Iron-Catalyzed Reductive Coupling of Alkyl Iodides with Alkynes to Yield Cis-Olefins: Mechanistics Insights from Computation

Andrea Darù,[a] Xile Hu,[b] Jeremy N. Harvey[a,*]

a: KU Leuven, Department of Chemistry, Division of Quantum Chemistry and Physical Chemistry, Celestijnenlaan 200F, 3001 Heverlee (Belgium)

b: Laboratory of Inorganic Synthesis and Catalysis, Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne (EPFL), ISIC-LSCI, BCH 3305, Lausanne 1015, Switzerland

Supporting Information

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Extra computational details:

For some of the benchmark calculations performed we used a different set of different functionals called **BS3**. This is not listed in the computational details of the main text. Therefore, the details are reported here. **BS3** is composed by Def2QZVPP[1] for Fe and Zn; Def2TZVPP[2,3] for O, I, and Br; Def2TZVP[2] for N and C; and Def2SVP[2] for H. Also, the relativistic Hamiltonian DKH is *not* used when this basis set is used.

Solvation and spin-state energetic study:

In this section we report detailed tables with the free energy values for the solvation and spin-state study. The data refers to the structures for $FeBr_2$, FeBr, and $ZnBr_2$ by using 3 different functionals. The details and terminology of these methods are described in the computational details section of the article. All the xyz structures with also the electronic energy at the optimization level of theory are reported at the bottom of this document.
For the 3 different species we tried to locate the structures starting from the mono- until the tetra- solvated one. The abbreviation "sv" indicates the DMA solvent molecules and the number in front of it the coordination number of the metal center. All the free energy values include implicit solvation using the model SMD. For the case of Fe(I) complexes the tetra solvated structure was impossible to locate due to the release of one ligand during the optimization process.
The spin state is denoted by the superscript in front of the metal center.

Table S1: Single-point total energy values (/hartree) at the B3LYP-D3BJ-DKH/**BS2**, M06L/**BS3**, MN15/**BS3** level of theory for Fe(I)Br, Fe(II)Br_2 and $ZnBr_2$ with different solvation number and spin-multiplicity. The structures were obtained at the B3LYP-D3BJ/**BS1** level in each case. For both optimizations are single point calculations the implicit solvation model SMD for the DMA solvent has been applied. The free energy correction (at 298 K) is calculated at the optimization level of theory with vibrations correction at 100 cm^{-1}.

Name	B3LYP	M06L	MN15	G corr
DMA	−288.093612	−287.896739	−287.587511	0.104696
^{2}FeBr_1sv	−4166.992744	−4125.701098	−4125.975688	0.097356
^{2}FeBr_2sv	−4455.137605	−4413.621173	−4413.626780	0.221785
^{2}FeBr_3sv	−4743.226575	−4701.528405	−4701.235880	0.344152
^{4}FeBr_1sv	−4167.056842	−4125.748616	−4126.067452	0.096360
^{4}FeBr_2sv	−4455.178104	−4413.652761	−4413.692400	0.219147
^{4}FeBr_3sv	−4743.266157	−4701.565462	−4701.283618	0.342867
^{1}FeBr2_cis_2sv	−7061.373472	−6987.745338	−6988.186409	0.220142
^{1}FeBr2_cis_3sv	−7349.496149	−7275.668528	−7275.802222	0.345486
^{1}FeBr2_trans_1sv	−6773.229905	−6699.799491	−6700.553406	0.096828
^{1}FeBr2_trans_3sv	−7349.497433	−7275.670875	−7275.805091	0.344530
^{1}FeBr2_cis_4sv	−7637.606497	−7563.580423	−7563.409260	0.470549
^{1}FeBr2_trans_4sv	−7637.611682	−7563.586588	−7563.413935	0.470745
^{3}FeBr2_cis_2sv	−7061.406505	−6987.780543	−6988.231455	0.219605
^{3}FeBr2_cis_3sv	−7349.530870	−7275.700018	−7275.856310	0.343888
^{3}FeBr2_trans_1sv	−6773.268884	−6699.848363	−6700.625476	0.095111
^{3}FeBr2_trans_3sv	−7349.531188	−7275.700586	−7275.857363	0.343289
^{3}FeBr2_cis_4sv	−7637.622472	−7563.586467	−7563.447730	0.468764
^{5}FeBr2_cis_2sv	−7061.459887	−6987.832699	−6988.284227	0.217435
^{5}FeBr2_cis_3sv	−7349.565129	−7275.737652	−7275.883629	0.341848
^{5}FeBr2_cis_4sv	−7637.667306	−7563.641818	−7563.481305	0.466360
^{5}FeBr2_trans_1sv	−6773.329757	−6699.909516	−6700.659871	0.094291
^{5}FeBr2_trans_3sv	−7349.560941	−7275.734010	−7275.881214	0.341000
^{5}FeBr2_trans_4sv	−7637.669023	−7563.641340	−7563.481231	0.465880
ZnBr2_cis_2sv	−7584.673939	−7503.496042	−7504.151642	0.219617
ZnBr2_cis_3sv	−7872.771752	−7791.397816	−7791.743978	0.342714
ZnBr2_cis_4sv	−8160.862375	−8079.292391	−8079.331642	0.468633
ZnBr2_trans_3sv	−7872.771169	−7791.397839	−7791.744168	0.343101
ZnBr2_trans_4sv	−8160.876013	−8079.298152	−8079.338569	0.470433

Table S2: Single-point free energy values (/hartree) and relative free energy values (kcal/mol) calculated comparing each complex to the most stable one; at the B3LYP-D3BJ-DKH/**BS2**, M06L/**BS3**, MN15/**BS3** level of theory for Fe(I)Br, Fe(II)Br_2 and $ZnBr_2$ with different solvation number and spin-multiplicity. The structures were obtained at the B3LYP-D3BJ/**BS1** level in each case. For both optimizations are single point calculations the implicit solvation model SMD for the DMA solvent has been applied. The free energy correction (at 298 K) is calculated at the optimization level of theory with vibrations correction at 100 cm^{-1}. All the listed structures have the same amount of explicit solvent summed on the total free energy values for easier comparison.

Name	G (/hartree)	ΔG (kcal/mol)
^{2}FeBr_1sv + 2sv	−4742.87322	19.78
^{2}FeBr_2sv + 1sv	−4742.90473	0.00
^{2}FeBr_3sv	−4742.88242	14.00
^{4}FeBr_1sv + 2sv	−4742.93831	6.00
^{4}FeBr_2sv + 1sv	−4742.94787	0.00
^{4}FeBr_3sv	−4742.92329	15.43
^{1}FeBr2_cis_2sv + 2sv	−7637.13116	5.93
^{1}FeBr2_cis_3sv + 1sv	−7637.13821	1.50
^{1}FeBr2_trans_1sv + 3sv	−7637.09982	25.59
^{1}FeBr2_trans_3sv + 1sv	−7637.14061	0.00
^{1}FeBr2_cis_4sv	−7637.13453	3.81
^{1}FeBr2_trans_4sv	−7637.13972	0.56
^{3}FeBr2_cis_2sv + 2sv	−7637.16473	7.58
^{3}FeBr2_cis_3sv + 1sv	−7637.1759	0.58
^{3}FeBr2_trans_1sv + 3sv	−7637.14052	22.78
^{3}FeBr2_trans_3sv + 1sv	−7637.17681	0.00
^{3}FeBr2_cis_4sv	−7637.15229	15.39
^{5}FeBr2_cis_2sv + 2sv	−7637.22028	0.00
^{5}FeBr2_cis_3sv + 1sv	−7637.2122	5.07
^{5}FeBr2_trans_1sv + 3sv	−7637.20221	11.34
^{5}FeBr2_trans_3sv + 1sv	−7637.20724	8.18
^{5}FeBr2_trans_4sv	−7637.19978	12.86

Free Energy Surface

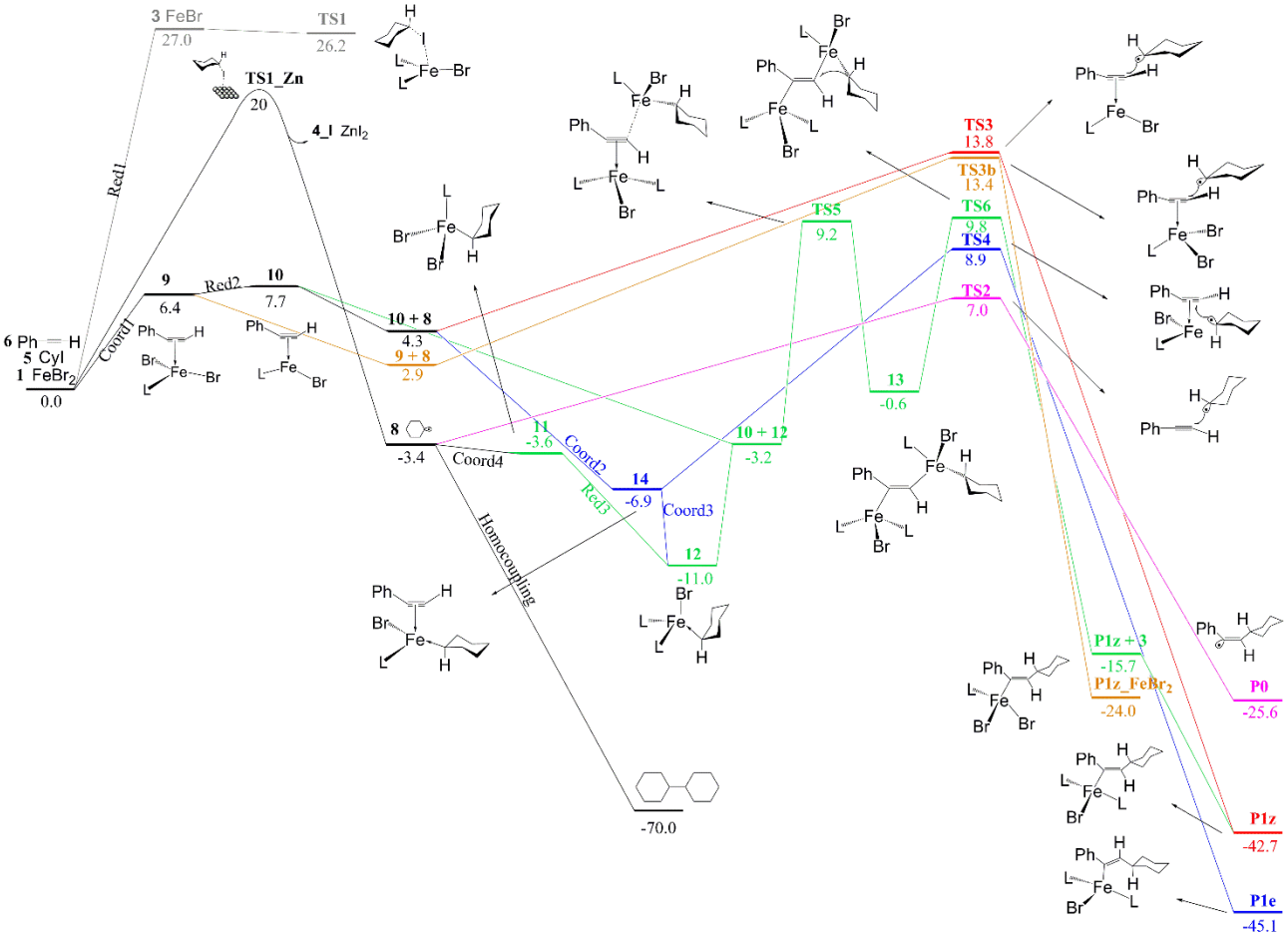

Figure S1. Reaction paths explored during this study at B3LYP-D3BJ-DKH level of theory, **BS2** basis set. The values are free energy in kcal/mol calculated according with the computational detail section (298 K). L = DMA solvent molecule.

In Fig. S1, some TSs have estimated free energy values obtained using various approximate protocols described in the kinetic modelling section. The TSs for which this has been done are those for the processes labelled with the labels listed here. The estimated free energy barrier is given relative to overall reactants, and in parentheses relative to the corresponding reactant state. The type of estimate used is also given: 'diff' = diffusion-limited step; 'Marcus' = Marcus theory estimate.

Red1: 33.6 kcal/mol ($\Delta\Delta G_{act}$ = 33.6 kcal/mol), Marcus
Coord1: 10.4 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Red2: 24.8 kcal/mol ($\Delta\Delta G_{act}$ = 18.2 kcal/mol), Marcus
Coord2: 8.3 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Coord3: −2.9 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Homocoupling: 0.6 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Coord4: 0.6 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Red3: 10.9 kcal/mol ($\Delta\Delta G_{act}$ = 14.5 kcal/mol), Marcus

Free energy calculation of Zn(0) halogen abstraction

The activation free energy of the halogen abstraction made by Zn(0) to the cyclohexyl iodide has been calculated by using the kinetic rate equation from the experimental observations made in three papers available in the literature[4–7] . To do so we used the following equation and the data of Table S3.

The free energy barriers for halogen abstraction reactions from cyclohexyl iodide or iron bromide complexes have been estimated using a multi-step procedure ultimately based on combining Marcus theory with experimentally observed rate constants for the reaction with benzyl iodide $PhCH_2I$. This procedure is described in detail here.

