857	3.471	0.979	-0.103	-0.004	-0.240	-0.223
H	2.147	2.361	1.705	0.147	0.096	0.120	0.226
C	4.867	3.566	-0.015	0.063	0.082	0.169	0.061
H	5.601	2.546	-1.796	0.157	0.110	0.178	0.252
H	3.783	4.208	1.771	0.151	0.125	0.175	0.248
C	-5.884	4.718	-0.008	0.063	0.054	0.287	-0.005
C	-5.911	-4.708	0.018	0.063	0.087	0.288	-0.005
C	5.883	4.719	0.007	0.063	0.056	0.286	-0.005
C	5.910	-4.710	0.005	0.063	0.083	0.285	-0.005
C	5.762	-5.490	1.348	-0.292	-0.150	-0.431	-0.638
H	6.513	-6.288	1.389	0.121	0.056	0.146	0.240
H	5.917	-4.846	2.222	0.097	0.078	0.122	0.216
H	4.771	-5.954	1.434	0.108	0.068	0.130	0.227
C	7.333	-4.077	-0.076	-0.292	-0.118	-0.430	-0.638
H	8.087	-4.873	-0.042	0.122	0.089	0.148	0.240
H	7.471	-3.521	-1.011	0.105	0.053	0.127	0.225
H	7.535	-3.398	0.762	0.096	0.029	0.120	0.215
C	5.740	-5.703	-1.170	-0.298	-0.108	-0.436	-0.659
H	4.766	-6.210	-1.145	0.100	0.044	0.125	0.222
H	5.860	-5.215	-2.146	0.100	0.025	0.124	0.222
H	6.509	-6.480	-1.100	0.122	0.064	0.147	0.244
C	6.668	4.674	1.354	-0.292	-0.087	-0.438	-0.638
H	7.386	5.501	1.385	0.121	0.073	0.147	0.240
H	6.007	4.778	2.224	0.096	0.006	0.122	0.215
H	7.228	3.736	1.459	0.105	0.053	0.129	0.225
C	5.111	6.071	-0.101	-0.292	-0.047	-0.431	-0.637
H	5.827	6.900	-0.073	0.121	0.052	0.146	0.239
H	4.552	6.138	-1.042	0.108	0.055	0.131	0.227
H	4.407	6.214	0.728	0.096	0.004	0.121	0.215
C	6.895	4.631	-1.162	-0.298	-0.106	-0.436	-0.659
H	7.492	3.710	-1.124	0.099	0.041	0.123	0.221
H	6.402	4.692	-2.141	0.101	0.034	0.125	0.223
H	7.594	5.472	-1.099	0.122	0.079	0.148	0.245
C	-5.742	-5.705	-1.154	-0.298	-0.115	-0.435	-0.659
H	-4.768	-6.212	-1.129	0.100	0.046	0.124	0.222
H	-6.512	-6.480	-1.082	0.122	0.063	0.147	0.244
H	-5.862	-5.219	-2.131	0.100	0.035	0.123	0.222
C	-5.763	-5.486	1.363	-0.292	-0.147	-0.434	-0.638
H	-5.918	-4.840	2.235	0.097	0.070	0.121	0.216
H	-6.514	-6.283	1.406	0.121	0.056	0.146	0.240
H	-4.773	-5.949	1.450	0.108	0.068	0.131	0.227
C	-7.334	-4.075	-0.063	-0.292	-0.075	-0.431	-0.638
H	-7.535	-3.394	0.772	0.096	0.049	0.120	0.215
H	-7.472	-3.521	-1.000	0.105	0.020	0.127	0.225

H	-8.088	-4.870	-0.028	0.121	0.059	0.147	0.240
C	-6.672	4.673	1.338	-0.292	-0.101	-0.436	-0.638
H	-7.391	5.500	1.365	0.121	0.070	0.147	0.240
H	-7.232	3.736	1.442	0.105	0.055	0.128	0.225
H	-6.014	4.779	2.209	0.096	0.021	0.120	0.215
C	-6.892	4.628	-1.179	-0.298	-0.092	-0.436	-0.659
H	-6.397	4.689	-2.157	0.101	0.027	0.125	0.223
H	-7.489	3.707	-1.142	0.099	0.040	0.123	0.221
H	-7.592	5.469	-1.119	0.122	0.081	0.147	0.245
C	-5.112	6.069	-0.114	-0.292	-0.042	-0.430	-0.637
H	-4.410	6.214	0.716	0.096	0.018	0.121	0.215
H	-4.550	6.136	-1.054	0.108	0.043	0.130	0.227
H	-5.827	6.899	-0.089	0.121	0.047	0.147	0.239

Atom	X_A	Y_A	Z_A	ASM						
				MBS	NPA	Bader	$\chi_{spin}=1$	$\chi_{spin}=3/14$	$\chi_{spin}=1/2$	LSF
Cu	1.572	-0.007	-0.011	0.613	0.530	0.591	0.592	0.580	0.587	0.562
N	0.000	1.240	-0.193	0.107	0.142	0.105	0.105	0.115	0.110	0.130
Cu	-1.571	-0.008	-0.010	0.613	0.530	0.591	0.592	0.580	0.587	0.562
N	0.000	2.450	-0.520	-0.039	-0.038	-0.021	-0.012	-0.031	-0.022	-0.045
N	0.001	-2.464	0.500	-0.039	-0.038	-0.021	-0.012	-0.031	-0.022	-0.045
N	0.001	-1.254	0.175	0.106	0.141	0.105	0.105	0.115	0.110	0.130
N	-0.001	3.585	-0.815	0.129	0.128	0.120	0.113	0.126	0.120	0.134
N	0.002	-3.599	0.793	0.129	0.128	0.120	0.113	0.126	0.120	0.134
N	-2.953	1.456	-0.007	0.096	0.118	0.095	0.089	0.100	0.095	0.116
C	-2.931	2.431	0.952	-0.007	-0.007	-0.002	0.002	-0.004	-0.001	-0.012
C	-3.914	1.520	-0.971	-0.008	-0.007	-0.004	0.000	-0.006	-0.003	-0.017
C	-3.860	3.471	0.971	0.007	0.007	0.006	0.005	0.007	0.006	0.013
H	-2.153	2.362	1.705	0.003	0.002	0.002	0.001	0.002	0.002	0.004
C	-4.864	2.547	-1.009	0.007	0.007	0.006	0.005	0.007	0.006	0.013
H	-3.918	0.732	-1.716	0.003	0.002	0.002	0.001	0.002	0.002	0.004
C	-4.867	3.565	-0.025	-0.006	-0.006	-0.005	-0.004	-0.006	-0.005	-0.011
H	-3.789	4.209	1.764	0.001	0.001	0.001	0.001	0.001	0.001	0.000
H	-5.595	2.543	-1.808	0.001	0.001	0.001	0.001	0.001	0.001	0.000
N	-2.951	-1.473	-0.020	0.096	0.118	0.095	0.089	0.100	0.094	0.116
C	-2.926	-2.443	-0.979	-0.008	-0.007	-0.003	0.001	-0.004	-0.001	-0.013
C	-3.918	-1.539	0.942	-0.008	-0.007	-0.003	0.000	-0.006	-0.002	-0.016
C	-3.856	-3.488	-1.008	0.007	0.007	0.006	0.005	0.007	0.006	0.013
H	-2.144	-2.373	-1.729	0.003	0.003	0.002	0.001	0.002	0.002	0.004
C	-4.864	-2.565	0.972	0.007	0.007	0.006	0.005	0.007	0.006	0.013
H	-3.924	-0.753	1.689	0.003	0.002	0.002	0.001	0.002	0.002	0.004
C	-4.864	-3.583	-0.018	-0.006	-0.006	-0.005	-0.004	-0.006	-0.005	-0.011
H	-3.782	-4.221	-1.801	0.001	0.001	0.001	0.001	0.001	0.001	0.000
H	-5.599	-2.563	1.769	0.001	0.001	0.001	0.001	0.001	0.001	0.000
N	2.951	-1.473	-0.025	0.096	0.118	0.095	0.089	0.100	0.094	0.116
C	3.919	-1.542	0.937	-0.008	-0.007	-0.003	0.000	-0.006	-0.002	-0.016
C	2.926	-2.440	-0.986	-0.008	-0.007	-0.003	0.001	-0.004	-0.001	-0.013
C	4.864	-2.568	0.964	0.007	0.007	0.006	0.005	0.007	0.006	0.013
H	3.925	-0.758	1.686	0.003	0.002	0.002	0.001	0.002	0.002	0.004