The starting point is an empirical equation that has been fit[4] (based on a Langmuir-Hinshelwood model of surface reactivity) to multiple experimental observations of the rate of reaction of benzyl halides with solid zinc in DMF, a solvent similar to that used in the present chemistry. It is known[4] that this reaction involves as rate-limiting step a halogen atom transfer step that is similar to those we wish to model. The fitted expression yields the rate of reaction *w* (expressed in

terms of weight of zinc reacting per unit of solid zinc surface area per unit time) in terms of the concentrations of benzyl halide and DMF as well as two equilibrium constants K_1 and K_2 and a rate constant k. K_1 and K_2 correspond to assumed equilibrium constants for adsorption on the zinc surface of benzyl halide and DMF respectively, while k is the assumed rate constant for the bond cleavage step starting from adsorbed reagents. Values of k, K_1 and K_2 are available for both $PhCH_2Br$ and $PhCH_2Cl$ from Tables 3 and 2, respectively, of ref. 4.

We first calculate w using this expression, the literature values of k, K_1 and K_2, and the concentrations of cyclohexyl iodide and solvent appropriate for the experiments performed in ref. 4, namely 0.5 M and 10.755 M. The values of w thus obtained are shown in the Table below. We obtain a reaction rate w per surface area equal to 0.1053 g m^{-2} s^{-1} and 0.4890 g m^{-2} s^{-1} for bromide and chloride abstraction respectively.

$$w = \frac{kK_1K_2[\mathrm{PhCH_2Hal}][\mathrm{DMF}]}{(1 + K_1[\mathrm{PhCH_2Hal}] + K_2[\mathrm{DMF}])^2} \quad (1)$$

Next, we wish to re-express the rate of reaction of alkyl halide in terms of an apparent rate constant k_{app} for its consumption, with the rate 'constant' encompassing the reactivity but also the conditions (amount of zinc metal and surface area of the zinc, and solvent concentration). k_{app} is such that the rate of consumption of alkyl halide is given by:

$$W = -\frac{d[RX]}{dt} = k_{app}\,[RX] \quad (2)$$

This equation is too simple to take into account the full Langmuir-Hinshelwood dependence of rate on surface binding constants, but should be realistic enough to account at least roughly for the rate of the activation process. Here we obtain a value of k_{app} by identifying eq. 1 and eq. 2 using, as much as possible, the reaction conditions relevant for the present iron-catalyzed process.

We derive a value for k_{app} in this way. First of all, we divide w by the molar mass of Zn so as to obtain a rate in mol m^{-2} s^{-1}. Next, we multiply by the surface area per g of the zinc powder used in the experiments of ref. 8. Typically, the sort of zinc powder used in such experiments has a surface area of 0.25 m^2 g^{-1}.[7] We also multiply by the total mass of zinc used in the experiments,[8] which is typically of 82 mg (corresponding to 2.5 equivalents of zinc for a reaction carried out with 0.5 mmol of substrate). This yields an overall rate (which we denote W, eq. 2) of 3.3×10^{-5} and 1.53×10^{-4} mol s^{-1} for bromide and chloride respectively. Finally, we divide W by the number of moles of cyclohexyl iodide present in the typical experimental conditions of ref. 8, to obtain an estimate for the k_{app} value we would need to use for describing reactivity of benzyl bromide or chloride, k_{benzyl} in Table S3.

For our purposes, we want to be able to describe reaction of cyclohexyl iodide, rather than benzyl bromide or chloride. Here, we have used the relative reactivity of benzyl bromide and cyclopentyl bromide (factor 100) reported in ref. 5 to estimate the k_{app} value for cyclopentyl bromide. We have furthermore noted that observed rates for reaction of zinc with benzyl bromide and benzyl chloride are rather similar. Also, the experiments for cross-coupling that we model can use alkyl bromides in place of alkyl iodides under rather similar conditions and giving similar yields. Hence we assume that our estimated k_{app} for cyclopentyl bromide is also a reasonable estimate for k_{app} for cyclohexyl iodide. Finally, we invert the Eyring equation to generate an estimate for the activation free energy of this reaction. The value obtained is 22 kcal/mol but for the subsequent kinetic analysis we have used a value of 20 kcal/mol which is within the uncertainty of this estimate.

$$k = \frac{k_B T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}} \Rightarrow \Delta G^{\ddagger} = -\mathrm{RTln}\left(\frac{k\,h}{k_B T}\right) \quad (3)$$

k_B is the Boltzmann constant with value 1.38×10^{-23} m^2 kg s^{-2} K^{-1}, h is the Planck constant with value 6.63×10^{-34} m^2 kg s^{-1}, and T is the temperature set as 300K.

And finally from that we are able to get the intrinsic activation barrier (λ) applying Marcus theory as explained in the "*Kinetic study"* section below in this document, and on the main text in the section "*kinetics*".

Table S3. Kinetic and thermodynamic parameters used to estimate the activation barrier for steps involving solid zinc and halide atom abstraction from a benzyl -bromide and -chloride molecules. These values are divided in subcategories: (a) taken from experimental paper by Hu group;[8] (b) calculated values by us; (c) taken from experimental paper by Egorov[4].

	Br	Cl
[CyX] (mol l^{-1})[a]	0.5	0.5
[DMF] (mol l^{-1})[b]	10.755	10.755
k (g cm^{-2} min^{-1})[c]	1.9	1.13
k (g m^{-2} s^{-1})[c]	1.14	6.78
K_1 (mol l^{-1})[c]	1.2	0.86
K_2 (mol l^{-1})[c]	0.19	0.2
w (g m^{-2} s^{-1})[b]	0.1053	0.4890
W (mol s^{-1})[b]	3.30×10^{-5}	1.53×10^{-4}
k_{benzyl} (s^{-1})[b]	6.60×10^{-2}	3.07×10^{-1}
$k_{cyclohexyl}$ (s^{-1})[b]	6.60×10^{-4}	3.07×10^{-3}
$\Delta G^{\ddagger}$ (J mol^{-1})[b]	86536.09	82731.27
$\Delta G^{\ddagger}$ (kcal mol^{-1})[b]	21.78	20.87

Iodide group

As described in the main text we have carried out some calculations in order to understand the effect of the halide group throughout the reaction mechanism. In fact, both bromide and iodide groups can be present in the metal complexes involved in the reaction. But our main model is calculated with all bromide groups except on **5**, **7**, **TS1** and **11** where the atom abstraction is involved. We selected the coordination and reduction reaction for two fundamental steps of the proposed reaction mechanism and calculate both with each of those substituent group. We can conclude that the results are pretty similar therefore we can consider our model realistic.

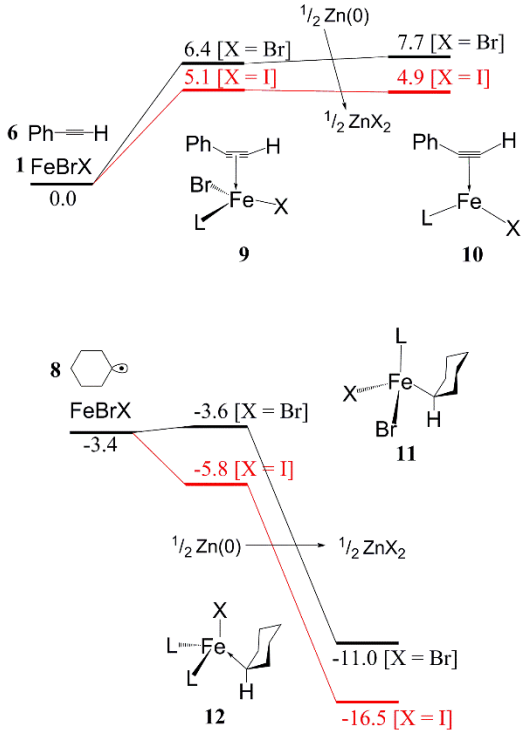

Figure S2. Halide study to confirm that a model with all bromide is suitable for the study of the reaction mechanism. Free energy in kcal/mol (T = 298 K) calculated at B3LYP-D3BJ-DKH/**BS2** level of theory. L = DMA solvent molecule.

Coupled cluster calculations

In order to validate our previous calculations and to have a clearer idea about the Fe(II) reduction by metallic zinc we decided to perform some Coupled Cluster calculation with singles, doubles and perturbative triple excitations (CCSD(T))[9,10] for a similar although simple system $FeCl_2(DMF)_2$ + ½ Zn(0) + DMF → $FeCl(DMF)_2$ + ½ $ZnCl_2(DMF)_2$. In order to increase the accuracy of the results we included the relativistic effect in the calculation using the scalar-relativistic Douglass-Kroll-Hess (DKH) Hamiltonian[11,12] and the appropriate correlation-consistent basis set, including appropriate polarization functions to describe correlation of the outer core electrons, cc-pwCVQZ family of basis sets, for Zn and Fe. This is the same basis set **BS2** as used for the DFT calculations, see computational details section of the main text for full specification. We then compared the CCSD(T) results with those obtained with B3LYP-D3BJ,[13,14] MN15,[15] M06L[16] using the same **BS2** basis set. For consistency, these DFT calculations were also performed with Douglas-Kroll-Hess one-electron integrals. All of these calculations are carried out in vacuum, and the Zn(0) species here simply refers to a zinc atom. The electronic energies at the different levels of theory are shown in Table S4, as well as the relative energy change for the reaction above. As can be seen, CCSD(T) and B3LYP-D3BJ agree to within better than 2 kcal/mol, while MN15 and M06L are slightly less accurate. This is one of our motivations for using B3LYP-D3BJ in the results in the main text.

Table S4. Benchmark of the functional B3LYP-D3BJ, M06L, and MN15 against CCSD(T) with basis set **BS2**, for the reaction $FeCl_2(DMF)_2$ + ½ Zn(0) + DMF → $FeCl(DMF)_2$ + ½ $ZnCl_2(DMF)_2$

	CCSD(T)	B3LYP-D3BJ	MN15	M06L
DMF	−248.1980144	**−248.7350428**	−248.4682993	−248.677091
Zn(0)	−1795.24577	**−1795.9469637**	−1797.200277	−1795.820278
[$C2_v$] $FeCl(DMF)_2$	−2229.68920	**−2231.9232163**	−2232.229673	−2231.665422
[$C2_v$] $FeCl_2(DMF)_2$	−2690.95339	**−2693.6874758**	−2694.056932	−2693.414700
[$C2_v$] $ZnCl_2(DMF)_2$	−3214.11834	**−3216.8992468**	−3217.754833	−3216.601592
Reaction [kcal/mol]	16.26	**14.58**	11.47	22.41

Different functionals

The choice of the functional in a DFT study is always difficult, mainly for the non-noble transition metals that still lack on a complete reactivity description. From the literature has been shown that B3LYP and B3LYP* can describe well the behavior for the non-noble metal series, in particular about iron.[17,18] Here we report the results obtained when we calculate the system under study by using different functionals. We choose them from different families, the first of them is the local meta-GGA M06L (0% exact HF exchange), and the second the global-hybrid exchange correlation MN15 (44% exact HF exchange). We then performed single point calculations for all the structures previously located in the different routes of the reaction mechanism. Finally, we compared the values with our chosen level of theory (B3LYP-D3BJ-DKH). The most significant changes of M06L compared to B3LYP-D3BJ are (a) a lower free energy value for the migratory insertion transition state **TS4**, (b) a higher free energy value for the bimetallic reductive elimination **TS6**, and (c) a more accessible isomerization transition state **TS_iso** that can compete with the transmetalation process **TS7**. MN15, instead, gives a similar description than B3LYP. The only differences were (a) a coordination step between cyclohexyl radical **8** and $FeBr_2$ slightly more reversible, and (b) a more favorable reduction step of complex **9** to **10**. Therefore, MN15 cannot be completely discarded if compared with B3LYP but we didn't consider it as main method for the deviation it has when compared with CCSD(T).

The different reaction paths for those functionals are shown for comparison in Figure S3 and S4 for M06L; S5 and S6 for MN15.