C	3.856	-3.486	-1.018	0.007	0.007	0.006	0.005	0.007	0.006	0.013
H	2.144	-2.369	-1.736	0.003	0.003	0.002	0.001	0.002	0.002	0.004
C	4.863	-3.584	-0.028	-0.006	-0.006	-0.005	-0.004	-0.006	-0.005	-0.011
H	5.600	-2.569	1.761	0.001	0.001	0.001	0.001	0.001	0.001	0.000
H	3.781	-4.217	-1.813	0.001	0.001	0.001	0.001	0.001	0.001	0.000
N	2.953	1.456	-0.004	0.096	0.118	0.095	0.089	0.100	0.094	0.116
C	3.917	1.521	-0.965	-0.008	-0.007	-0.004	0.000	-0.006	-0.003	-0.017
C	2.929	2.430	0.955	-0.007	-0.007	-0.002	0.002	-0.004	-0.001	-0.012
C	4.867	2.549	-1.000	0.007	0.007	0.006	0.005	0.007	0.006	0.013
H	3.924	0.734	-1.711	0.003	0.002	0.002	0.001	0.002	0.002	0.004
C	3.857	3.471	0.979	0.007	0.007	0.006	0.005	0.007	0.006	0.013
H	2.147	2.361	1.705	0.003	0.002	0.002	0.001	0.002	0.002	0.004
C	4.867	3.566	-0.015	-0.006	-0.006	-0.005	-0.004	-0.006	-0.005	-0.011
H	5.601	2.546	-1.796	0.001	0.001	0.001	0.001	0.001	0.001	0.000
H	3.783	4.208	1.771	0.001	0.001	0.001	0.001	0.001	0.001	0.000
C	-5.884	4.718	-0.008	0.001	0.000	0.000	0.000	0.001	0.000	0.002
C	-5.911	-4.708	0.018	0.001	0.001	0.000	0.000	0.001	0.000	0.002
C	5.883	4.719	0.007	0.001	0.000	0.000	0.000	0.001	0.000	0.002
C	5.910	-4.710	0.005	0.001	0.001	0.000	0.000	0.001	0.000	0.002
C	5.762	-5.490	1.348	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
H	6.513	-6.288	1.389	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	5.917	-4.846	2.222	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	4.771	-5.954	1.434	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	7.333	-4.077	-0.076	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
H	8.087	-4.873	-0.042	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	7.471	-3.521	-1.011	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	7.535	-3.398	0.762	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	5.740	-5.703	-1.170	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	4.766	-6.210	-1.145	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	5.860	-5.215	-2.146	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	6.509	-6.480	-1.100	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	6.668	4.674	1.354	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
H	7.386	5.501	1.385	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	6.007	4.778	2.224	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	7.228	3.736	1.459	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	5.111	6.071	-0.101	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
H	5.827	6.900	-0.073	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	4.552	6.138	-1.042	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	4.407	6.214	0.728	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	6.895	4.631	-1.162	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	7.492	3.710	-1.124	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	6.402	4.692	-2.141	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	7.594	5.472	-1.099	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	-5.742	-5.705	-1.154	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-4.768	-6.212	-1.129	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-6.512	-6.480	-1.082	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-5.862	-5.219	-2.131	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	-5.763	-5.486	1.363	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
H	-5.918	-4.840	2.235	0.000	0.000	0.000	0.000	0.000	0.000	0.000

H	-6.514	-6.283	1.406	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-4.773	-5.949	1.450	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	-7.334	-4.075	-0.063	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
H	-7.535	-3.394	0.772	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-7.472	-3.521	-1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-8.088	-4.870	-0.028	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	-6.672	4.673	1.338	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
H	-7.391	5.500	1.365	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-7.232	3.736	1.442	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-6.014	4.779	2.209	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	-6.892	4.628	-1.179	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-6.397	4.689	-2.157	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-7.489	3.707	-1.142	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-7.592	5.469	-1.119	0.000	0.000	0.000	0.000	0.000	0.000	0.000
C	-5.112	6.069	-0.114	0.000	0.000	0.000	0.000	0.000	0.000	-0.001
H	-4.410	6.214	0.716	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-4.550	6.136	-1.054	0.000	0.000	0.000	0.000	0.000	0.000	0.000
H	-5.827	6.899	-0.089	0.000	0.000	0.000	0.000	0.000	0.000	0.000

5.2 DFT Optimized Singlet Geometry

computational details: Calculation performed when symmetry was removed in the initial guess (using guess=mix) converged to a symmetric state, and this indicates the singlet state is closed shell. For a closed shell singlet, the ASMs are zero for all atoms. The singlet state was 0.78 eV higher in energy than the triplet state.

Atom	X_A	Y_A	Z_A
H	-2.181	2.308	1.800
H	-3.942	0.904	-1.722
H	-3.822	4.142	1.982
H	-5.631	2.707	-1.688
H	-2.184	-2.326	-1.841
H	-3.946	-0.894	1.669
H	-3.831	-4.158	-2.014
H	-5.637	-2.692	1.644
H	3.819	0.792	-1.846
H	2.249	2.402	1.678
H	5.536	2.558	-1.980
H	3.931	4.213	1.691
H	3.770	-0.789	1.879
H	2.303	-2.405	-1.686
H	5.492	-2.549	2.060
H	3.991	-4.207	-1.653
H	6.580	6.240	-1.615
H	5.917	4.819	-2.432
H	4.830	5.953	-1.599
H	8.165	4.776	-0.245
H	7.547	3.437	0.740
H	7.544	3.320	-1.035

H	4.920	6.193	0.982
H	6.029	5.170	1.936
H	6.666	6.423	0.870
H	7.585	-5.405	-1.034
H	6.246	-4.709	-1.956
H	7.381	-3.644	-1.096
H	5.973	-6.869	0.295
H	4.615	-6.158	1.187
H	4.590	-6.211	-0.590
H	7.468	-3.648	1.498
H	6.343	-4.677	2.426
H	7.625	-5.405	1.457
H	-4.821	-6.185	-1.436
H	-6.566	-6.446	-1.414
H	-5.903	-5.138	-2.395
H	-5.990	-4.973	1.984
H	-6.596	-6.367	1.080
H	-4.851	-6.056	1.154
H	-7.581	-3.440	0.577
H	-7.505	-3.487	-1.199
H	-8.141	-4.873	-0.294
H	-7.430	5.443	1.675
H	-7.270	3.677	1.629
H	-6.052	4.667	2.466
H	-6.437	4.870	-1.896
H	-7.524	3.819	-0.948
H	-7.635	5.575	-0.808
H	-4.455	6.208	1.073
H	-4.597	6.250	-0.699
H	-5.876	6.941	0.317
C	-2.960	2.425	1.052
C	-3.940	1.640	-0.925
C	-3.892	3.459	1.142
C	-4.896	2.663	-0.893
C	-4.901	3.614	0.155
C	-2.963	-2.435	-1.092
C	-3.946	-1.637	0.878
C	-3.899	-3.471	-1.179
C	-4.900	-2.655	0.849
C	-4.907	-3.616	-0.196
C	3.869	1.566	-1.088
C	2.993	2.465	0.889
C	4.839	2.568	-1.149
C	3.948	3.488	0.886
C	4.910	3.573	-0.149
C	3.843	-1.563	1.122
C	3.026	-2.466	-0.878
C	4.819	-2.562	1.212
C	3.984	-3.481	-0.847

C	4.921	-3.562	0.215
C	-5.923	4.759	0.250
C	-5.963	-4.733	-0.224
C	5.971	-4.686	0.248
C	5.983	4.672	-0.217
C	5.810	5.463	-1.550
C	7.392	4.001	-0.189
C	5.882	5.664	0.967
C	6.843	-4.599	-1.042
C	5.233	-6.060	0.286
C	6.898	-4.586	1.483
C	-5.792	-5.672	-1.442
C	-5.836	-5.578	1.082
C	-7.380	-4.084	-0.287
C	-6.711	4.621	1.590
C	-6.932	4.743	-0.924
C	-5.157	6.118	0.235
N	-0.018	-1.213	0.167
N	-0.019	-2.438	0.505
N	-0.018	2.429	-0.553
N	-0.018	1.206	-0.208
N	-0.020	-3.568	0.809
N	-0.018	3.557	-0.863
N	-2.977	1.516	0.030
N	-2.979	-1.521	-0.080
N	2.947	1.509	-0.081
N	2.951	-1.508	0.094
Cu	1.616	-0.002	-0.009
Cu	-1.655	-0.004	-0.025

6. Optimized Geometry and NACs for Fe_3Si solid

computational details: experimental geometry**,** PBE functional, Methfessel-Paxton smearing of order 1, smearing parameter = 0.05 eV, no Vosko-Wilk-Nusair interpolation

experimental lattice vectors (Å):
(0.0000, 2.8350, 2.8350), (2.8350, 0.0000, 2.8350), (2.8350, 2.8350, 0.0000)

Atom	X_A	Y_A	Z_A	NAC	
				Bader	DDEC
Fe	2.835	2.835	2.835	0.298	0.384
Fe	1.418	1.418	1.418	-0.152	-0.347
Fe	4.253	4.253	4.253	-0.150	-0.348
Si	0.000	0.000	0.000	0.005	0.311

7. Optimized Geometry and NACs for $[Cr(CN)_6]^{3-}$

Atom	X_A	Y_A	Z_A	MBS ASM	net atomic charge (NAC)			
					MBS	Bader	DDEC	NPA
Cr	0.000	0.000	0.000	0.017	-11.966	1.454	0.284	-0.779
C	0.000	0.000	2.136	0.694	-2.454	0.618	0.098	0.253
C	0.000	2.136	0.000	0.199	-1.958	0.618	0.097	0.253
C	-2.136	0.000	0.000	0.694	-2.454	0.618	0.097	0.253
C	0.000	0.000	-2.136	0.694	-2.454	0.618	0.098	0.253
C	0.000	-2.136	0.000	0.199	-1.958	0.618	0.097	0.253
C	2.136	0.000	0.000	0.694	-2.454	0.618	0.097	0.253
N	3.304	0.000	0.000	-0.036	4.120	-1.360	-0.643	-0.623
N	0.000	0.000	3.304	-0.036	4.120	-1.360	-0.645	-0.623
N	0.000	3.304	0.000	-0.025	4.109	-1.360	-0.645	-0.623
N	0.000	0.000	-3.304	-0.036	4.120	-1.360	-0.645	-0.623
N	-3.304	0.000	0.000	-0.036	4.120	-1.360	-0.643	-0.623
N	0.000	-3.304	0.000	-0.025	4.109	-1.360	-0.645	-0.623

8. Optimized Geometries and Sample Input Files for Magnetite

8.1 $U_{eff} = 0$

computational details: DFT optimized geometry, PBE functional, Gaussian smearing, smearing parameter = 0.05 eV, no Vosko-Wilk-Nusair interpolation

optimized lattice vectors (Å) :
(-0.0038, 4.1517, 4.1517), (4.1517, -0.0038, 4.1517), (4.1517, 4.1517, -0.0038)

Atom	X_A	Y_A	Z_A
O	2.113	2.113	2.113
O	2.110	4.113	4.113
O	4.113	2.110	4.113
O	4.113	4.113	2.110
O	6.186	6.186	6.186
O	6.190	4.186	4.186
O	4.186	6.190	4.186
O	4.186	4.186	6.190
Fe	7.263	7.263	7.263
Fe	1.037	1.037	1.037
Fe	4.150	4.150	4.150
Fe	4.148	6.226	6.226
Fe	2.074	4.152	2.074
Fe	2.074	2.074	4.152

Example INCAR for electron density generation with previously optimized geometry

```
SYSTEM = periodic system

#### SCF Routine
ENCUT = 400.00 eV
PREC = Accurate
LREAL = .FALSE.
NELMIN = 5; # minimum number of SCF cycles
NSW=0
NGX =  56
NGY =  56
NGZ =  56

ALGO = Fast; # uses Davidson initially then switches to DIIS

LWAVE = .FALSE.
LCHARG = .TRUE.
ISPIN = 2
MAGMOM =  0 0 0 0 0 0 0 0 -3.33 -3.33 3.33 3.33 3.33 3.33
ISYM = 0
LORBIT=10

### Parameters related to fractional occupations of the orbitals
ISMEAR = 0; # Gaussian smearing
SIGMA = 0.05; # in eV for smearing width

### Selection of GGA exchange-correlation functional
GGA = PE;

LAECHG = .TRUE.
NUPDOWN = 8
```

8.2 U_{eff} = 3.2 eV

computational details: DFT+U optimized geometry, PBE functional, Methfessel-Paxton smearing of order 1, smearing parameter = 0.02 eV, no Vosko-Wilk-Nusair interpolation.

optimized lattice vectors (Å) :
(0.0000, 4.2175, 4.2175), (4.2175, 0.0000, 4.2175), (4.2175, 4.2175, 0.0000)

Atom	X_A	Y_A	Z_A
O	2.160	2.182	2.094
O	2.102	4.151	4.138
O	4.226	2.176	4.138
O	4.166	4.146	2.091
O	6.275	6.253	6.341
O	6.333	4.284	4.297
O	4.209	6.259	4.297
O	4.269	4.289	6.344

Fe	7.380	7.380	7.418
Fe	1.055	1.055	1.017
Fe	4.218	4.218	4.218
Fe	4.218	2.109	2.109
Fe	6.326	4.218	6.326
Fe	2.109	2.109	4.218

Example INCAR for electron density generation with previously optimized geometry
(Note: only the difference U_{eff} = U-J effects the calculation result.)

```
SYSTEM = periodic system

#### SCF Routine
ENCUT = 400.00 eV
PREC = Accurate
LREAL = .FALSE.
NELMIN = 5; # minimum number of SCF cycles
NSW=0
ALGO = Fast; # uses Davidson initially then switches to DIIS

LWAVE = F
LCHARG = .TRUE.
ISPIN = 2
MAGMOM =  0 0 0 0 0 0 0 0 -3.33 -3.33 3.33 3.33 3.33 3.33
LDAU = .TRUE.
LDAUU = 0.0 4.0
LDAUJ = 0.0 0.8
ISYM = 0
LORBIT = 10

### Parameters related to fractional occupations of the orbitals
ISMEAR = 1; #
SIGMA = 0.02; # in eV for smearing width

### Selection of GGA exchange-correlation functional
GGA = PE;

LAECHG = .TRUE.
```

8.3 HSE06 range-separated hybrid functional

computational details: HSE06 optimized geometry, Methfessel-Paxton smearing of order 1, smearing parameter = 0.02 eV, no Vosko-Wilk-Nusair interpolation

optimized lattice vectors (Å) :
(0.0158, 4.1469, 4.1751), (4.1682, 0.0043, 4.1868), (4.1841, 4.1745, -0.0117)

Atom	X_A	Y_A	Z_A
O	2.094	2.094	2.145
O	2.120	4.124	4.067
O	4.155	2.115	4.072

O	4.176	4.162	2.137
O	6.274	6.232	6.205
O	6.248	4.202	4.283
O	4.213	6.211	4.278
O	4.192	4.164	6.213
Fe	7.327	7.283	7.324
Fe	1.041	1.042	1.026
Fe	4.184	4.163	4.175
Fe	4.192	6.236	6.262
Fe	2.100	4.161	2.082
Fe	6.276	6.250	4.169

Example INCAR for geometry optimization

```
SYSTEM = periodic system

#### SCF Routine
ENCUT = 400.00 eV
PREC = Accurate
PRECFOCK = Normal
LREAL = .FALSE.
NELMIN = 10; # minimum number of SCF cycles
NELMDL = -9
NELM = 400
NSW=200
ISIF=3
IBRION=1
NFREE=3
EDIFFG=-0.03
ALGO = All;
TIME = 0.4

LWAVE = .TRUE.
LCHARG = .TRUE.
LAECHG = .TRUE.

LHFCALC = .TRUE.
HFSCREEN = 0.2
MAGMOM =  0 0 0 0 0 0 0 0 -3.33 -3.33 3.33 3.33 3.33 3.33

ISPIN = 2
ISYM = 0
LORBIT = 10

### Parameters related to fractional occupations of the orbitals
ISMEAR = 1; #
SIGMA = 0.02; # in eV for smearing width

### Selection of GGA exchange-correlation functional
GGA = PE;
```

Example INCAR for electron density generation with previously optimized geometry

```
SYSTEM = periodic system

#### SCF Routine
ENCUT = 400.00 eV
PREC = Accurate
PRECFOCK = Normal
LREAL = .FALSE.
NELMIN = 10; # minimum number of SCF cycles
NELMDL = -9
NELM = 400
NSW=0
ISIF=3
IBRION=1
NFREE=3
EDIFFG=-0.03
ALGO = All;
TIME = 0.4

LWAVE = .TRUE.
LCHARG = .TRUE.
LAECHG = .TRUE.

LHFCALC = .TRUE.
HFSCREEN = 0.2
MAGMOM =  0 0 0 0 0 0 0 0 -3.33 -3.33 3.33 3.33 3.33 3.33

ISPIN = 2
ISYM = 0
LORBIT = 10

### Parameters related to fractional occupations of the orbitals
ISMEAR = 1; #
SIGMA = 0.02; # in eV for smearing width

### Selection of GGA exchange-correlation functional
GGA = PE;
NBANDS=60
```

9. Optimized Geometry, NACs, ASMs, Spin-Orbit Coupling Energies, Canted ASMs, and Sample Input Files for Ferrous Cube Complex

9.1 Sample input files

Example INCAR for geometry optimization calculation

```
SYSTEM = periodic system

#### SCF Routine
ISYM = 0 # symmetry turned off
ENCUT = 400.00 eV
```

```
PREC = Accurate # select the accurate grid spacine
ALGO = Fast; # uses Davidson initially then switches to DIIS
LREAL = .FALSE.
NELMIN = 10; # minimum number of SCF cycles
NELMDL = -5
NELM = 200 # maximum number of SCF cycles per ionic step

### geometry optimization parameters
NSW=200 # maximum number of ionic steps
ISIF = 1
EDIFFG= -0.03
IBRION=2

### print out the charge densities and Lorbit populations
LMAXMIX = 4
LWAVE = T
LCHARG = T
LAECHG = .TRUE.
LORBIT = 10

### smearing method
ISMEAR = 1; # Methfessel-Paxton of order 1
SIGMA = 0.05; # in eV for smearing width

### Selection of GGA exchange-correlation functional
GGA = 91;
VOSKOWN=1

### perform a non-collinear calculation
ISPIN = 2
LNONCOLLINEAR= .TRUE.
GGA_COMPAT = .FALSE.

### the initial guess for the magnetic moments
MAGMOM = 120*0.0 0.456 1.648 1.077 -1.454 1.390 -0.221 1.390 -1.451 0.228 -0.517 -1.655 -1.034 272*0.0

### manually specify the mixing parameters
IMIX=4
AMIX = 0.40
BMIX = 1.0
AMIX_MAG = 0.40
BMIX_MAG = 1.0
AMIN = 0.10
WC = 100.0
INIMIX = 1
MIXPRE = 1

### parameters for parallelization
LPLANE = T
NPAR = 4
```

Example INCAR for relaxing magnetization at fixed geometry

```
SYSTEM = periodic system

#### SCF Routine
ISTART = 2 # restart the calculation from the saved WAVECAR and CHGCAR
ICHARG = 1 # read initial charge from CHGCAR file
ISYM = 0 # symmetry turned off
ENCUT = 400.00 eV
PREC = Accurate # select the accurate grid spacine
ALGO = Fast; # uses Davidson initially then switches to DIIS
LREAL = .FALSE.
NELMIN = 200; # minimum number of SCF cycles, set large to relax magnetization
NELMDL = -9
NELM = 800 # maximum number of SCF cycles per ionic step

### geometry optimization parameters
NSW=10 # number of ionic steps
ISIF = 1
EDIFFG= -0.03
IBRION= -1 # the ions are not moved but outer loops are performed

### print out the charge densities and Lorbit populations
LMAXMIX = 4
LWAVE = T
LCHARG = T
LAECHG = .TRUE.
LORBIT = 10

### smearing method
ISMEAR = 1; # Methfessel-Paxton of order 1
SIGMA = 0.05; # in eV for smearing width

### Selection of GGA exchange-correlation functional
GGA = 91;
VOSKOWN=1

### perform a non-collinear calculation
LNONCOLLINEAR= .TRUE.
GGA_COMPAT = .FALSE.

### manually specify the mixing parameters
IMIX=4
AMIX = 0.40
BMIX = 1.0
AMIX_MAG = 0.40
BMIX_MAG = 1.0
AMIN = 0.10
WC = 100.0
```

```
INIMIX = 1
MIXPRE = 1

### parameters for parallelization
LPLANE = T
NPAR = 4

### Specify NBANDS to insure the WAVECAR is properly read
### Use the value of NBANDS from the OUTCAR of the run that generated the WAVECAR being used.
### This insures the correct number of bands is used to read the WAVECAR  to form the initial guess.
NBANDS = 452
```