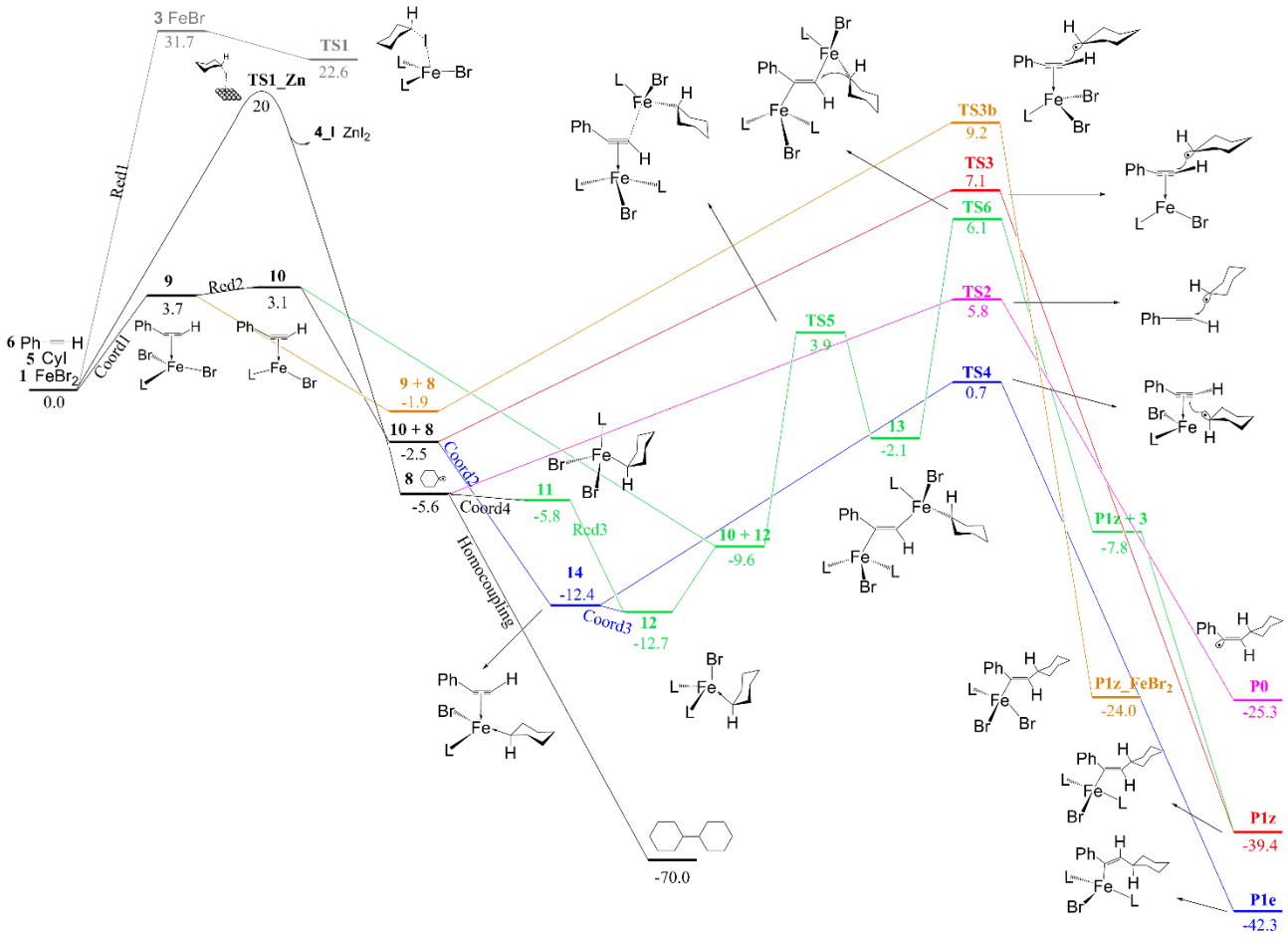

Figure S3. Reaction paths calculated at M06L level of theory on top of the geometry optimized using B3LYP-D3BJ. The values are free energy in kcal/mol (T = 298 K) calculated according with the computational detail section. L = DMA solvent molecule.

In Fig. S3, some TSs have estimated free energy values obtained using various approximate protocols described in the kinetic modelling section. The TSs for which this has been done are those for the processes labelled with the labels listed here. The estimated free energy barrier is given relative to overall reactants, and in parentheses relative to the corresponding reactant state. The type of estimate used is also given: 'diff' = diffusion-limited step; 'Marcus' = Marcus theory estimate.

Red1: 36.9 kcal/mol ($\Delta\Delta G_{act}$ = 36.9 kcal/mol), Marcus
Coord1: 7.7 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Red2: 20.9 kcal/mol ($\Delta\Delta G_{act}$ = 17.2 kcal/mol), Marcus
Coord2: 1.5 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Coord3: −8.4 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Homocoupling: −1.6 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Coord4: −1.6 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Red3: 7.6 kcal/mol ($\Delta\Delta G_{act}$ = 13.4 kcal/mol), Marcus

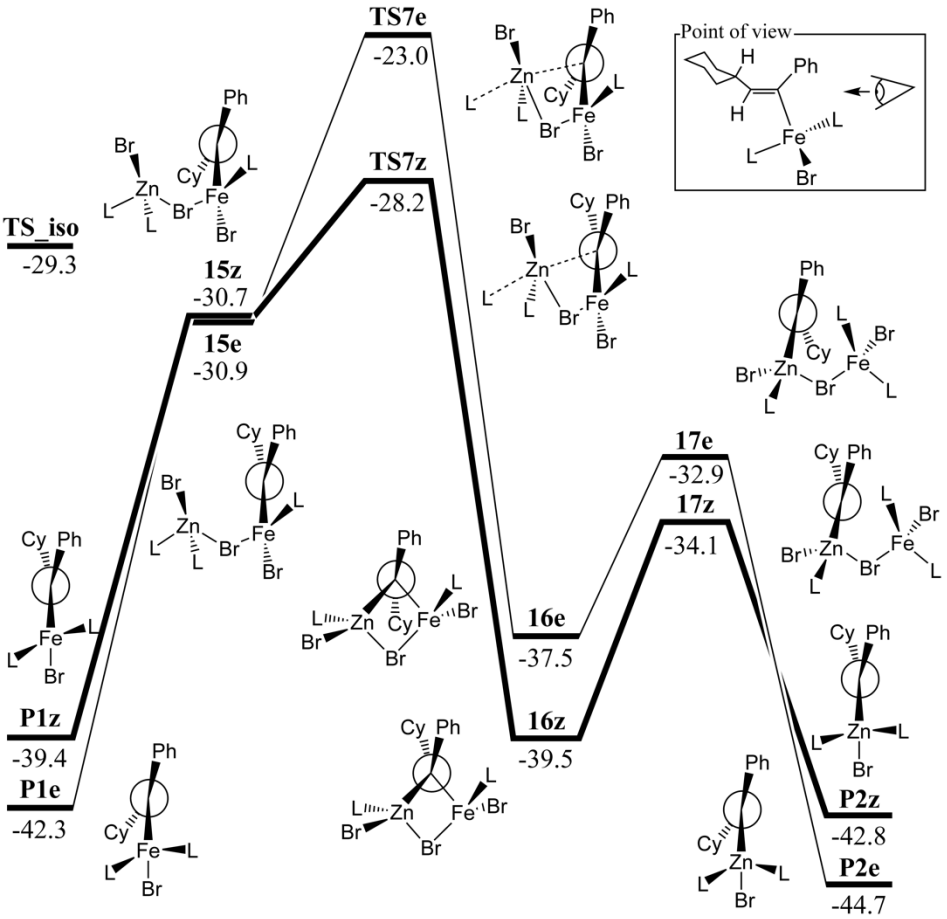

Figure S4. Transmetallation paths calculated using M06L functional on top of the geometry optimized using B3LYP-D3BJ. The values are free energy in kcal/mol (T = 298 K) calculated according with the computational detail section. L = DMA solvent molecule.

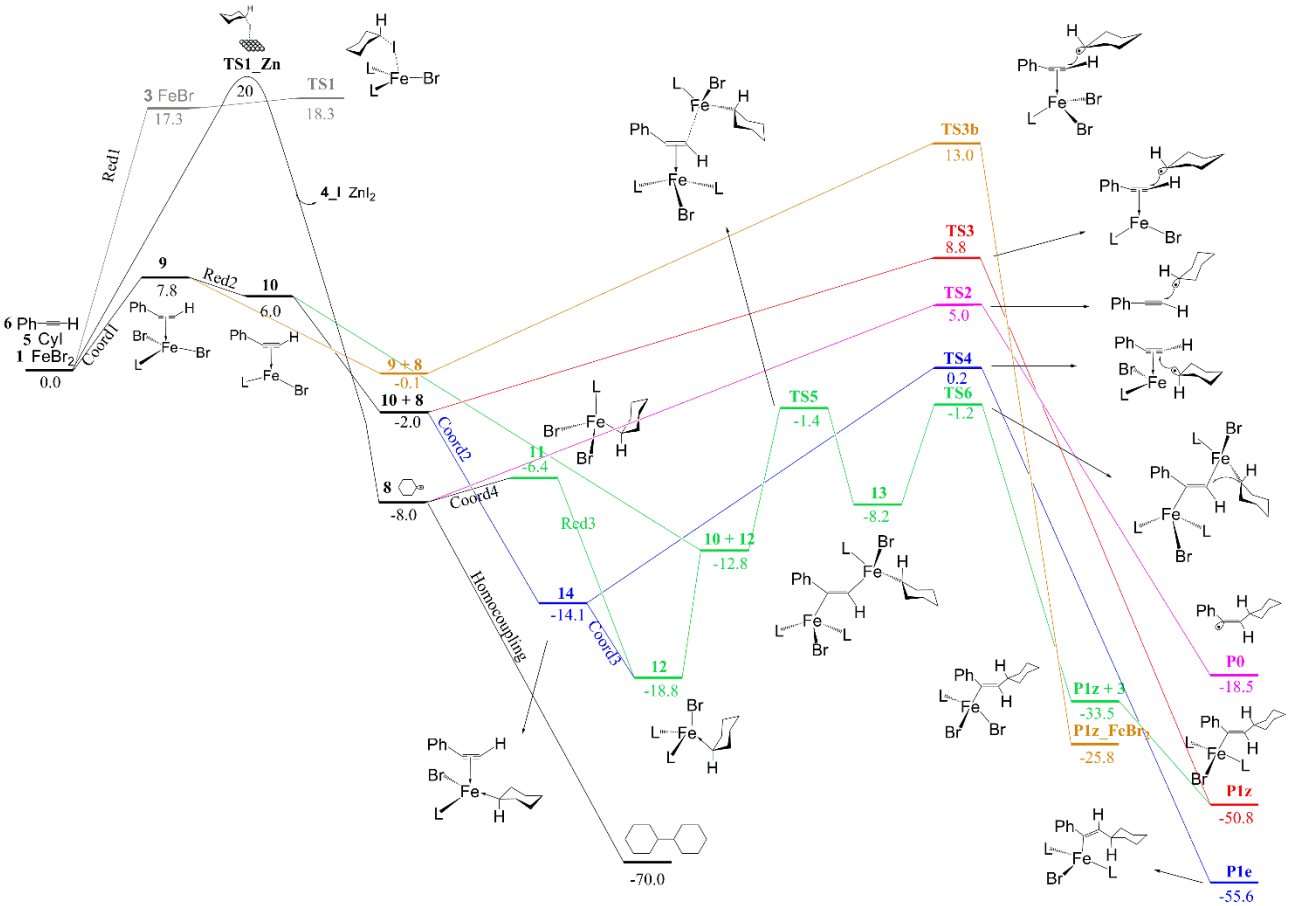

Figure S5. Reaction paths calculated using MN15 functional on top of the geometry optimized using B3LYP-D3BJ. The values are free energy in kcal/mol (T = 298 K) calculated according with the computational detail section. L = DMA solvent molecule.

In Fig. S5, some TSs have estimated free energy values obtained using various approximate protocols described in the kinetic modelling section. The TSs for which this has been done are those for the processes labelled with the labels listed here. The estimated free energy barrier is given relative to overall reactants, and in parentheses relative to the corresponding reactant state. The type of estimate used is also given: 'diff' = diffusion-limited step; 'Marcus' = Marcus theory estimate.

Red1: 27.2 kcal/mol ($\Delta\Delta G_{act}$ = 27.2 kcal/mol), Marcus
Coord1: 11.8 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Red2: 24.4 kcal/mol ($\Delta\Delta G_{act}$ = 16.6 kcal/mol), Marcus
Coord2: 2.0 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Coord3: −10.1 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Homocoupling: −4.0 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Coord4: −4.0 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Red3: 5.6 kcal/mol ($\Delta\Delta G_{act}$ = 12.0 kcal/mol), Marcus

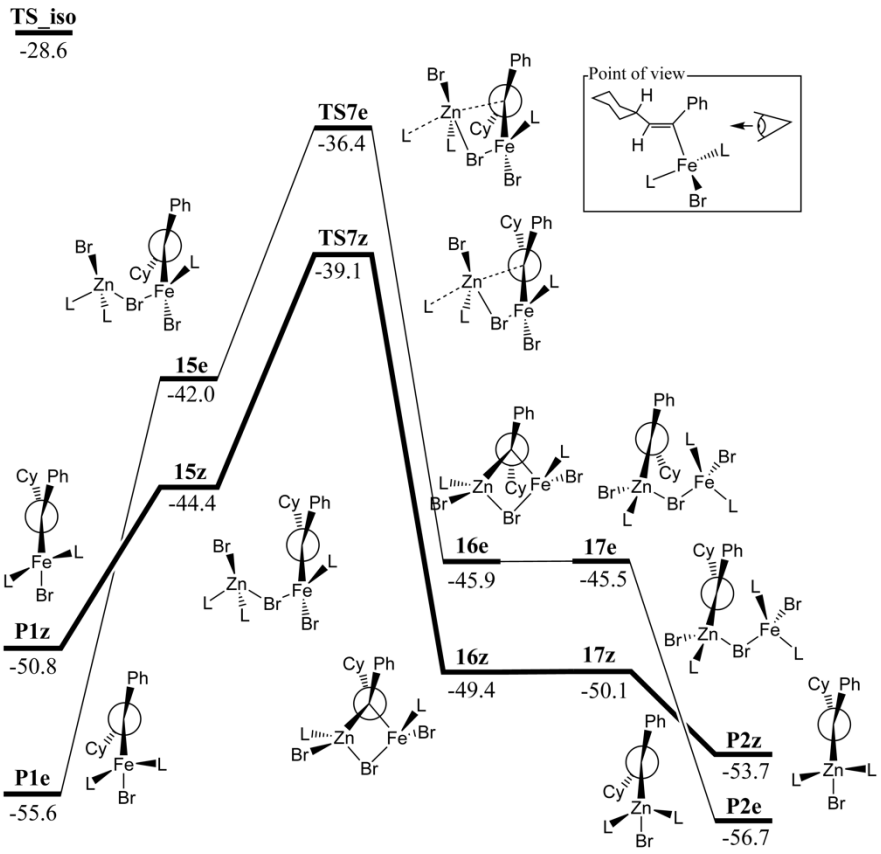

Figure S6. Transmetallation paths calculated using MN15 functional on top of the geometry optimized using B3LYP-D3BJ. The values are free energy in kcal/mol (T = 298 K) calculated according with the computational detail section. L = DMA solvent molecule.

Kinetic study

In this section we report a detailed description of our kinetic study. In Table S5 the values of free energy and rate constants are shown. Some free energy values are marked with a star (*) in order to indicate when that value is calculated by using Marcus theory. Some other values are marked with a hash (#) to indicate the barrierless step where we used 4 kcal/mol as activation barrier or in case of a reversible reaction where the product are less stable than reactant this value has been summed to the product free energy.

Table S5. Free energy values (kcal/mol) and kinetic rate constants (s^{-1}) divided in the different steps of the reaction mechanism. The label we used are the same that in the free energy profiles.

Reaction	5 + 2 → 8 + 4	1 + 6 → 9	9 → 10	10 + 8 → 14	1 + 8 → 11	14 → 12 + 6
$\Delta G^{\ddagger}$	20	$10.35^{\#}$	22.4*	$4^{\#}$	$4^{\#}$	$4^{\#}$
ΔG_{rea}	−3.4	6.35	1.38	−11.3	−0.2	−4
k_f	1.49×10^{-2}	1.69×10^{5}	2.79×10^{-4}	7.43×10^{9}	7.43×10^{9}	7.43×10^{9}
k_b	4.87×10^{-5}	7.43×10^{9}	2.85×10^{-3}	40.7	5.31×10^{9}	8.84×10^{6}

Reaction	10 + 12 → 13	13 → P1z + 3	3 + 6 → 10	8 + 8 → homocoupling	11 → 12	8 + 6 → P0
$\Delta G^{\ddagger}$	12.4	10.37	$4^{\#}$	5	18.13*	10.36
ΔG_{rea}	2.65	−15.13	−19.3	−70	−7.4	−22.14
k_f	5.37×10^{3}	1.64×10^{5}	7.43×10^{9}	1.38×10^{9}	3.5×10^{-1}	1.66×10^{5}
k_b	8.84×10^{6}	0	5.76×10^{-5}	0	1.36×10^{-6}	0

Reaction	10 + 8 → P1z	14 → P1e	1 → 3	3 + 8 → 12	3 + 5 → 8 + 1
$\Delta G^{\ddagger}$	9.44	15.8	33.6*	$4^{\#}$	−0.82
ΔG_{rea}	−47	−38.1	27	−34.57	−27.88
k_f	7.83×10^{5}	17.5	1.69×10^{-12}	7.43×10^{9}	2.48×10^{13}
k_b	0	0	9.28×10^{7}	3.94×10^{-16}	1.03×10^{-7}

Reaction	10 + 8 → P1z_$FeBr_2$	P1z → P2z	P1e → P2e	P1z → P1e
$\Delta G^{\ddagger}$	10.5	13.92	19.72	22
ΔG_{rea}	−26.9	−3.86	−3.66	−2.34
k_f	1.31×10^{5}	415	2.39×10^{-2}	5.14×10^{-4}
k_b	0	0.625	5.03×10^{-5}	1×10^{-5}

We used Marcus theory in order to guess the solid-zinc reduction barriers of the steps **1 → 3**, **9 → 10**, and **11 → 12** detailed during the explanation of the reaction mechanism. We made use of the following equation (4) and the data of the atom abstraction reaction made by solid zinc (first column of the previous Table S5) to calculate the intrinsic barrier height λ. Those values come from the experimental work made by Egorov[4] previously discussed here in the previous section "*Free energy calculation of Zn(0) halogen abstraction*" and on the main text in the section "*kinetics*". Resolving the equation we obtained a λ value of 86.7 kcal/mol. This value can now be used to estimate the activation free energy for the reduction steps of which we calculated the free energy difference. To do so we used the same equation in a backword way with $\Delta G^{\ddagger}$ as unknown variable. Therefore we could estimate the barrier for the solid-zinc reduction reaction step of which we don't have a transition state structure.

$$\Delta G^{\ddagger} = \frac{(\lambda + \Delta G^{0})^{2}}{4\lambda} \tag{4}$$

For all the other values we used the Eyring equation. We calculate the forward and backward rate constants by using the following equations:

$$k_f = \frac{k_B T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}} \tag{5}$$

$$k_b = \frac{k_B T}{h} e^{-\frac{(\Delta G^{\ddagger} - \Delta G_{rea})}{RT}} \tag{6}$$

k_B is the Boltzmann constant with value 1.38×10^{-23} m^2 kg s^{-2} K^{-1}, h is the Planck constant with value 6.63×10^{-34} m^2 kg s^{-1}, and T is the temperature set as 300K.

For the modified model the steps that got adjusted are shown in Table S6 with a reference for the raw model.

Table S6. Adjusted values for selected steps, in order to show the steps that have to be adjusted in order to see the bimetallic route dominate. All the free energy values are shown in kcal/mol.

Reaction	1 + 6 → 9	9 → 10
$\Delta G^{\ddagger}$ raw model	10.35#	22.4*
$\Delta G^{\ddagger}$ adjusted	4.35#	15.4*
ΔG_{rea}	0.35	1.4
k_f	4.12×10^{9}	36.6
k_b	7.43×10^{9}	373

A scheme showing the result of the adjustments to the thermodynamics of the reaction mechanism is shown in Figure S7.

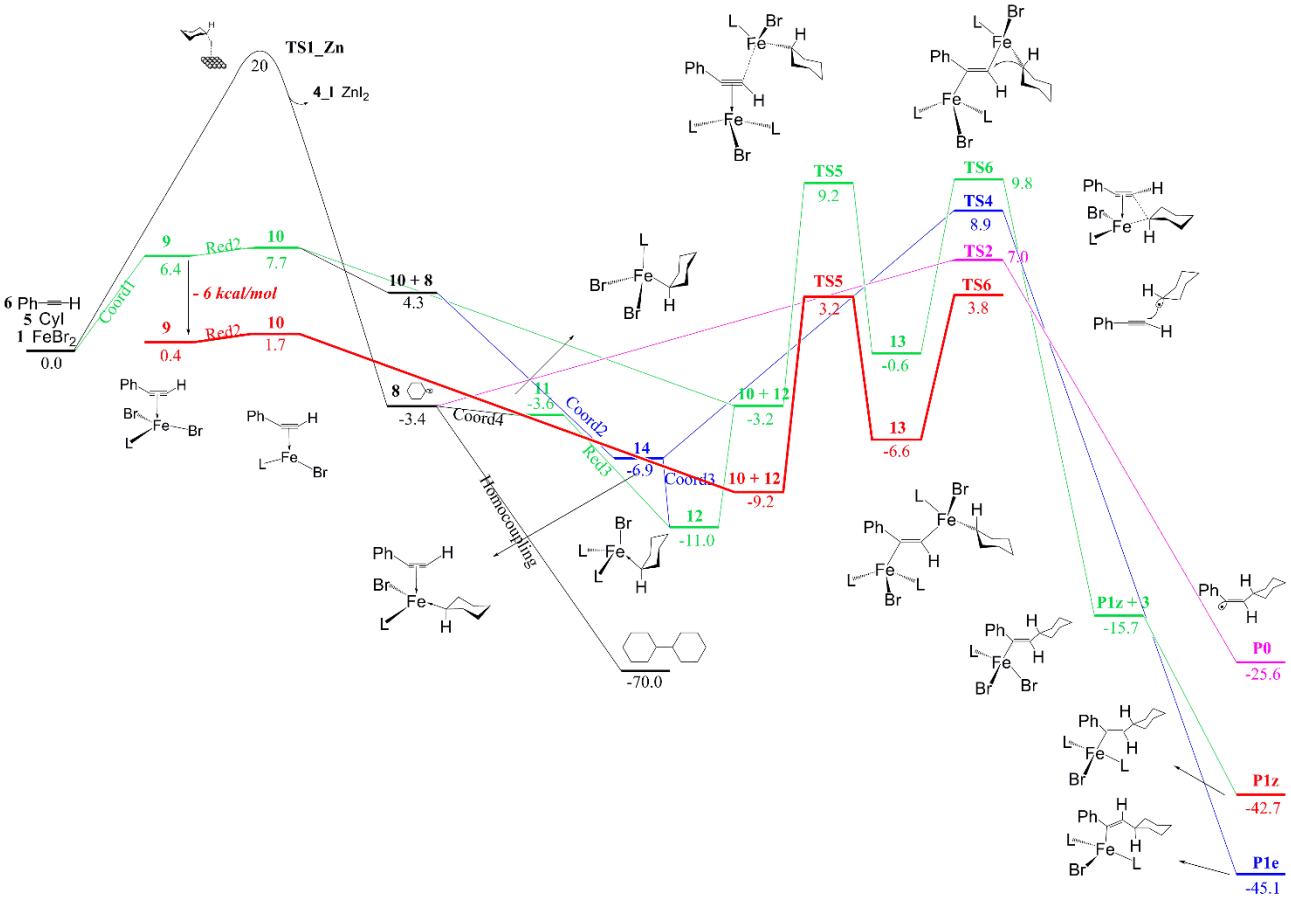

Figure S7. Free energy surface of the different reaction mechanism explored during this study. The adjusted value for the modified kinetics are highlighted for giving a clearer and visual understanding. The values are free energy in kcal/mol.

In Fig. S7, some TSs have estimated free energy values obtained using various approximate protocols described in the kinetic modelling section. The TSs for which this has been done are those for the processes labelled with the labels listed here. The estimated free energy barrier is given relative to overall reactants, and in parentheses relative to the corresponding reactant state. The type of estimate used is also given: 'diff' = diffusion-limited step; 'Marcus' = Marcus theory estimate.

Red1: 33.6 kcal/mol ($\Delta\Delta G_{act}$ = 33.6 kcal/mol), Marcus
~~Coord1: 10.4 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol)~~ → 4.4 kcal/mol (4 kcal/mol), adjusted
~~Red2: 28.8 kcal/mol ($\Delta\Delta G_{act}$ = 22.4 kcal/mol)~~ → 15.8 kcal/mol (15.4 kcal/mol), adjusted
Coord2: 8.3 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Coord3: −2.9 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Homocoupling: 0.6 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Coord4: 0.6 kcal/mol ($\Delta\Delta G_{act}$ = 4 kcal/mol), diff
Red3: 10.9 kcal/mol ($\Delta\Delta G_{act}$ = 14.5 kcal/mol), Marcus

The kinetic study has been done at the B3LYP-D3BJ level of theory but also testing the functionals M06L and MN15. The results are shown in Tab. S8 giving the same outcome with the free radical addition route dominating on the other reaction paths. The percentage are calculating based on the 1.2 eq of the reactant cyclohexyl iodide **5** in excess.

Table S7. Final yield of kinetic simulations at different levels of theory.