Example INCAR for computing the spin-orbit coupling energy with a chosen SAXIS value

```
SYSTEM = periodic system

#### SCF Routine
ISTART = 2 # restart the calculation from the saved WAVECAR and CHGCAR
ICHARG = 11  # read initial charge from CHGCAR file and keep it constant during the entire calculation
ISYM = 0 # symmetry turned off
ENCUT = 400.00 eV
PREC = Accurate # select the accurate grid spacine
ALGO = Fast; # uses Davidson initially then switches to DIIS
LREAL = .FALSE.
NELMIN = 5; # minimum number of SCF cycles, set small since charges kept constant
NELMDL = -4
NELM = 20 # maximum number of SCF cycles per ionic step, no need for large value

### geometry optimization parameters
NSW=0 # no ionic updates

### charge density and wavefunction printing options
LMAXMIX = 4
LWAVE = .FALSE. # optional to print WAVECAR
LCHARG = .FALSE.# no need to print this since it's kept constant throughout calculation
LORBIT = 10 # optional to print these

### smearing method
ISMEAR = 1; # Methfessel-Paxton of order 1
SIGMA = 0.05; # in eV for smearing width

### Selection of GGA exchange-correlation functional
GGA = 91;
VOSKOWN=1

### perform a non-collinear calculation with spin-orbit coupling turned on
ISPIN = 2
LNONCOLLINEAR= .TRUE.
GGA_COMPAT = .FALSE.
```

```
LSORBIT = .TRUE.

### choose the SAXIS value
SAXIS =  0.523  -0.126  0.843

### manually specify the mixing parameters
IMIX=4
AMIX = 0.40
BMIX = 1.0
AMIX_MAG = 0.40
BMIX_MAG = 1.0
AMIN = 0.10
WC = 100.0
INIMIX = 1
MIXPRE = 1

### parameters for parallelization
LPLANE = T

### Specify NBANDS to insure the WAVECAR is properly read
### Use the value of NBANDS from the OUTCAR of the run that generated the WAVECAR being used.
### This insures the correct number of bands is used to read the WAVECAR  to form the initial guess.
NBANDS = 452
```

9.2 Spin orbit coupling energies

computational details: SAXIS is a unit vector VASP uses to denote a global rotation of $\{\vec{m}(\vec{r})\}$. For a collinear calculation, SAXIS sets the direction of $\hat{h}_{global}$. For a non-collinear calculation, SAXIS is an auxiliary quantity that has no special meaning other than to globally rotate $\{\vec{m}(\vec{r})\}$. The spin orbit coupling energies are listed below for 60 different SAXIS values. The global minimum is assigned a relative energy of 0.0 meV. Using $\vec{\varsigma}$ to denote SAXIS, the ASMs rotate in space with constant magnitude as described below.[1] First, the rotation angles φ and θ are defined by

$$\varphi = a\tan\left(\varsigma_y/\varsigma_x\right) = a\tan 2\left(\varsigma_y,\varsigma_x\right) \qquad (31)$$

$$\theta = a\tan\left(\sqrt{\varsigma_x^{\,2}+\varsigma_y^{\,2}}\,/\varsigma_z\right) = a\tan 2\left(\sqrt{\varsigma_x^{\,2}+\varsigma_y^{\,2}},\varsigma_z\right). \qquad (32)$$

These angles determine the transformed spin magnetization components:

$$m_x = \cos(\varphi)\cos(\theta)m_x^{axis} - \sin(\varphi)m_y^{axis} + \cos(\varphi)\sin(\theta)m_z^{axis} \qquad (33)$$

$$m_y = \sin(\varphi)\cos(\theta)m_x^{axis} + \cos(\varphi)m_y^{axis} + \sin(\varphi)\sin(\theta)m_z^{axis} \qquad (34)$$

$$m_z = -\sin(\theta)m_x^{axis} + \cos(\theta)m_z^{axis}. \qquad (35)$$

In Eqs. (33), (34), and (35), $\vec{m}^{axis}$ are the spin magnetization components measured with respect to SAXIS, which includes the MAGMOM line in the INCAR, the total and local magnetizations in the OUTCAR and PROCAR, the spinor-like orbitals in the WAVECAR, and the magnetization density in the CHGCAR file. Since the four charge density components (measured with respect to SAXIS) are kept constant for all the spin-orbit coupling calculations, $\vec{m}^{axis}$ is the same for all 60 SAXIS values. The

[1] Kresse, G.; Marsman, M.; Furthmüller, J. *VASP the Guide*, Universitat Wien, 2011.

specific $\vec{m}^{axis}$ values for each atom equal the ASMs listed in section 9.3. For each SAXIS value, the spin magnetization $\vec{m}$ with respect to the xyz-coordinate sytem can be computed using Eqs. (33), (34), and (35) to give the relative orientation of the ASMs with respect to the molecular structure.

SAXIS			relative energy (meV)
x-component	y-component	z-component	
-0.7813	-0.6250	0.0000	3.78
0.6826	-0.6250	0.0000	1.52
1.3749	0.5742	0.0000	2.27
0.6429	1.8420	0.0000	2.89
-0.7417	1.8419	0.0000	2.10
-1.4736	0.5741	0.0000	3.76
-1.2336	-1.7314	-0.8451	3.70
-0.0493	-2.4151	-1.3675	2.87
1.1350	-1.7313	-0.8452	2.02
2.2552	-1.5786	-1.6447	2.44
2.5592	0.7356	-0.8453	2.78
1.3748	2.7869	-0.8453	2.32
0.6824	3.6807	-1.6447	1.19
-0.7815	3.6806	-1.6446	0.46
-1.4737	2.7868	-0.8452	1.16
-2.6581	2.1030	-1.3675	1.73
-2.6580	0.7355	-0.8451	3.33
-3.0859	-0.3110	-1.6445	3.87
-2.3539	-1.5788	-1.6445	4.15
-0.0494	-2.9092	-2.6610	3.13
-1.2337	-2.7479	-3.5061	3.62
-2.3539	-2.1011	-3.0120	4.06
-3.0860	-1.1562	-3.8572	4.00
-3.5383	-0.0499	-3.0120	3.47
-3.5384	1.2437	-3.5061	2.38
-3.0860	2.3500	-2.6610	1.27
-2.3541	3.2950	-3.5062	0.36
-1.2339	3.9418	-3.0122	0.00
2.5591	2.1032	-1.3676	2.92
1.1347	2.9253	-5.6733	2.62
2.2550	2.7727	-4.8739	3.03
2.9869	1.5050	-4.8739	3.66
2.5590	0.4585	-5.6733	3.31
1.3747	0.6199	-6.5184	2.94
-0.7816	1.8190	-6.5184	2.34
-1.2340	2.9253	-5.6732	1.29
-0.0496	3.6091	-5.1509	1.17
-0.0496	4.1032	-3.8574	0.48
1.1348	3.9418	-3.0122	1.21
2.2550	3.2951	-3.5063	2.39
3.4393	1.2438	-3.5064	3.62
3.4394	-0.0497	-3.0123	3.47
2.9870	-1.1561	-3.8574	3.21

2.5591	-0.9091	-5.1509	2.84
1.3748	-1.5928	-5.6732	1.95
0.6428	-0.6479	-6.5184	0.94
-0.7419	-0.6480	-6.5183	2.88
-1.4739	0.6198	-6.5183	3.74
-2.3542	2.7726	-4.8737	1.07
-3.0861	1.5048	-4.8737	2.34
-2.6582	0.4584	-5.6731	3.53
-2.6581	-0.9092	-5.1507	3.98
-1.4738	-1.5929	-5.6731	3.49
-0.7814	-2.4867	-4.8737	3.18
0.6825	-2.4867	-4.8737	2.56
1.1349	-2.7478	-3.5063	2.85
2.2551	-2.1010	-3.0122	2.86
2.9870	2.3502	-2.6612	3.08
2.9871	-0.3108	-1.6447	2.86
0.6823	1.8190	-6.5184	3.47

9.3 DFT Optimized Geometry, NACs, and ASMs

The molecule was placed in the center of a supercell with lattice vectors in Å: (19.0000, 0.0000, 0.0000), (0.0000, 19.0000, 0.0000), (0.0000, 0.0000, 19.0000). The ASMs below used the default value SAXIS = (0+, 0, 1).

Atom	X_A	Y_A	Z_A	NAC	
				Bader	DDEC
C	13.813	13.499	5.941	0.546	0.360
C	14.822	14.393	6.357	0.017	-0.282
C	15.188	15.486	5.583	-0.088	-0.038
C	14.551	15.733	4.356	-0.055	-0.184
C	13.554	14.874	3.929	-0.133	-0.080
C	13.155	13.748	4.691	0.068	-0.139
C	12.087	12.931	4.201	0.444	0.066
C	10.432	11.187	4.262	0.277	-0.002
C	10.460	9.750	4.753	0.459	0.094
C	11.158	10.972	12.328	0.559	0.362
C	10.292	11.485	13.316	-0.036	-0.280
C	10.512	11.250	14.667	-0.063	-0.039
C	11.617	10.488	15.084	-0.036	-0.183
C	12.484	9.982	14.133	-0.084	-0.088
C	12.292	10.201	12.747	0.017	-0.127
C	13.218	9.619	11.825	0.408	0.052
C	14.097	8.985	9.675	0.209	-0.007
C	14.159	9.675	8.322	0.384	0.094
C	12.909	6.224	6.003	0.600	0.369
C	13.713	5.823	4.915	-0.051	-0.287
C	14.321	4.575	4.883	-0.126	-0.036
C	14.149	3.675	5.947	-0.035	-0.181
C	13.367	4.047	7.026	-0.038	-0.085