	B3LYP-D3BJ	M06L	MN15
P0	82.5%	82.5%	31.5%
P2e	0%	0%	0%
P2z	0%	0%	0%
CyCy homocoupling	3.8%	8.3%	34.2%
CyI	9.2%	0.1%	0.1%

Following the *raw* inputs for the software Tenua[19] we used for the kinetic calculations. From that it's possible to see the kinetic constant used for the forward and back reaction steps. The first column is made by using calculations at the B3LYP-D3BJ/DKH level of theory, second MN15 and third M06L.

```
cyi+zn<->cy+znx2;
k(+1):1.49e-2;
k(-1):4.87e-5;
fex2+alk<->alkfex2;
k(+2):1.69e5;
k(-2):7.43e9;
alkfex2+zn<->alkfex+znx2;
k(+3):2.79e-4;
k(-3):2.85e-3;
alkfex+cy<->alkcyfex;
k(+4):7.43e9;
k(-4):40.7;
fex2+cy<->cyfex2;
k(+5):7.43e9;
k(-5):5.31e9;
alkcyfex<->cyfex+alk;
k(+6):7.43e9;
k(-6):8.84e6;
alkfex+cyfex<->dimcomp;
k(+7):5.37e3;
k(-7):4.65e5;
dimcomp<->Zfepdim+fex;
k(+8):1.64e5;
k(-8):0;
Zfepdim+znx2<->Zznpdim+fex2;
k(+9):4.15e2;
k(-9):0.625;
fex+alk<->alkfex;
k(+10):7.43e9;
k(-10):5.76e-5;
cy+cy<->cycy;
k(+11):1.38e9;
k(-11):0;
cyfex2+zn<->cyfex+znx2;
k(+12):0.35;
k(-12):1.36e-6;
cy+alk<->prad;
k(+13):1.66e5;
k(-13):0;
alkfex+cy<->Zfeprad;
k(+14):7.83e5;
k(-14):0;
Zfeprad+znx2<->Zznprad+fex2;
k(+15):4.15e2;
k(-15):0.625;
alkcyfex<->Efepmi;
k(+16):17.5;
k(-16):0;
Efepmi+znx2<->Eznpmi+fex2;
k(+17):2.39e-2;
k(-17):5.03e-5;
fex2+zn<->fex+znx2;
k(+18):3.52e-15;
k(-18):1.94e5;
fex+cy<->cyfex;
k(+19):7.43e9;
k(-19):3.94e-16;
fex+cyi<->cy+fex2;
k(+20):2.48e13;
k(-20):1.03e-7;
alkfex2+cy<->PZ_febr2;
k(+21):1.31e5;
k(-21):0;

*script;
mechanism.solver="stiff";
go;
```

```
cyi+zn<->cy+znx2;
k(+1):1.49e-2;
k(-1):2.29e-8;
fex2+alk<->alkfex2;
k(+2):1.47e4;
k(-2):7.95e9;
alkfex2+zn<->alkfex+znx2;
k(+3):4.2e-3;
k(-3):1.86e-4;
alkfex+cy<->alkcyfex;
k(+4):7.43e9;
k(-4):9.89;
fex2+cy<->cyfex2;
k(+5):7.43e9;
k(-5):9.45e10;
alkcyfex<->cyfex+alk;
k(+6):7.43e9;
k(-6):2.72e6;
alkfex+cyfex<->dimcomp;
k(+7):3.09e4;
k(-7):7.5e7;
dimcomp<->Zfepdim+fex;
k(+8):4.93e7;
k(-8):0;
Zfepdim+znx2<->Zznpdim+fex2;
k(+9):2.06e4;
k(-9):13.2;
fex+alk<->alkfex;
k(+10):7.43e9;
k(-10):38.7;
cy+cy<->cycy;
k(+11):1.38e9;
k(-11):0;
cyfex2+zn<->cyfex+znx2;
k(+12):11.7;
k(-12):1.67e-8;
cy+alk<->prad;
k(+13):2.13e3;
k(-13):0;
alkfex+cy<->Zfeprad;
k(+14):8.63e4;
k(-14):0;
Zfeprad+znx2<->Zznprad+fex2;
k(+15):2.06e4;
k(-15):13.2;
alkcyfex<->Efepmi;
k(+16):219;
k(-16):0;
Efepmi+znx2<->Eznpmi+fex2;
k(+17):5.45e-2;
k(-17):1.01e-2;
fex2+zn<->fex+znx2;
k(+18):7.85e-8;
k(-18):3.5e5;
fex+cy<->cyfex;
k(+19):7.43e9;
k(-19):1.79e-11;
fex+cyi<->cy+fex2;
k(+20):1.28e12;
k(-20):7.77e-6;
alkfex2+cy<->PZ_febr2;
k(+21):1.65e3;
k(-21):0;

*script;
mechanism.solver="stiff";
go;
```

```
cyi+zn<->cy+znx2;
k(+1):1.49e-2;
k(-1):1.2e-6;
fex2+alk<->alkfex2;
k(+2):1.47e7;
k(-2):7.43e9;
alkfex2+zn<->alkfex+znx2;
k(+3):1.49e-3;
k(-3):5.42e-4;
alkfex+cy<->alkcyfex;
k(+4):7.43e9;
k(-4):437;
fex2+cy<->cyfex2;
k(+5):7.43e9;
k(-5):5.3e9;
alkcyfex<->cyfex+alk;
k(+6):7.43e9;
k(-6):4.88e9;
alkfex+cyfex<->dimcomp;
k(+7):4.57e5;
k(-7):1.32e11;
dimcomp<->Zfepdim+fex;
k(+8):6.87e6;
k(-8):0;
Zfepdim+znx2<->Zznpdim+fex2;
k(+9):4.05e4;
k(-9):156;
fex+alk<->alkfex;
k(+10):7.43e9;
k(-10):9.1e-12;
cy+cy<->cycy;
k(+11):1.38e9;
k(-11):0;
cyfex2+zn<->cyfex+znx2;
k(+12):0.35;
k(-12):1.36e-6;
cy+alk<->prad;
k(+13):3.14e4;
k(-13):0;
alkfex+cy<->Zfeprad;
k(+14):6.19e5;
k(-14):0;
Zfeprad+znx2<->Zznprad+fex2;
k(+15):4.05e4;
k(-15):156;
alkcyfex<->Efepmi;
k(+16):1520;
k(-16):0;
Efepmi+znx2<->Eznpmi+fex2;
k(+17):5.01e-2;
k(-17):7.44e-4;
fex2+zn<->fex+znx2;
k(+18):6.14e-15;
k(-18):9.23e8;
fex+cy<->cyfex;
k(+19):7.43e9;
k(-19):3.77e-19;
fex+cyi<->cy+fex2;
k(+20):3e14;
k(-20):1.65e-11;
alkfex2+cy<->PZ_febr2;
k(+21):4.71e4;
k(-21):0;

*script;
mechanism.solver="stiff";
go;
```

Next the input for the adjusted kinetics:

```
cyi+zn<->cy+znx2;
k(+1):1.49e-2;
k(-1):4.87e-5;
fex2+alk<->alkfex2;
k(+2):4.12e9;
k(-2):7.43e9;
alkfex2+zn<->alkfex+znx2;
k(+3):36.6;
k(-3):373;
alkfex+cy<->alkcyfex;
k(+4):7.43e9;
k(-4):40.7;
fex2+cy<->cyfex2;
k(+5):7.43e9;
k(-5):5.31e9;
alkcyfex<->cyfex+alk;
k(+6):7.43e9;
k(-6):8.84e6;
alkfex+cyfex<->dimcomp;
k(+7):5.37e3;
k(-7):4.65e5;
dimcomp<->Zfepdim+fex;
k(+8):1.64e5;
k(-8):0;
Zfepdim+znx2<->Zznpdim+fex2;
k(+9):4.15e2;
k(-9):0.625;
fex+alk<->alkfex;
k(+10):7.43e9;
k(-10):5.76e-5;
cy+cy<->cycy;
k(+11):1.38e9;
k(-11):0;
cyfex2+zn<->cyfex+znx2;
k(+12):0.35;
k(-12):1.36e-6;
cy+alk<->prad;
k(+13):1.66e5;
k(-13):0;
alkfex+cy<->Zfeprad;
k(+14):7.83e5;
k(-14):0;
Zfeprad+znx2<->Zznprad+fex2;
k(+15):4.15e2;
k(-15):0.625;
alkcyfex<->Efepmi;
k(+16):17.5;
k(-16):0;
Efepmi+znx2<->Eznpmi+fex2;
k(+17):2.39e-2;
k(-17):5.03e-5;
fex2+zn<->fex+znx2;
k(+18):0;
k(-18):0;
fex+cy<->cyfex;
k(+19):7.43e9;
k(-19):3.94e-16;
fex+cyi<->cy+fex2;
k(+20):2.48e13;
k(-20):1.03e-7;
alkfex2+cy<->PZ_febr2;
k(+21):1.31e5;
k(-21):0;



*script;
mechanism.solver="stiff";
go;
```

Labels used during the kinetic study and the related one used in the free energy description:
fex2: **1**
zn: **2**
fex: **3**
znx2: **4**
cyi: **5**
alk: **6**
cy: **8**
alkfex2: **9**
alkfex: **10**
cyfex2: **11**
cyfex: **12**
dimcomp: **13**
alkcyfex: **14**
prad: **P0**
Zfeprad: **P1z** (from TS3)
Zfepdim: **P1z** (from bimetallic process)
Efepmi: **P1e** (from TS4)
Zznprad: **P2z** (from Zfeprad)
Zznpdim: **P2z** (from Zfepdim)
Eznpmi: **P2e** (from Zfepmi)
cycy: product of homocoupling of 2 Cy radical **8**

Relaxed scan of species 16e and 16z:

In this section the relaxed scans of the C—Fe bond of the diamond-like complexes **16e/z** is showsn. We did so because we were not able to locate a transition state structure for the releasing of the Fe(II) salt **1** in the last step of the transmetalation. In order to show the potential barrierless character of this step we performed a relaxed scan of the C—Fe bond highlighted in the next figures. It is possible to see the electronic energy increasing as the bond elongates starting from **16** and going to a structure similar to **17** but with the absence of one of the explicit solvents (Figure S8 for Z-diastereomer and S10 for E-diastereomer). However, when one more explicit solvent is add in order to resemble the structure of **17** we can see the energy decreasing during the process (Figure S11). The calculations have been performed by setting a step-size of 0.1 Å using as starting geometry the one optimized and described in the *transmetalation* section.

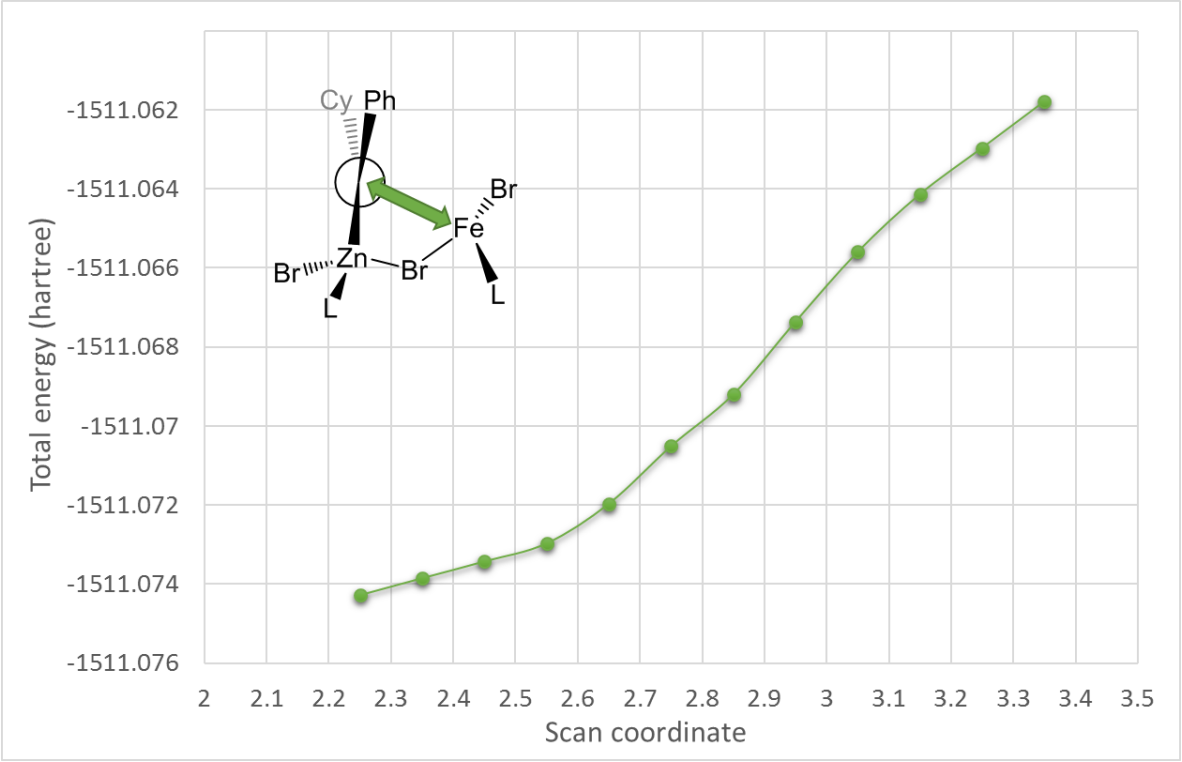

Figure S8. Electronic energy raising when performing a relaxed scan to the C-Fe bond of the diamond-like Z-diastereomer **16z** becoming a complex similar to **17z** but without one solvent.