C	12.733	5.312	7.094	-0.028	-0.139
C	11.979	5.639	8.265	0.478	0.063
C	10.729	7.045	9.768	0.194	0.001
C	9.653	8.099	9.560	0.384	0.090
C	6.535	9.895	6.934	0.582	0.366
C	5.547	8.917	6.699	-0.013	-0.285
C	4.271	9.262	6.274	-0.060	-0.035
C	3.934	10.608	6.058	-0.099	-0.185
C	4.891	11.585	6.270	-0.120	-0.086
C	6.202	11.271	6.705	-0.003	-0.138
C	7.145	12.335	6.870	0.477	0.061
C	9.283	13.342	7.334	0.254	-0.002
C	10.323	13.074	8.408	0.443	0.090
C	14.172	9.710	3.884	0.341	0.014
C	14.416	12.951	10.141	0.302	0.026
C	7.400	11.841	10.500	0.402	0.016
C	8.559	6.134	6.492	0.340	0.016
Fe	12.272	11.077	6.354	1.266	0.691
Fe	11.925	10.726	9.542	1.272	0.692
Fe	11.176	8.177	7.260	1.268	0.698
Fe	9.159	10.619	7.914	1.264	0.687
H	15.318	14.197	7.308	0.057	0.123
H	15.975	16.153	5.933	0.076	0.093
H	14.835	16.593	3.749	0.066	0.111
H	13.040	15.060	2.983	0.042	0.093
H	11.612	13.235	3.259	0.070	0.064
H	10.416	11.247	3.162	0.002	0.063
H	9.530	11.692	4.645	0.052	0.068
H	9.477	9.268	4.655	0.059	0.063
H	11.191	9.152	4.183	0.027	0.046
H	9.441	12.083	12.988	0.069	0.125
H	9.824	11.662	15.406	0.069	0.093
H	11.789	10.297	16.143	0.060	0.109
H	13.343	9.384	14.444	0.034	0.094
H	14.031	9.014	12.245	0.075	0.067
H	13.718	7.957	9.552	0.095	0.068
H	15.089	8.932	10.153	0.054	0.064
H	14.779	10.585	8.374	0.069	0.045
H	14.582	9.020	7.547	0.077	0.067
H	13.839	6.524	4.089	0.084	0.124
H	14.934	4.295	4.027	0.056	0.093
H	14.625	2.695	5.926	0.057	0.110
H	13.234	3.360	7.864	0.054	0.095
H	11.944	4.889	9.065	0.067	0.065
H	11.500	7.433	10.454	0.071	0.065
H	10.319	6.119	10.203	0.077	0.064
H	8.746	7.655	9.117	0.057	0.047
H	9.367	8.579	10.507	0.092	0.066
H	5.810	7.873	6.878	0.052	0.126

H	3.529	8.481	6.110	0.046	0.094
H	2.934	10.881	5.724	0.070	0.114
H	4.646	12.636	6.096	0.107	0.095
H	6.815	13.347	6.605	0.073	0.066
H	8.727	14.275	7.520	0.032	0.062
H	9.781	13.430	6.354	0.068	0.068
H	11.199	13.729	8.294	0.074	0.066
H	9.904	13.237	9.415	0.018	0.048
H	14.598	10.710	3.742	0.069	0.080
H	14.949	8.959	3.665	0.042	0.046
H	13.340	9.580	3.171	0.068	0.038
H	14.548	12.193	10.926	0.075	0.057
H	15.316	12.959	9.505	0.076	0.042
H	14.312	13.937	10.620	0.056	0.052
H	7.175	11.746	11.575	0.042	0.045
H	7.694	12.884	10.287	0.005	0.036
H	6.492	11.611	9.929	0.068	0.080
H	8.238	5.921	7.527	0.058	0.037
H	7.693	6.015	5.820	0.030	0.047
H	9.328	5.406	6.208	0.083	0.079
H	13.275	8.735	5.394	0.639	0.335
H	13.452	12.661	8.397	0.677	0.329
H	9.276	11.117	10.572	0.685	0.331
H	8.488	8.128	6.716	0.667	0.334
N	11.622	11.862	4.814	-1.109	-0.302
N	13.146	9.741	10.514	-1.086	-0.291
N	11.352	6.782	8.457	-1.115	-0.302
N	8.379	12.178	7.303	-1.114	-0.299
O	13.508	12.462	6.732	-1.110	-0.484
O	10.847	9.798	6.133	-1.045	-0.470
O	10.881	11.222	11.042	-1.105	-0.486
O	12.810	10.030	7.980	-1.051	-0.480
O	12.352	7.441	5.973	-1.107	-0.492
O	10.199	9.076	8.660	-1.042	-0.466
O	7.741	9.498	7.359	-1.109	-0.486
O	10.715	11.701	8.265	-1.048	-0.463
O	13.738	9.611	5.241	-1.149	-0.467
O	13.244	12.650	9.379	-1.177	-0.468
O	8.409	10.909	10.109	-1.195	-0.468
O	9.126	7.439	6.363	-1.170	-0.470

DDEC χ_{spin} = 1/2 ASMs

Atom	X_A	Y_A	Z_A	ASM magnitude	ASM vector		
					x-component	y-component	z-component
C	13.813	13.499	5.941	0.031	0.005	0.030	-0.008
C	14.822	14.393	6.357	0.013	-0.002	-0.012	0.003
C	15.188	15.486	5.583	0.038	0.006	0.036	-0.010
C	14.551	15.733	4.356	0.016	-0.003	-0.016	0.004

C	13.554	14.874	3.929	0.029	0.005	0.028	-0.008
C	13.155	13.748	4.691	0.010	-0.002	-0.010	0.003
C	12.087	12.931	4.201	0.104	0.017	0.099	-0.028
C	10.432	11.187	4.262	0.004	0.000	0.004	0.000
C	10.460	9.750	4.753	0.003	-0.001	0.003	0.000
C	11.158	10.972	12.328	0.031	0.022	-0.015	-0.017
C	10.292	11.485	13.316	0.013	-0.009	0.006	0.007
C	10.512	11.250	14.667	0.038	0.027	-0.018	-0.020
C	11.617	10.488	15.084	0.016	-0.011	0.008	0.009
C	12.484	9.982	14.133	0.029	0.021	-0.014	-0.016
C	12.292	10.201	12.747	0.010	-0.007	0.005	0.005
C	13.218	9.619	11.825	0.106	0.074	-0.050	-0.056
C	14.097	8.985	9.675	0.004	0.003	-0.001	-0.002
C	14.159	9.675	8.322	0.002	0.002	0.001	-0.002
C	12.909	6.224	6.003	0.031	-0.021	0.014	0.017
C	13.713	5.823	4.915	0.013	0.009	-0.006	-0.007
C	14.321	4.575	4.883	0.038	-0.026	0.017	0.021
C	14.149	3.675	5.947	0.016	0.011	-0.008	-0.009
C	13.367	4.047	7.026	0.029	-0.020	0.013	0.016
C	12.733	5.312	7.094	0.010	0.007	-0.005	-0.006
C	11.979	5.639	8.265	0.103	-0.071	0.048	0.058
C	10.729	7.045	9.768	0.004	-0.003	0.001	0.003
C	9.653	8.099	9.560	0.003	-0.002	0.000	0.002
C	6.535	9.895	6.934	0.031	-0.004	-0.029	0.008
C	5.547	8.917	6.699	0.013	0.002	0.012	-0.004
C	4.271	9.262	6.274	0.037	-0.005	-0.036	0.010
C	3.934	10.608	6.058	0.017	0.002	0.016	-0.004
C	4.891	11.585	6.270	0.029	-0.004	-0.027	0.008
C	6.202	11.271	6.705	0.010	0.001	0.010	-0.003
C	7.145	12.335	6.870	0.102	-0.013	-0.098	0.028
C	9.283	13.342	7.334	0.004	0.000	-0.004	0.000
C	10.323	13.074	8.408	0.003	0.001	-0.003	0.000
C	14.172	9.710	3.884	0.003	0.000	-0.002	0.001
C	14.416	12.951	10.141	0.003	-0.002	0.001	0.002
C	7.400	11.841	10.500	0.002	0.000	0.002	-0.001
C	8.559	6.134	6.492	0.003	0.002	-0.001	-0.001
Fe	12.272	11.077	6.354	2.058	-0.332	-1.957	0.544
Fe	11.925	10.726	9.542	2.062	-1.444	0.976	1.101
Fe	11.176	8.177	7.260	2.060	1.416	-0.942	-1.163
Fe	9.159	10.619	7.914	2.058	0.252	1.965	-0.559
H	15.318	14.197	7.308	0.000	0.000	0.000	0.000
H	15.975	16.153	5.933	0.001	0.000	0.001	0.000
H	14.835	16.593	3.749	0.001	0.000	-0.001	0.000
H	13.040	15.060	2.983	0.000	0.000	0.000	0.000
H	11.612	13.235	3.259	0.007	0.001	0.007	-0.002
H	10.416	11.247	3.162	0.002	0.000	0.002	0.000
H	9.530	11.692	4.645	0.001	0.000	0.001	0.000
H	9.477	9.268	4.655	0.001	0.000	0.001	0.000
H	11.191	9.152	4.183	0.001	0.000	0.000	0.000