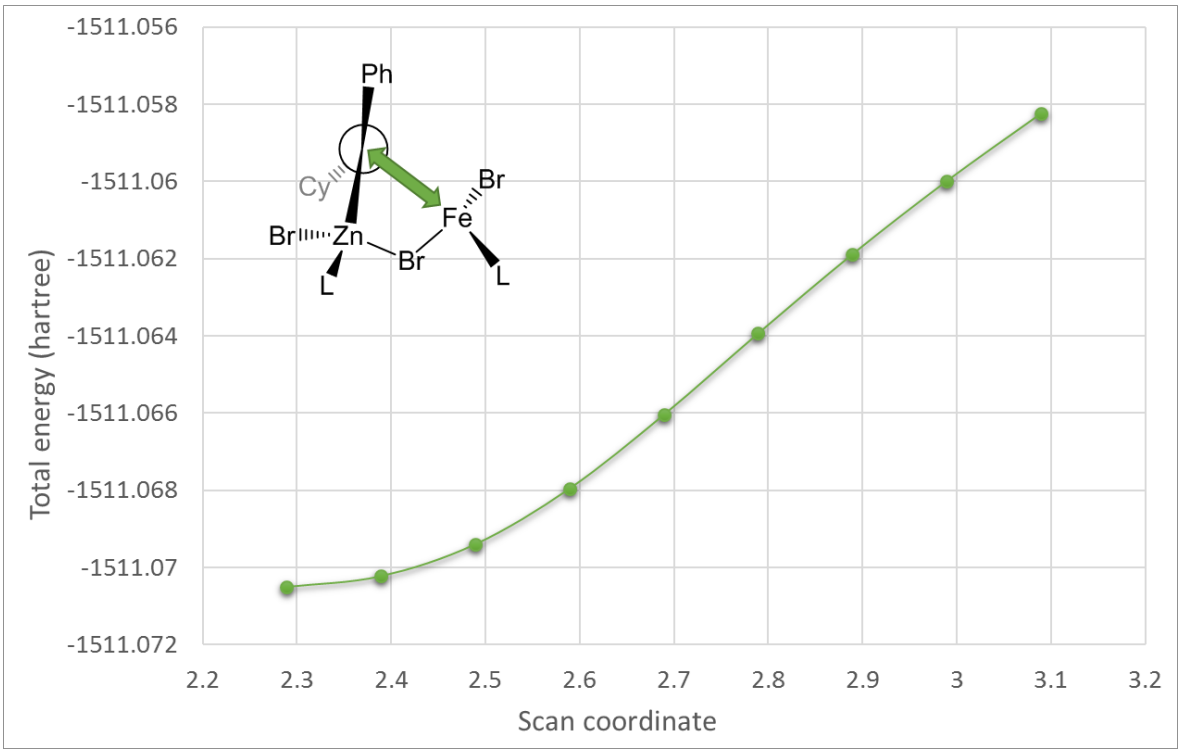

Figure S9. Electronic energy raising when performing a relaxed scan to the C-Fe bond of the diamond-like E-diastereomer **16e** becoming a complex similar to **17e** but without one solvent.

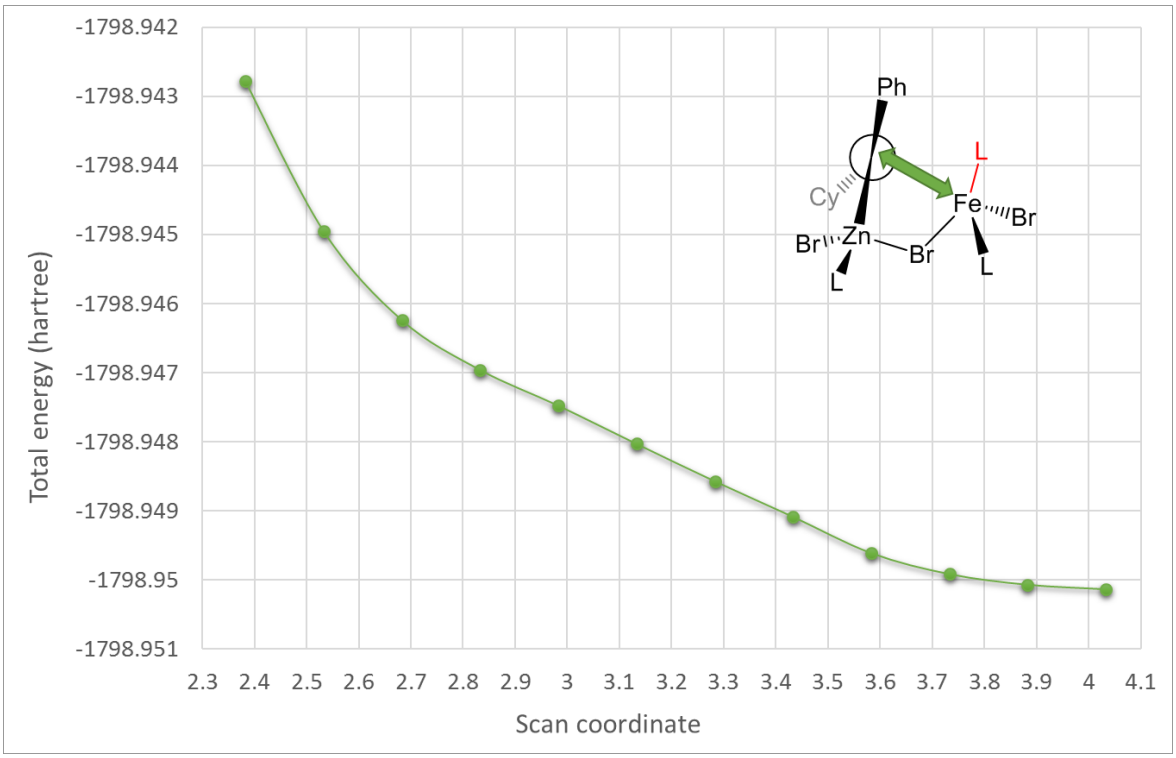

Figure S10. Electronic energy decreasing when performing a relaxed scan to the C-Fe bond of the diamond-like E-diastereomer **16e** becoming **17e** with an extra solvent coordinated.

Cartesian coordinates

Structure coordinate of spin state energetics and solvation study:

1FeBr2_cis_2sv
Opt Eel: -726.551720
SP Eel B3LYP: -7061.37347213
SP Eel M06L: -6987.74533825
SP Eel MN15: -6988.18640877
Gcorr: 0.220142
C -4.934798 0.401453 -1.312667
H -5.283431 1.392354 -1.624455
C -2.615420 0.145165 -0.496337
N -3.488905 0.312576 -1.491846
C -2.985706 0.531720 -2.848739
H -2.186467 -0.176874 -3.072882
H -3.809344 0.383960 -3.548757
H -2.598051 1.550778 -2.959656
C 4.941619 0.221096 -1.337847
Fe 0.000534 -0.128529 0.535853
C 2.618761 0.075332 -0.507449
N 3.493958 0.345279 -1.478990
C 2.999495 0.668551 -2.817653
H 5.416675 1.176537 -1.582842
H 2.715356 -0.241994 -3.357931
H 2.131135 1.324978 -2.747388
H 3.795931 1.175289 -3.365343
O 1.381980 0.105874 -0.781561
O -1.378289 0.174186 -0.769532
H 5.215645 -0.060486 -0.323885
H 5.312069 -0.544483 -2.028669
H -5.213964 0.243173 -0.273596
H -5.426565 -0.356086 -1.931313
Br -0.073663 -2.579990 0.730120
Br 0.064815 2.060001 1.662443
C 3.107005 -0.258021 0.878333
H 3.652931 -1.207032 0.877589
H 3.765803 0.524217 1.266772
H 2.262103 -0.358285 1.563613
C -3.104670 -0.075336 0.911479
H -3.657506 0.798112 1.271876
H -3.758383 -0.951047 0.968654
H -2.260764 -0.237000 1.586173

1FeBr2_cis_3sv
Opt Eel: -1014.443161
SP Eel B3LYP: -7349.49614855
SP Eel M06L: -7275.66852842
SP Eel MN15: -7275.80222243
Gcorr: 0.345486
Fe 0.175639 -0.548957 0.031653
Br 0.385828 -0.628929 2.521278
H -2.970519 1.455437 -1.198889
C -3.151183 2.501254 -0.963630
N -2.044716 3.028485 -0.169143
H -4.088012 2.594689 -0.401877
H -3.241947 3.076507 -1.891314
C -1.046363 2.228830 0.246277
C -2.173594 4.428880 0.218982
O -1.039257 1.023078 -0.115930
H -2.550272 4.995062 -0.637891
H -2.883748 4.538157 1.048285
H -1.213174 4.849069 0.511526
H 2.110977 1.485840 -2.684611
C 2.918094 2.106786 -2.294038
N 3.620196 1.399876 -1.225355
H 2.493441 3.050405 -1.929529
H 3.630099 2.323885 -3.092907
C 5.047444 1.674447 -1.105732
C 2.909479 0.688042 -0.334436
H 5.545564 1.433737 -2.050453
H 5.496659 1.081366 -0.312638
H 5.208864 2.737120 -0.886314
O 1.655699 0.664766 -0.456487
Br 1.534494 -2.552735 -0.744378
H -2.092756 -1.551551 -2.516074
C -3.164720 -1.705207 -2.403032
N -3.586850 -1.276347 -1.073308
H -3.394059 -2.766643 -2.558549
H -3.704166 -1.116242 -3.150481
C -5.011807 -1.000010 -0.931791
C -2.697417 -1.202911 -0.069327
H -5.278339 -0.095541 -1.491148
H -5.286242 -0.867961 0.112153
H -5.583226 -1.841917 -1.337596
O -1.511567 -1.586374 -0.265890
C 3.617535 -0.023459 0.786185
H 4.406761 -0.677982 0.405658
H 4.076367 0.706745 1.463714
H 2.889768 -0.614565 1.337435
C -3.147312 -0.692368 1.274934
H -3.662843 0.268412 1.189711
H -3.836780 -1.406906 1.740714
H -2.268474 -0.581821 1.908984
C 0.028067 2.802819 1.131851
H 0.629576 3.532828 0.578483
H -0.407437 3.311122 1.997864
H 0.667290 1.993405 1.474889

1FeBr2_cis_4sv
Opt Eel: -1302.321576
SP Eel B3LYP: -7637.60649743
SP Eel M06L: -7563.58042255
SP Eel MN15: -7563.40925979
Gcorr: 0.470549
Fe 0.056567 -0.309684 0.158913
Br 0.475593 -1.862109 2.206077
H 2.070656 1.109926 -2.291119
C 3.088980 0.882362 -2.602596
N 3.543046 -0.322391 -1.916501
H 3.743203 1.733024 -2.374243
H 3.117004 0.704200 -3.683063
C 2.884570 -0.766372 -0.828876
C 4.699446 -0.985273 -2.503709
O 1.995972 -0.044784 -0.316900
H 5.459840 -0.232857 -2.739253
H 5.134238 -1.704708 -1.812166
H 4.422754 -1.500576 -3.432320
H -3.333253 1.599063 0.346611
C -4.289860 1.142088 0.587168
N -4.154316 -0.310574 0.582710
H -5.038848 1.440436 -0.153236
H -4.620044 1.489332 1.575269
C -2.929800 -0.887626 0.591649
C -5.391376 -1.050700 0.797926
O -1.915518 -0.160183 0.502838
H -5.688187 -1.026464 1.855066
H -6.185229 -0.585681 0.205896
H -5.291416 -2.087216 0.480199
H 1.559134 2.384346 -0.255060
C 2.263055 2.957577 0.339666
N 2.157966 2.557635 1.739136
H 2.062203 4.032719 0.246629
H 3.281479 2.763737 -0.012196
C 3.190153 3.107414 2.608579
C 1.152380 1.765936 2.156954
H 4.163467 2.661371 2.369667
H 2.966973 2.928844 3.657924
H 3.258189 4.189311 2.447055
O 0.250568 1.391895 1.370902
Br -0.057169 -2.282930 -1.541108
H -0.576211 3.117606 -0.059680
C -1.085809 3.658489 -0.855405
N -1.860922 2.714190 -1.654842
H -0.346659 4.186005 -1.471975
H -1.772063 4.394862 -0.427549
C -3.030505 3.262864 -2.328117
C -1.426150 1.445991 -1.783778
H -3.762486 3.607663 -1.588757
H -3.499797 2.522382 -2.971755
H -2.731042 4.119350 -2.943906
O -0.308922 1.124506 -1.307975
C -2.288522 0.452819 -2.522980
H -3.320421 0.456006 -2.160500
H -2.306769 0.691204 -3.593686
H -1.850221 -0.535797 -2.389022
C -2.841958 -2.386140 0.711084
H -3.353454 -2.728948 1.617513
H -3.314255 -2.871821 -0.149568
H -1.792980 -2.667805 0.751536
C 3.273277 -2.091209 -0.225886
H 3.361694 -2.873638 -0.983962
H 4.239486 -1.999165 0.287627
H 2.506751 -2.363608 0.498952
C 1.089364 1.384476 3.619057
H 2.021625 0.925544 3.961423
H 0.895048 2.267053 4.240769
H 0.283326 0.662769 3.736403

1FeBr2_trans_1sv
Opt Eel: -438.610280
SP Eel B3LYP: -6773.22990500
SP Eel M06L: -6699.79949145
SP Eel MN15: -6700.55340573
Gcorr: 0.096828
C 4.399801 -0.238942 1.007576
H 4.976640 -1.167822 1.057393
C 2.099595 -0.517851 0.214148
N 3.380738 -0.349099 -0.039778
C 3.886846 -0.240392 -1.411217
H 3.141256 -0.600647 -2.115993
H 4.128743 0.805383 -1.626378
H 4.795148 -0.842851 -1.489824
Fe -0.555418 -0.166722 -0.655600
O 1.265252 -0.573945 -0.774098
H 3.949961 -0.030776 1.975288
H 5.068526 0.584397 0.744556
Br -0.986489 2.022860 0.148834
Br -2.491190 -1.318530 0.149605
C 1.598477 -0.660535 1.622077
H 2.166664 -1.422025 2.163576
H 1.690967 0.289480 2.159100
H 0.546235 -0.950319 1.608267

1FeBr2_trans_3sv
Opt Eel: -1014.444414
SP Eel B3LYP: -7349.49743262
SP Eel M06L: -7275.67087462
SP Eel MN15: -7275.80509056
Gcorr: 0.344530
C 5.395970 -1.264099 -0.302365
H 5.895008 -0.949925 -1.227427
N 4.259359 -0.392399 -0.031956
H 5.083696 -2.300092 -0.411702
H 6.115564 -1.197782 0.520745
C 2.972686 -0.784608 -0.078392
C 4.570343 1.027373 0.107077
O 2.069211 0.081930 0.017671
H 3.827181 1.510050 0.741505
H 5.558722 1.124309 0.562816
H 4.580689 1.525468 -0.870941
Br 0.216510 -1.010226 2.448942
Fe 0.105184 -0.201637 0.028926
Br 0.143314 -0.531754 -2.492095
H -4.734648 0.326758 -0.637767
C -4.504880 -0.122203 0.336702
N -3.861957 -1.423521 0.173369
H -5.436889 -0.260727 0.890071
H -3.847403 0.547599 0.889929
C -2.526801 -1.485401 0.024789
C -4.760141 -2.556158 -0.017521
O -1.860749 -0.420643 0.067383
H -5.319714 -2.442724 -0.954588
H -4.211843 -3.495124 -0.047825
H -5.473753 -2.595024 0.811658
H 1.299646 3.520821 1.068202
C 0.433274 4.155219 1.255998
N -0.604203 3.892043 0.261939
H 0.726094 5.205178 1.182369
H 0.064753 3.959641 2.270899
C -1.460216 5.023052 -0.074716
C -0.792690 2.635299 -0.181340
H -1.906285 5.430737 0.840126
H -2.261942 4.725910 -0.746538
H -0.868132 5.810749 -0.554062
O -0.057071 1.729145 0.289403
C 2.655575 -2.250354 -0.238243
H 2.930961 -2.596940 -1.239717
H 3.186458 -2.858585 0.499765
H 1.585665 -2.406459 -0.103829
C -1.869044 -2.825666 -0.182503
H -2.098423 -3.510375 0.639617
H -2.204804 -3.282480 -1.119140
H -0.788783 -2.695664 -0.234936
C -1.853490 2.371424 -1.217859
H -2.850713 2.519662 -0.789414
H -1.744625 3.052190 -2.067972
H -1.762145 1.345091 -1.562451

1FeBr2_trans_4sv
Opt Eel: -1302.326361
SP Eel B3LYP: -7637.61168208
SP Eel M06L: -7563.58658769
SP Eel MN15: -7563.41393537
Gcorr: 0.470745
C -4.398017 -3.373695 0.282061
H -5.247550 -3.422571 0.972321
N -3.609866 -2.186498 0.578727
H -3.806702 -4.279442 0.404267
H -4.787616 -3.335071 -0.743326
C -2.266250 -2.169455 0.680569
C -4.362276 -0.949135 0.749472
O -1.697402 -1.127486 1.080322
H -3.678076 -0.106100 0.669611
H -5.126659 -0.886316 -0.032736
H -4.862675 -0.928725 1.726625
Br 0.358318 0.763363 2.798618
Fe -0.168000 -0.035292 0.350102
Br -0.889703 -0.836630 -2.105779
H -3.152622 1.181625 -1.601140
C -3.604973 2.162384 -1.452187
N -2.594543 3.082268 -0.937391
H -4.449876 2.073163 -0.755800
H -3.978828 2.549781 -2.404254
C -1.607763 2.595914 -0.151004
C -2.863432 4.502425 -1.117884
O -1.588400 1.371021 0.098059
H -3.687343 4.831755 -0.470152
H -1.980833 5.100133 -0.897069
H -3.149971 4.682125 -2.158665
H 1.200935 -2.948684 -1.475857
C 2.091580 -3.520842 -1.215373
N 2.918207 -2.745744 -0.294954
H 2.675054 -3.729889 -2.117644
H 1.794898 -4.476077 -0.763596
C 2.365100 -1.756484 0.433567
C 4.317150 -3.143160 -0.219353
O 1.124025 -1.583764 0.376427
H 4.379359 -4.220036 -0.024871
H 4.822471 -2.933355 -1.169845
H 4.834585 -2.618280 0.580543
H 2.397007 2.523802 1.227630
C 3.138922 2.956209 0.556951
N 3.305726 2.091893 -0.607079
H 4.100808 3.039131 1.072835
H 2.817600 3.961100 0.255297
C 4.548385 2.267231 -1.346056
C 2.338021 1.212161 -0.936348
H 4.690503 3.331187 -1.566782
H 4.530633 1.721026 -2.286617
H 5.400164 1.921252 -0.747603
O 1.265423 1.224568 -0.289671
C -1.489942 -3.423668 0.366419
H -1.638545 -4.166994 1.160380
H -1.798972 -3.869305 -0.582426

H -0.437113 -3.154554 0.316083
C 3.255784 -0.896494 1.295523
H 3.679750 -1.492239 2.112482
H 4.087232 -0.474194 0.723138
H 2.649839 -0.101869 1.727864
C 2.586241 0.246737 -2.068820
H 2.659446 0.787658 -3.019590
H 3.518496 -0.308270 -1.926222
H 1.740851 -0.436355 -2.129925
C -0.582325 3.548489 0.411207
H -0.022886 4.046850 -0.387556
H -1.069090 4.322253 1.015647
H 0.099147 2.977595 1.036242

1ZnBr2_cis_2sv
Opt Eel: -829.840591
SP Eel B3LYP: -7061.37347213
SP Eel M06L: -6987.74533825
SP Eel MN15: -6988.18640877
Gcorr: 0.219617
C -5.007896 -1.743225 -0.006661
H -5.350666 -2.324906 -0.868902
C -2.742257 -0.756197 0.087746
N -3.551156 -1.817908 0.067599
C -2.985457 -3.166576 0.028993
H -2.040487 -3.190306 0.570477
H -3.694323 -3.851667 0.499087
H -2.815618 -3.483623 -1.006641
C 5.008108 -1.742642 0.005908
Zn -0.000007 0.388698 0.000039
C 2.742241 -0.756090 -0.087628
N 3.551330 -1.817658 -0.067362
C 2.986169 -3.166519 -0.028373
H 5.448564 -2.165697 -0.903419
H 2.819526 -3.484565 1.007477
H 2.039639 -3.190001 -0.567098
H 3.693867 -3.850980 -0.501180
O 1.488850 -0.943695 -0.059572
O -1.488840 -0.943712 0.060386
H 5.346967 -0.716262 0.124301
H 5.351598 -2.325577 0.867001
H -5.346957 -0.716749 -0.123623
H -5.448827 -2.167814 0.901710
Br 0.116640 1.641408 2.081570
Br -0.116874 1.641099 -2.081617
C 3.329492 0.630122 -0.147364
H 3.849729 0.866850 0.787127
H 4.045046 0.723553 -0.969626
H 2.530821 1.357075 -0.292887
C -3.329664 0.629981 0.146678
H -3.849659 0.866224 -0.788070
H -4.045453 0.723743 0.968695
H -2.531103 1.357082 0.292090

1ZnBr2_cis_3sv
Opt Eel: -1117.706338
SP Eel B3LYP: -7349.49614855
SP Eel M06L: -7275.66852842
SP Eel MN15: -7275.80222243
Gcorr: 0.342714
Zn 0.223571 -0.709505 0.052372
Br 1.051478 -0.842333 2.399336
H -2.898337 1.268371 -1.602353
C -2.896721 2.355301 -1.645309
N -1.946306 2.885862 -0.671155
H -3.894062 2.735889 -1.406623
H -2.629086 2.680489 -2.657982
C -0.979487 2.101641 -0.168344
C -2.118923 4.295778 -0.339826
O -0.878814 0.914183 -0.575153
H -2.180210 4.875835 -1.266877
H -3.047918 4.439628 0.224039
H -1.283185 4.669900 0.247015
H 2.277811 2.663460 -1.219890
C 3.330482 2.791782 -0.978104
N 3.899928 1.506162 -0.589510
H 3.434324 3.514766 -0.160498
H 3.864924 3.176817 -1.854084
C 5.351766 1.485430 -0.452925
C 3.113902 0.419577 -0.450465
H 5.836893 1.450493 -1.436767
H 5.681505 0.633778 0.139429
H 5.668359 2.400378 0.057178
O 1.872668 0.521238 -0.598107
Br 0.560720 -2.503888 -1.620418
H -2.856183 -1.979829 -1.425285
C -3.878161 -1.686141 -1.189888
N -3.867560 -0.778896 -0.047716
H -4.472737 -2.581269 -0.966389
H -4.327851 -1.175003 -2.047106
C -5.116596 -0.069624 0.192987
C -2.778710 -0.712281 0.744398
H -5.369867 0.541226 -0.680648
H -5.044885 0.576573 1.064807
H -5.926992 -0.790375 0.357388
O -1.794312 -1.458047 0.531491
C 3.769477 -0.902130 -0.130552
H 4.567024 -1.128638 -0.845867
H 4.206053 -0.885668 0.873228
H 3.016318 -1.686671 -0.174333
C -2.772791 0.263657 1.900048
H -3.042094 1.276924 1.587857
H -3.486945 -0.049633 2.670620
H -1.772086 0.267150 2.333376
C -0.055905 2.657997 0.885772
H 0.579101 3.444713 0.465505
H -0.623104 3.088523 1.716751
H 0.580402 1.858224 1.260284

1ZnBr2_cis_4sv
Opt Eel: -1405.566622
SP Eel B3LYP: -7637.60649743
SP Eel M06L: -7563.58042255
SP Eel MN15: -7563.40925979
Gcorr: 0.468633
Zn 0.142192 -0.402298 0.266903
Br 0.655587 -2.142352 2.160508
H 1.610414 1.190458 -2.247246
C 2.562592 1.049209 -2.755347
N 3.275399 -0.074883 -2.156434
H 3.162167 1.966152 -2.691691
H 2.384435 0.825423 -3.812252
C 2.928602 -0.518373 -0.939732
C 4.287302 -0.707759 -2.992052
O 2.112702 0.131378 -0.236177
H 4.843479 0.071752 -3.521626
H 4.991919 -1.280132 -2.390500
H 3.822680 -1.369970 -3.734112
H -3.444805 1.421312 0.731796
C -4.387439 0.885589 0.804504
N -4.151888 -0.542354 0.618535
H -5.076977 1.246314 0.035060
H -4.838699 1.064583 1.788704
C -2.897039 -1.037971 0.590349
C -5.344581 -1.381769 0.656662
O -1.919159 -0.252254 0.617125
H -5.659348 -1.575892 1.690284
H -6.153604 -0.857164 0.140876
H -5.175505 -2.330488 0.149333
H 1.168051 2.610425 -0.174476
C 1.954249 3.177768 0.315517
N 2.178297 2.651320 1.657359
H 1.682440 4.239404 0.373784
H 2.881292 3.089251 -0.261109
C 3.371804 3.155071 2.325132
C 1.373082 1.704958 2.174049
H 4.273990 2.679556 1.918596
H 3.331315 2.983142 3.399257
H 3.443145 4.233751 2.152593
O 0.335664 1.327004 1.578414
Br 0.066598 -2.087847 -1.756332
H -0.935927 3.066702 0.428696
C -1.558394 3.659716 -0.240611
N -2.243395 2.772311 -1.173671
H -0.931103 4.389037 -0.770134
H -2.311155 4.204444 0.336699
C -3.497754 3.270757 -1.718565
C -1.626641 1.636407 -1.574841
H -4.198792 3.485885 -0.904645
H -3.953087 2.544721 -2.388502
H -3.323328 4.199498 -2.277419
O -0.460263 1.384250 -1.208144
C -2.379662 0.684816 -2.477066
H -3.374799 0.451912 -2.086104
H -2.503050 1.115179 -3.478346
H -1.793894 -0.231954 -2.549847
C -2.723640 -2.534264 0.537417
H -3.286922 -3.016874 1.343343
H -3.086903 -2.931169 -0.416452
H -1.667066 -2.770005 0.638485
C 3.561526 -1.778124 -0.403757
H 3.594491 -2.573285 -1.152687
H 4.587937 -1.576268 -0.071044
H 2.965312 -2.107241 0.448585
C 1.720560 1.127465 3.527967
H 2.757441 0.779468 3.568177
H 1.585509 1.877940 4.316521
H 1.058816 0.281268 3.706137