H	9.441	12.083	12.988	0.000	0.000	0.000	0.000
H	9.824	11.662	15.406	0.001	0.001	-0.001	-0.001
H	11.789	10.297	16.143	0.001	0.000	0.000	0.000
H	13.343	9.384	14.444	0.000	0.000	0.000	0.000
H	14.031	9.014	12.245	0.007	0.005	-0.003	-0.004
H	13.718	7.957	9.552	0.000	0.000	0.000	0.000
H	15.089	8.932	10.153	0.002	0.001	-0.001	-0.001
H	14.779	10.585	8.374	0.001	0.000	0.001	0.000
H	14.582	9.020	7.547	0.001	0.001	-0.001	-0.001
H	13.839	6.524	4.089	0.000	0.000	0.000	0.000
H	14.934	4.295	4.027	0.001	-0.001	0.001	0.001
H	14.625	2.695	5.926	0.001	0.000	0.000	0.000
H	13.234	3.360	7.864	0.000	0.000	0.000	0.000
H	11.944	4.889	9.065	0.007	-0.005	0.003	0.004
H	11.500	7.433	10.454	0.000	0.000	0.000	0.000
H	10.319	6.119	10.203	0.002	-0.001	0.001	0.001
H	8.746	7.655	9.117	0.000	0.000	0.000	0.000
H	9.367	8.579	10.507	0.001	-0.001	0.001	0.001
H	5.810	7.873	6.878	0.000	0.000	0.000	0.000
H	3.529	8.481	6.110	0.001	0.000	-0.001	0.000
H	2.934	10.881	5.724	0.001	0.000	0.001	0.000
H	4.646	12.636	6.096	0.000	0.000	0.000	0.000
H	6.815	13.347	6.605	0.007	-0.001	-0.006	0.002
H	8.727	14.275	7.520	0.002	0.000	-0.002	0.000
H	9.781	13.430	6.354	0.000	0.000	0.000	0.000
H	11.199	13.729	8.294	0.001	0.000	-0.001	0.001
H	9.904	13.237	9.415	0.000	0.000	0.000	0.000
H	14.598	10.710	3.742	0.000	0.000	0.000	0.000
H	14.949	8.959	3.665	0.003	0.000	-0.003	0.001
H	13.340	9.580	3.171	0.000	0.000	0.000	0.000
H	14.548	12.193	10.926	0.001	-0.001	0.000	0.000
H	15.316	12.959	9.505	0.001	0.000	0.000	0.000
H	14.312	13.937	10.620	0.002	-0.001	0.001	0.001
H	7.175	11.746	11.575	0.003	0.000	0.003	-0.001
H	7.694	12.884	10.287	0.000	0.000	0.000	0.000
H	6.492	11.611	9.929	0.000	0.000	0.000	0.000
H	8.238	5.921	7.527	0.000	0.000	0.000	0.000
H	7.693	6.015	5.820	0.003	0.002	-0.001	-0.002
H	9.328	5.406	6.208	0.000	0.000	0.000	0.000
H	13.275	8.735	5.394	0.001	-0.001	0.000	0.001
H	13.452	12.661	8.397	0.001	0.000	0.001	0.000
H	9.276	11.117	10.572	0.001	0.001	0.000	-0.001
H	8.488	8.128	6.716	0.001	0.000	-0.001	0.000
N	11.622	11.862	4.814	0.034	0.005	0.032	-0.009
N	13.146	9.741	10.514	0.034	0.024	-0.016	-0.018
N	11.352	6.782	8.457	0.034	-0.023	0.015	0.019
N	8.379	12.178	7.303	0.034	-0.004	-0.032	0.009
O	13.508	12.462	6.732	0.026	-0.004	-0.025	0.006
O	10.847	9.798	6.133	0.016	-0.001	0.016	-0.002

O	10.881	11.222	11.042	0.025	-0.018	0.011	0.013
O	12.810	10.030	7.980	0.015	0.011	-0.004	-0.010
O	12.352	7.441	5.973	0.026	0.018	-0.011	-0.015
O	10.199	9.076	8.660	0.018	-0.013	0.007	0.010
O	7.741	9.498	7.359	0.026	0.003	0.025	-0.007
O	10.715	11.701	8.265	0.019	-0.001	-0.018	0.003
O	13.738	9.611	5.241	0.052	-0.009	-0.049	0.014
O	13.244	12.650	9.379	0.052	-0.036	0.025	0.028
O	8.409	10.909	10.109	0.054	0.007	0.051	-0.015
O	9.126	7.439	6.363	0.051	0.035	-0.024	-0.029
total spin moment of molecule							
				0.135	-0.102	0.044	-0.076

DDEC χ_{spin} = 3/14 ASMs

Atom	X_A	Y_A	Z_A	ASM magnitude	ASM vector		
					x-component	y-component	z-component
C	13.813	13.499	5.941	0.037	0.006	0.035	-0.010
C	14.822	14.393	6.357	0.019	-0.003	-0.018	0.005
C	15.188	15.486	5.583	0.046	0.007	0.044	-0.012
C	14.551	15.733	4.356	0.023	-0.004	-0.022	0.006
C	13.554	14.874	3.929	0.035	0.006	0.033	-0.009
C	13.155	13.748	4.691	0.019	-0.003	-0.018	0.005
C	12.087	12.931	4.201	0.118	0.020	0.112	-0.032
C	10.432	11.187	4.262	0.002	-0.001	0.002	0.000
C	10.460	9.750	4.753	0.002	0.000	0.002	0.000
C	11.158	10.972	12.328	0.037	0.026	-0.018	-0.020
C	10.292	11.485	13.316	0.019	-0.013	0.009	0.010
C	10.512	11.250	14.667	0.046	0.032	-0.022	-0.025
C	11.617	10.488	15.084	0.023	-0.016	0.011	0.012
C	12.484	9.982	14.133	0.035	0.024	-0.016	-0.019
C	12.292	10.201	12.747	0.019	-0.014	0.009	0.010
C	13.218	9.619	11.825	0.120	0.084	-0.057	-0.064
C	14.097	8.985	9.675	0.001	0.001	0.000	-0.001
C	14.159	9.675	8.322	0.002	0.001	0.000	-0.001
C	12.909	6.224	6.003	0.037	-0.025	0.017	0.021
C	13.713	5.823	4.915	0.019	0.013	-0.009	-0.011
C	14.321	4.575	4.883	0.046	-0.031	0.021	0.026
C	14.149	3.675	5.947	0.023	0.016	-0.010	-0.013
C	13.367	4.047	7.026	0.034	-0.023	0.016	0.019
C	12.733	5.312	7.094	0.019	0.013	-0.009	-0.011
C	11.979	5.639	8.265	0.117	-0.080	0.054	0.066
C	10.729	7.045	9.768	0.001	-0.001	-0.001	0.001
C	9.653	8.099	9.560	0.002	-0.002	0.000	0.001
C	6.535	9.895	6.934	0.036	-0.005	-0.035	0.010
C	5.547	8.917	6.699	0.019	0.002	0.018	-0.005
C	4.271	9.262	6.274	0.045	-0.006	-0.043	0.012
C	3.934	10.608	6.058	0.023	0.003	0.022	-0.006
C	4.891	11.585	6.270	0.034	-0.004	-0.033	0.009

C	6.202	11.271	6.705	0.019	0.002	0.018	-0.005
C	7.145	12.335	6.870	0.116	-0.015	-0.111	0.032
C	9.283	13.342	7.334	0.002	0.001	-0.001	0.000
C	10.323	13.074	8.408	0.003	0.000	-0.003	0.000
C	14.172	9.710	3.884	0.000	0.000	0.000	0.000
C	14.416	12.951	10.141	0.001	-0.001	0.000	0.000
C	7.400	11.841	10.500	0.000	0.000	0.000	0.000
C	8.559	6.134	6.492	0.000	0.000	0.000	0.000
Fe	12.272	11.077	6.354	2.099	-0.339	-1.995	0.555
Fe	11.925	10.726	9.542	2.103	-1.473	0.996	1.122
Fe	11.176	8.177	7.260	2.103	1.445	-0.963	-1.186
Fe	9.159	10.619	7.914	2.100	0.258	2.004	-0.571
H	15.318	14.197	7.308	0.000	0.000	0.000	0.000
H	15.975	16.153	5.933	0.000	0.000	0.000	0.000
H	14.835	16.593	3.749	0.000	0.000	0.000	0.000
H	13.040	15.060	2.983	0.002	0.000	-0.002	0.000
H	11.612	13.235	3.259	0.004	0.001	0.004	-0.001
H	10.416	11.247	3.162	0.002	0.000	0.002	0.000
H	9.530	11.692	4.645	0.001	0.000	0.001	0.000
H	9.477	9.268	4.655	0.001	0.000	0.001	0.000
H	11.191	9.152	4.183	0.001	-0.001	-0.001	0.001
H	9.441	12.083	12.988	0.000	0.000	0.000	0.000
H	9.824	11.662	15.406	0.000	0.000	0.000	0.000
H	11.789	10.297	16.143	0.000	0.000	0.000	0.000
H	13.343	9.384	14.444	0.002	-0.001	0.001	0.001
H	14.031	9.014	12.245	0.004	0.003	-0.002	-0.002
H	13.718	7.957	9.552	0.001	0.000	0.000	0.000
H	15.089	8.932	10.153	0.002	0.001	-0.001	-0.001
H	14.779	10.585	8.374	0.001	-0.001	0.001	0.000
H	14.582	9.020	7.547	0.001	0.001	0.000	-0.001
H	13.839	6.524	4.089	0.000	0.000	0.000	0.000
H	14.934	4.295	4.027	0.000	0.000	0.000	0.000
H	14.625	2.695	5.926	0.000	0.000	0.000	0.000
H	13.234	3.360	7.864	0.002	0.001	-0.001	-0.001
H	11.944	4.889	9.065	0.004	-0.003	0.002	0.002
H	11.500	7.433	10.454	0.000	0.000	0.000	0.000
H	10.319	6.119	10.203	0.002	-0.001	0.001	0.001
H	8.746	7.655	9.117	0.001	0.000	-0.001	0.000
H	9.367	8.579	10.507	0.001	-0.001	0.001	0.001
H	5.810	7.873	6.878	0.000	0.000	0.000	0.000
H	3.529	8.481	6.110	0.000	0.000	0.000	0.000
H	2.934	10.881	5.724	0.000	0.000	0.000	0.000
H	4.646	12.636	6.096	0.002	0.000	0.002	0.000
H	6.815	13.347	6.605	0.004	-0.001	-0.004	0.001
H	8.727	14.275	7.520	0.002	0.000	-0.002	0.000
H	9.781	13.430	6.354	0.001	0.000	0.000	0.000
H	11.199	13.729	8.294	0.001	0.000	-0.001	0.000
H	9.904	13.237	9.415	0.001	0.000	0.001	-0.001
H	14.598	10.710	3.742	0.000	0.000	0.000	0.000

H	14.949	8.959	3.665	0.004	-0.001	-0.004	0.001
H	13.340	9.580	3.171	0.000	0.000	0.000	0.000
H	14.548	12.193	10.926	0.001	-0.001	0.000	0.000
H	15.316	12.959	9.505	0.001	-0.001	0.000	0.000
H	14.312	13.937	10.620	0.002	-0.001	0.001	0.001
H	7.175	11.746	11.575	0.004	0.000	0.004	-0.001
H	7.694	12.884	10.287	0.000	0.000	0.000	0.000
H	6.492	11.611	9.929	0.000	0.000	0.000	0.000
H	8.238	5.921	7.527	0.000	0.000	0.000	0.000
H	7.693	6.015	5.820	0.004	0.002	-0.002	-0.002
H	9.328	5.406	6.208	0.000	0.000	0.000	0.000
H	13.275	8.735	5.394	0.002	-0.001	0.001	0.001
H	13.452	12.661	8.397	0.002	0.000	0.002	0.000
H	9.276	11.117	10.572	0.002	0.001	-0.001	-0.001
H	8.488	8.128	6.716	0.002	0.000	-0.001	0.001
N	11.622	11.862	4.814	0.044	0.007	0.042	-0.012
N	13.146	9.741	10.514	0.044	0.031	-0.021	-0.023
N	11.352	6.782	8.457	0.044	-0.030	0.020	0.025
N	8.379	12.178	7.303	0.044	-0.006	-0.042	0.012
O	13.508	12.462	6.732	0.020	-0.003	-0.020	0.005
O	10.847	9.798	6.133	0.032	-0.006	0.032	-0.001
O	10.881	11.222	11.042	0.020	-0.014	0.009	0.011
O	12.810	10.030	7.980	0.028	0.021	-0.002	-0.019
O	12.352	7.441	5.973	0.020	0.014	-0.009	-0.012
O	10.199	9.076	8.660	0.030	-0.023	0.004	0.019
O	7.741	9.498	7.359	0.021	0.002	0.020	-0.005
O	10.715	11.701	8.265	0.034	0.003	-0.034	0.001
O	13.738	9.611	5.241	0.053	-0.009	-0.050	0.014
O	13.244	12.650	9.379	0.054	-0.038	0.026	0.029
O	8.409	10.909	10.109	0.055	0.007	0.052	-0.015
O	9.126	7.439	6.363	0.053	0.036	-0.025	-0.030
total spin moment of molecule							
				0.135	-0.102	0.044	-0.076

DDEC χ_{spin} = 1 ASMs

Atom	X_A	Y_A	Z_A	ASM magnitude	ASM vector		
					x-component	y-component	z-component
C	13.813	13.499	5.941	0.025	0.004	0.024	-0.007
C	14.822	14.393	6.357	0.009	-0.001	-0.008	0.002
C	15.188	15.486	5.583	0.032	0.005	0.030	-0.008
C	14.551	15.733	4.356	0.011	-0.002	-0.011	0.003
C	13.554	14.874	3.929	0.026	0.004	0.024	-0.007
C	13.155	13.748	4.691	0.004	-0.001	-0.003	0.001
C	12.087	12.931	4.201	0.090	0.015	0.085	-0.024
C	10.432	11.187	4.262	0.005	0.000	0.005	-0.001
C	10.460	9.750	4.753	0.002	0.000	0.002	0.000
C	11.158	10.972	12.328	0.026	0.018	-0.012	-0.014
C	10.292	11.485	13.316	0.009	-0.006	0.004	0.005

C	10.512	11.250	14.667	0.032	0.023	-0.015	-0.017
C	11.617	10.488	15.084	0.011	-0.008	0.005	0.006
C	12.484	9.982	14.133	0.026	0.018	-0.012	-0.014
C	12.292	10.201	12.747	0.004	-0.003	0.002	0.002
C	13.218	9.619	11.825	0.091	0.064	-0.044	-0.049
C	14.097	8.985	9.675	0.004	0.003	-0.001	-0.003
C	14.159	9.675	8.322	0.002	0.001	0.000	-0.001
C	12.909	6.224	6.003	0.025	-0.017	0.012	0.014
C	13.713	5.823	4.915	0.009	0.006	-0.004	-0.005
C	14.321	4.575	4.883	0.032	-0.022	0.015	0.018
C	14.149	3.675	5.947	0.011	0.008	-0.005	-0.007
C	13.367	4.047	7.026	0.025	-0.017	0.012	0.014
C	12.733	5.312	7.094	0.004	0.003	-0.002	-0.002
C	11.979	5.639	8.265	0.089	-0.061	0.041	0.050
C	10.729	7.045	9.768	0.004	-0.003	0.001	0.003
C	9.653	8.099	9.560	0.002	-0.001	0.000	0.001
C	6.535	9.895	6.934	0.025	-0.003	-0.024	0.007
C	5.547	8.917	6.699	0.009	0.001	0.008	-0.002
C	4.271	9.262	6.274	0.031	-0.004	-0.030	0.009
C	3.934	10.608	6.058	0.012	0.001	0.011	-0.003
C	4.891	11.585	6.270	0.025	-0.003	-0.024	0.007
C	6.202	11.271	6.705	0.004	0.000	0.004	-0.001
C	7.145	12.335	6.870	0.089	-0.011	-0.084	0.024
C	9.283	13.342	7.334	0.005	0.000	-0.005	0.001
C	10.323	13.074	8.408	0.002	0.000	-0.002	0.000
C	14.172	9.710	3.884	0.004	-0.001	-0.004	0.001
C	14.416	12.951	10.141	0.005	-0.003	0.002	0.002
C	7.400	11.841	10.500	0.004	0.001	0.004	-0.001
C	8.559	6.134	6.492	0.004	0.003	-0.002	-0.002
Fe	12.272	11.077	6.354	2.013	-0.325	-1.914	0.532
Fe	11.925	10.726	9.542	2.017	-1.413	0.954	1.077
Fe	11.176	8.177	7.260	2.014	1.385	-0.921	-1.137
Fe	9.159	10.619	7.914	2.012	0.246	1.921	-0.546
H	15.318	14.197	7.308	0.000	0.000	0.000	0.000
H	15.975	16.153	5.933	0.002	0.000	0.002	-0.001
H	14.835	16.593	3.749	0.001	0.000	-0.001	0.000
H	13.040	15.060	2.983	0.001	0.000	0.001	0.000
H	11.612	13.235	3.259	0.008	0.001	0.008	-0.002
H	10.416	11.247	3.162	0.002	0.000	0.002	0.000
H	9.530	11.692	4.645	0.001	0.000	0.001	0.000
H	9.477	9.268	4.655	0.001	0.000	0.001	-0.001
H	11.191	9.152	4.183	0.000	0.000	0.000	0.000
H	9.441	12.083	12.988	0.000	0.000	0.000	0.000
H	9.824	11.662	15.406	0.002	0.001	-0.001	-0.001
H	11.789	10.297	16.143	0.001	0.000	0.000	0.000
H	13.343	9.384	14.444	0.001	0.001	0.000	-0.001
H	14.031	9.014	12.245	0.008	0.006	-0.004	-0.004
H	13.718	7.957	9.552	0.001	0.000	0.000	0.000
H	15.089	8.932	10.153	0.002	0.001	-0.001	-0.001

H	14.779	10.585	8.374	0.000	0.000	0.000	0.000
H	14.582	9.020	7.547	0.001	0.001	-0.001	-0.001
H	13.839	6.524	4.089	0.000	0.000	0.000	0.000
H	14.934	4.295	4.027	0.002	-0.001	0.001	0.001
H	14.625	2.695	5.926	0.001	0.000	0.000	0.000
H	13.234	3.360	7.864	0.001	-0.001	0.000	0.001
H	11.944	4.889	9.065	0.008	-0.006	0.004	0.005
H	11.500	7.433	10.454	0.000	0.000	0.000	0.000
H	10.319	6.119	10.203	0.002	-0.001	0.001	0.001
H	8.746	7.655	9.117	0.000	0.000	0.000	0.000
H	9.367	8.579	10.507	0.001	-0.001	0.001	0.001
H	5.810	7.873	6.878	0.000	0.000	0.000	0.000
H	3.529	8.481	6.110	0.002	0.000	-0.002	0.001
H	2.934	10.881	5.724	0.001	0.000	0.001	0.000
H	4.646	12.636	6.096	0.001	0.000	-0.001	0.000
H	6.815	13.347	6.605	0.008	-0.001	-0.008	0.002
H	8.727	14.275	7.520	0.002	0.000	-0.002	0.000
H	9.781	13.430	6.354	0.000	0.000	0.000	0.000
H	11.199	13.729	8.294	0.001	0.000	-0.001	0.001
H	9.904	13.237	9.415	0.000	0.000	0.000	0.000
H	14.598	10.710	3.742	0.000	0.000	0.000	0.000
H	14.949	8.959	3.665	0.003	0.000	-0.003	0.001
H	13.340	9.580	3.171	0.000	0.000	0.000	0.000
H	14.548	12.193	10.926	0.001	-0.001	0.000	0.001
H	15.316	12.959	9.505	0.001	-0.001	0.000	0.000
H	14.312	13.937	10.620	0.002	-0.001	0.001	0.001
H	7.175	11.746	11.575	0.003	0.000	0.003	-0.001
H	7.694	12.884	10.287	0.000	0.000	0.000	0.000
H	6.492	11.611	9.929	0.000	0.000	0.000	0.000
H	8.238	5.921	7.527	0.000	0.000	0.000	0.000
H	7.693	6.015	5.820	0.003	0.002	-0.001	-0.002
H	9.328	5.406	6.208	0.000	0.000	0.000	0.000
H	13.275	8.735	5.394	0.002	0.000	-0.001	0.000
H	13.452	12.661	8.397	0.002	-0.001	0.001	0.001
H	9.276	11.117	10.572	0.002	0.000	0.001	0.000
H	8.488	8.128	6.716	0.002	0.001	-0.001	-0.001
N	11.622	11.862	4.814	0.025	0.004	0.024	-0.007
N	13.146	9.741	10.514	0.026	0.018	-0.012	-0.014
N	11.352	6.782	8.457	0.025	-0.017	0.011	0.014
N	8.379	12.178	7.303	0.025	-0.003	-0.024	0.007
O	13.508	12.462	6.732	0.030	-0.005	-0.028	0.008
O	10.847	9.798	6.133	0.006	0.001	0.005	-0.003
O	10.881	11.222	11.042	0.029	-0.020	0.014	0.016
O	12.810	10.030	7.980	0.008	0.004	-0.005	-0.004
O	12.352	7.441	5.973	0.030	0.021	-0.014	-0.017
O	10.199	9.076	8.660	0.011	-0.007	0.008	0.004
O	7.741	9.498	7.359	0.031	0.004	0.029	-0.008
O	10.715	11.701	8.265	0.009	-0.004	-0.008	0.003
O	13.738	9.611	5.241	0.050	-0.008	-0.047	0.013

O	13.244	12.650	9.379	0.050	-0.035	0.024	0.027
O	8.409	10.909	10.109	0.052	0.007	0.050	-0.014
O	9.126	7.439	6.363	0.049	0.034	-0.023	-0.028
total spin moment of molecule							
				0.135	-0.102	0.044	-0.076

Bader ASMs

Atom	X_A	Y_A	Z_A	ASM magnitude	ASM vector		
					x-component	y-component	z-component
C	13.813	13.499	5.941	0.034	0.006	0.032	-0.009
C	14.822	14.393	6.357	0.015	-0.003	-0.015	0.004
C	15.188	15.486	5.583	0.040	0.006	0.038	-0.011
C	14.551	15.733	4.356	0.018	-0.003	-0.017	0.005
C	13.554	14.874	3.929	0.031	0.005	0.030	-0.008
C	13.155	13.748	4.691	0.015	-0.003	-0.015	0.004
C	12.087	12.931	4.201	0.106	0.018	0.100	-0.028
C	10.432	11.187	4.262	0.004	0.000	0.004	0.000
C	10.460	9.750	4.753	0.002	-0.001	0.002	0.000
C	11.158	10.972	12.328	0.034	0.024	-0.016	-0.018
C	10.292	11.485	13.316	0.015	-0.011	0.007	0.008
C	10.512	11.250	14.667	0.040	0.028	-0.019	-0.021
C	11.617	10.488	15.084	0.018	-0.013	0.009	0.010
C	12.484	9.982	14.133	0.031	0.022	-0.015	-0.017
C	12.292	10.201	12.747	0.015	-0.011	0.007	0.008
C	13.218	9.619	11.825	0.108	0.075	-0.051	-0.057
C	14.097	8.985	9.675	0.003	0.003	-0.001	-0.002
C	14.159	9.675	8.322	0.002	0.001	0.000	-0.001
C	12.909	6.224	6.003	0.034	-0.023	0.016	0.019
C	13.713	5.823	4.915	0.015	0.011	-0.007	-0.009
C	14.321	4.575	4.883	0.039	-0.027	0.018	0.022
C	14.149	3.675	5.947	0.018	0.013	-0.008	-0.010
C	13.367	4.047	7.026	0.031	-0.021	0.014	0.017
C	12.733	5.312	7.094	0.015	0.011	-0.007	-0.009
C	11.979	5.639	8.265	0.105	-0.072	0.049	0.059
C	10.729	7.045	9.768	0.003	-0.003	0.001	0.002
C	9.653	8.099	9.560	0.002	-0.001	0.000	0.001
C	6.535	9.895	6.934	0.033	-0.004	-0.032	0.009
C	5.547	8.917	6.699	0.015	0.002	0.015	-0.004
C	4.271	9.262	6.274	0.039	-0.005	-0.037	0.011
C	3.934	10.608	6.058	0.018	0.002	0.018	-0.005
C	4.891	11.585	6.270	0.031	-0.004	-0.029	0.008
C	6.202	11.271	6.705	0.015	0.002	0.015	-0.004
C	7.145	12.335	6.870	0.104	-0.013	-0.099	0.029
C	9.283	13.342	7.334	0.004	0.000	-0.004	0.000
C	10.323	13.074	8.408	0.002	0.000	-0.002	0.000
C	14.172	9.710	3.884	0.003	-0.001	-0.003	0.001
C	14.416	12.951	10.141	0.003	-0.002	0.001	0.002
C	7.400	11.841	10.500	0.002	0.000	0.002	-0.001

C	8.559	6.134	6.492	0.003	0.002	-0.001	-0.002
Fe	12.272	11.077	6.354	2.056	-0.332	-1.955	0.544
Fe	11.925	10.726	9.542	2.060	-1.444	0.975	1.100
Fe	11.176	8.177	7.260	2.058	1.415	-0.942	-1.161
Fe	9.159	10.619	7.914	2.056	0.252	1.963	-0.558
H	15.318	14.197	7.308	0.000	0.000	0.000	0.000
H	15.975	16.153	5.933	0.001	0.000	0.001	0.000
H	14.835	16.593	3.749	0.000	0.000	0.000	0.000
H	13.040	15.060	2.983	0.000	0.000	0.000	0.000
H	11.612	13.235	3.259	0.006	0.001	0.005	-0.002
H	10.416	11.247	3.162	0.002	0.000	0.002	0.000
H	9.530	11.692	4.645	0.001	0.000	0.001	0.000
H	9.477	9.268	4.655	0.001	0.001	0.001	-0.001
H	11.191	9.152	4.183	0.001	0.000	-0.001	0.000
H	9.441	12.083	12.988	0.000	0.000	0.000	0.000
H	9.824	11.662	15.406	0.001	0.001	0.000	-0.001
H	11.789	10.297	16.143	0.000	0.000	0.000	0.000
H	13.343	9.384	14.444	0.000	0.000	0.000	0.000
H	14.031	9.014	12.245	0.006	0.004	-0.003	-0.003
H	13.718	7.957	9.552	0.000	0.000	0.000	0.000
H	15.089	8.932	10.153	0.002	0.001	-0.001	-0.001
H	14.779	10.585	8.374	0.001	0.000	0.000	0.000
H	14.582	9.020	7.547	0.002	0.001	-0.001	-0.001
H	13.839	6.524	4.089	0.000	0.000	0.000	0.000
H	14.934	4.295	4.027	0.001	-0.001	0.000	0.001
H	14.625	2.695	5.926	0.000	0.000	0.000	0.000
H	13.234	3.360	7.864	0.000	0.000	0.000	0.000
H	11.944	4.889	9.065	0.006	-0.004	0.003	0.003
H	11.500	7.433	10.454	0.000	0.000	0.000	0.000
H	10.319	6.119	10.203	0.002	-0.001	0.001	0.001
H	8.746	7.655	9.117	0.000	0.000	0.000	0.000
H	9.367	8.579	10.507	0.002	-0.001	0.001	0.001
H	5.810	7.873	6.878	0.000	0.000	0.000	0.000
H	3.529	8.481	6.110	0.001	0.000	-0.001	0.000
H	2.934	10.881	5.724	0.000	0.000	0.000	0.000
H	4.646	12.636	6.096	0.000	0.000	0.000	0.000
H	6.815	13.347	6.605	0.005	-0.001	-0.005	0.002
H	8.727	14.275	7.520	0.002	0.000	-0.002	0.000
H	9.781	13.430	6.354	0.000	0.000	0.000	0.000
H	11.199	13.729	8.294	0.001	-0.001	-0.001	0.001
H	9.904	13.237	9.415	0.000	0.000	0.000	0.000
H	14.598	10.710	3.742	0.000	0.000	0.000	0.000
H	14.949	8.959	3.665	0.003	-0.001	-0.003	0.001
H	13.340	9.580	3.171	0.000	0.000	0.000	0.000
H	14.548	12.193	10.926	0.001	-0.001	0.001	0.001
H	15.316	12.959	9.505	0.001	-0.001	0.000	0.000
H	14.312	13.937	10.620	0.002	-0.001	0.001	0.001
H	7.175	11.746	11.575	0.003	0.000	0.003	-0.001
H	7.694	12.884	10.287	0.000	0.000	0.000	0.000

H	6.492	11.611	9.929	0.000	0.000	0.000	0.000
H	8.238	5.921	7.527	0.000	0.000	0.000	0.000
H	7.693	6.015	5.820	0.003	0.002	-0.001	-0.002
H	9.328	5.406	6.208	0.000	0.000	0.000	0.000
H	13.275	8.735	5.394	0.000	0.000	0.000	0.000
H	13.452	12.661	8.397	0.000	0.000	0.000	0.000
H	9.276	11.117	10.572	0.000	0.000	0.000	0.000
H	8.488	8.128	6.716	0.000	0.000	0.000	0.000
N	11.622	11.862	4.814	0.036	0.006	0.034	-0.009
N	13.146	9.741	10.514	0.036	0.025	-0.017	-0.019
N	11.352	6.782	8.457	0.035	-0.024	0.016	0.020
N	8.379	12.178	7.303	0.035	-0.004	-0.034	0.010
O	13.508	12.462	6.732	0.025	-0.004	-0.024	0.006
O	10.847	9.798	6.133	0.013	-0.001	0.013	-0.002
O	10.881	11.222	11.042	0.024	-0.017	0.011	0.013
O	12.810	10.030	7.980	0.012	0.009	-0.003	-0.008
O	12.352	7.441	5.973	0.025	0.017	-0.011	-0.014
O	10.199	9.076	8.660	0.015	-0.011	0.006	0.008
O	7.741	9.498	7.359	0.025	0.003	0.024	-0.007
O	10.715	11.701	8.265	0.016	-0.001	-0.015	0.002
O	13.738	9.611	5.241	0.050	-0.008	-0.047	0.013
O	13.244	12.650	9.379	0.050	-0.035	0.024	0.027
O	8.409	10.909	10.109	0.052	0.007	0.050	-0.014
O	9.126	7.439	6.363	0.049	0.034	-0.023	-0.028
total spin moment of molecule							
				0.135	-0.102	0.044	-0.076