1ZnBr2_trans_3sv
Opt Eel: -1117.705990
SP Eel B3LYP: -7349.49743262
SP Eel M06L: -7275.67087462
SP Eel MN15: -7275.80509056
Gcorr: 0.343101
C -5.889027 0.426388 -0.081152
H -6.443912 0.930085 0.716832
N -4.516097 0.916455 -0.084368
H -5.927714 -0.646125 0.096781
H -6.379849 0.648073 -1.037629
C -3.432103 0.130825 -0.250874
C -4.380178 2.368172 -0.049966
O -2.292784 0.648157 -0.335169
H -3.328785 2.631763 0.044092
H -4.785784 2.809983 -0.969000
H -4.939695 2.764749 0.803713
Br -0.255166 -1.446001 -2.175487
Zn -0.335482 -0.150200 -0.045559
Br -0.903275 -1.147677 2.175346
H 4.721227 0.649871 0.857176
C 4.430496 0.235180 -0.116781
N 3.944426 -1.134550 0.022482
H 5.305934 0.234178 -0.771826
H 3.649021 0.857815 -0.548354
C 2.627384 -1.352040 0.222383
C 4.971963 -2.161771 0.136421
O 1.839341 -0.379798 0.250525
H 5.540792 -2.032855 1.066351
H 4.535474 -3.158105 0.126935
H 5.664028 -2.076600 -0.707659
H 1.384396 2.323376 -2.131410
C 1.968101 3.161997 -1.755353
N 2.115063 3.046583 -0.306969
H 1.465767 4.100704 -2.019152
H 2.962386 3.155158 -2.210857
C 3.218650 3.804964 0.270556
C 1.238863 2.321699 0.402269
H 4.174299 3.399683 -0.080485
H 3.194996 3.772272 1.357277
H 3.144966 4.850410 -0.049070
O 0.242933 1.805141 -0.174769
C -3.634311 -1.362968 -0.339952
H -4.085948 -1.755112 0.576606
H -4.291935 -1.614741 -1.179125
H -2.668592 -1.839777 -0.492365
C 2.139234 -2.768253 0.408053
H 2.399550 -3.393483 -0.451781
H 2.584334 -3.217442 1.302982
H 1.057509 -2.748711 0.523893
C 1.431902 2.171019 1.890205
H 2.441236 1.831306 2.135225
H 1.259353 3.128768 2.395364
H 0.711347 1.440774 2.259640

1ZnBr2_trans_4sv
Opt Eel: -1405.582349
SP Eel B3LYP: -7637.61168208
SP Eel M06L: -7563.58658769
SP Eel MN15: -7563.41393537
Gcorr: 0.470433
C -1.870146 3.552049 -2.624177
H -2.049985 3.737771 -3.689140
N -1.139173 2.300959 -2.451498
H -1.326097 4.392673 -2.200217
H -2.836365 3.467839 -2.115760
C 0.114882 2.220383 -1.995875
C -1.892964 1.098508 -2.806488
O 0.663511 1.086670 -1.858620
H -1.215676 0.251231 -2.880265
H -2.662516 0.888439 -2.054648
H -2.380216 1.264840 -3.772617
Br 3.846865 1.285643 0.414662
Zn 1.631946 0.451873 -0.197371
Br -4.930800 -0.694859 -0.536707
H 0.920196 -2.214773 -3.018591
C 0.978633 -3.275015 -2.784716
N 1.723429 -3.460182 -1.542689
H 1.485940 -3.804294 -3.599850
H -0.029953 -3.686526 -2.674443
C 2.275593 -2.412908 -0.908018
C 1.906391 -4.849818 -1.137003
O 2.112123 -1.245978 -1.352797
H 2.643628 -5.345207 -1.780751
H 2.229887 -4.920892 -0.100624
H 0.949952 -5.371866 -1.238013
H -1.703535 1.661795 0.084987
C -2.281793 1.735087 1.001035
N -1.380999 1.680748 2.149302
H -2.999215 0.910940 1.047298
H -2.835963 2.682217 1.004169
C -0.053508 1.779440 1.978703
C -2.046520 1.561304 3.439913
O 0.429575 1.940554 0.826990
H -2.751858 2.390968 3.565751
H -2.608433 0.621284 3.477124
H -1.333015 1.583310 4.260227
H 0.571454 -1.450261 3.292977
C -0.430530 -1.863074 3.381280
N -1.072450 -1.878349 2.069926
H -1.019133 -1.257779 4.078051
H -0.372913 -2.886921 3.766877
C -2.357284 -2.573637 2.000218
C -0.450246 -1.390351 0.989399
H -2.210109 -3.647758 1.831065
H -2.991605 -2.160607 1.214643
H -2.868456 -2.439111 2.956667
O 0.675884 -0.825363 1.110749
C 0.880987 3.484085 -1.698177
H 0.936345 4.124138 -2.585165
H 0.407555 4.049503 -0.891669
H 1.889490 3.212558 -1.385393
C 0.858163 1.720648 3.180832
H 0.732851 2.617343 3.799126
H 0.659589 0.848033 3.806968
H 1.886817 1.679085 2.820952
C -1.105671 -1.555186 -0.354844
H -1.244007 -2.620190 -0.573041
H -2.095725 -1.086879 -0.388565
H -0.471304 -1.116292 -1.121797
C 3.102578 -2.663797 0.329991
H 2.495808 -3.093939 1.132497
H 3.924039 -3.356218 0.117359
H 3.516104 -1.713718 0.668189

2FeBr_1sv
Opt Eel: -425.227211
SP Eel B3LYP: -6773.22990500
SP Eel M06L: -6699.79949145
SP Eel MN15: -6700.55340573
Gcorr: 0.097356
C 4.513667 0.617448 0.014403
Fe -0.848208 -0.307052 -0.012816
C 2.063584 0.340844 0.003615
N 3.287766 -0.177260 -0.017899
C 3.482057 -1.628025 -0.010148
H 5.067793 0.474363 -0.919129
H 3.606675 -1.987960 1.017496
H 2.625465 -2.122474 -0.465283
H 4.384772 -1.858467 -0.580309
O 1.062764 -0.446366 0.042587
H 4.297389 1.674607 0.146879

H 5.134273 0.276447 0.849327
Br -3.187832 0.078249 0.004136
C 1.866892 1.832807 -0.013597
H 2.263919 2.284578 0.902097
H 2.375239 2.290737 -0.867710
H 0.798342 2.046119 -0.075945

2FeBr_2sv
Opt Eel: -713.086183
SP Eel B3LYP: -4455.13760489
SP Eel M06L: -4413.62117313
SP Eel MN15: -4413.62677952
Gcorr: 0.221785
C 2.757631 2.618564 0.147066
H 2.651678 3.662907 -0.172366
C 1.002641 1.277458 -0.940195
N 1.466028 1.933702 0.140160
C 0.638029 2.198044 1.311966
H 0.526136 3.282070 1.436444
H -0.346929 1.742935 1.188940
H 1.110803 1.785893 2.208488
Fe -1.227828 -0.330494 0.320052
O -0.095309 0.663900 -0.966465
H 3.475496 2.114528 -0.498319
H 3.147136 2.604710 1.168311
Br -3.581114 -0.019450 -0.117896
O 0.363467 -1.127509 1.167850
C 1.597051 -1.223878 0.918398
N 2.066316 -1.691067 -0.248248
C 3.497066 -1.829435 -0.516431
C 1.190096 -2.276452 -1.257974
H 3.863818 -2.811587 -0.193824
H 4.068221 -1.048364 -0.016331
H 3.654233 -1.735128 -1.593266
H 0.147141 -2.113170 -0.988141
H 1.387956 -1.812626 -2.228320
H 1.387667 -3.352705 -1.330636
C 2.583245 -0.815617 1.984254
H 3.161647 0.058698 1.667348
H 2.027980 -0.561290 2.887504
H 3.290477 -1.621088 2.207141
C 1.845904 1.270080 -2.192096
H 2.141896 2.280870 -2.489961
H 2.759354 0.684484 -2.039319
H 1.266166 0.810305 -2.993059

2FeBr_3sv
Opt Eel: -1000.979179
SP Eel B3LYP: -7349.49614855
SP Eel M06L: -7275.66852842
SP Eel MN15: -7275.80222243
Gcorr: 0.344152
C -4.093914 -0.588409 -1.707340
H -4.845761 -0.856130 -0.957455
N -2.932364 -0.026093 -1.032445
H -3.832485 -1.484055 -2.267229
H -4.536239 0.144917 -2.394171
C -1.652738 -0.325544 -1.345559
C -3.227108 1.028137 -0.068720
O -0.709548 0.257506 -0.764516
H -2.300866 1.371947 0.384444
H -3.721376 1.868704 -0.571947
H -3.900372 0.643300 0.705014
Fe 1.260630 -0.159428 -0.229759
Br 3.758761 -0.684948 -0.248603
H 0.758918 2.002510 2.192040
C 0.033596 2.812984 2.206993
N -0.307721 3.185252 0.839455
H 0.459320 3.673801 2.738569
H -0.870262 2.491655 2.734257
C 0.418090 2.720816 -0.198196
C -1.362662 4.183320 0.717157
O 1.379946 1.934212 -0.017406
H -1.004978 5.165983 1.050819
H -1.714742 4.264312 -0.308901
H -2.206306 3.889898 1.350050
H 0.043720 -0.355695 1.869558
C -0.888037 -0.735329 2.292308
N -1.318946 -1.917450 1.558444
H -1.654319 0.041602 2.229212
H -0.730857 -0.990465 3.349116
C -2.586283 -2.484863 2.004347
C -0.501256 -2.543827 0.680738
H -2.460804 -3.073024 2.923293
H -3.030960 -3.115050 1.235309
H -3.277535 -1.663188 2.212823
O 0.583561 -2.053812 0.291248
C 0.062824 3.181733 -1.592758
H -0.965470 2.910488 -1.850197
H 0.163474 4.268262 -1.693607
H 0.741220 2.693460 -2.293246
C -1.381232 -1.350255 -2.420867
H -1.813159 -2.325346 -2.178220
H -1.803696 -1.027315 -3.379198
H -0.300490 -1.457357 -2.522333
C -0.919445 -3.902786 0.164258
H -1.091000 -4.606192 0.986492
H -1.843988 -3.845690 -0.419788
H -0.123472 -4.284098 -0.476814

3FeBr2_cis_2sv
Opt Eel: -726.597436
SP Eel B3LYP: -7061.37347213
SP Eel M06L: -6987.74533825
SP Eel MN15: -6988.18640877
Gcorr: 0.219605
C -5.406861 0.160308 -0.006998
H -5.977438 0.965458 -0.481631
C -2.934810 0.146951 -0.005903
N -4.099950 0.056966 -0.650333
C -4.110691 -0.067506 -2.108084
H -3.295373 -0.714356 -2.434107
H -5.064542 -0.504888 -2.408742
H -4.000829 0.914349 -2.583027
C 5.406827 -0.159841 -0.006911
Fe -0.000014 -0.000058 -0.213645
C 2.934792 -0.146981 -0.005956
N 4.099939 -0.056944 -0.650363
C 4.110806 0.067818 -2.108084
H 5.954664 0.780814 -0.127868
H 4.001981 -0.914061 -2.583219
H 3.294921 0.713939 -2.434111
H 5.064290 0.506176 -2.408505
O 1.867681 -0.155237 -0.688976
O -1.867716 0.155154 -0.688949
H 5.309014 -0.383177 1.052823
H 5.978118 -0.964023 -0.482307
H -5.309036 0.382413 1.052993
H -5.955425 -0.779775 -0.129044
Br -0.224284 -2.364658 0.512885
Br 0.224277 2.364510 0.512990
C 2.904188 -0.242847 1.496072
H 3.331917 -1.196300 1.824840
H 3.476231 0.567667 1.956931
H 1.871963 -0.189514 1.839441
C -2.904171 0.242827 1.496126
H -3.331707 1.196377 1.824867
H -3.476348 -0.567561 1.957031
H -1.871951 0.189301 1.839480

3FeBr2_cis_3sv
Opt Eel: -1014.481309
SP Eel B3LYP: -7349.49614855
SP Eel M06L: -7275.66852842
SP Eel MN15: -7275.80222243
Gcorr: 0.343888
C -5.693175 0.487988 0.360024
H -6.026465 0.759778 1.367562
N -4.315483 0.924229 0.161549
H -5.789616 -0.587638 0.233056
H -6.341803 0.986417 -0.369413
C -3.297701 0.107238 -0.141312
C -4.097715 2.368500 0.198183
O -2.182388 0.617271 -0.443107
H -3.082459 2.579936 0.532650
H -4.248127 2.812405 -0.793612
H -4.814230 2.809408 0.895357
Br -0.367682 -1.626027 -2.281857
Fe -0.345193 -0.081678 -0.203972
Br -0.822829 -0.598854 2.284023
H 3.432666 0.765864 0.939982
C 4.167462 -0.001075 0.700596
N 3.549154 -1.322639 0.780765
H 4.991124 0.041723 1.417729
H 4.563639 0.184880 -0.304905
C 2.247282 -1.468248 0.484426
C 4.449594 -2.424435 1.099528
O 1.600992 -0.457425 0.104276
H 4.811401 -2.330580 2.129888
H 3.954123 -3.385505 0.982307
H 5.311063 -2.393958 0.422975
H 0.919941 2.738768 1.450243
C 1.685873 3.429076 1.099781
N 2.244085 2.947017 -0.160249
H 2.491054 3.492585 1.837124
H 1.244980 4.425622 0.972952
C 3.563145 3.466832 -0.500436
C 1.524926 2.130289 -0.943507
H 3.543881 4.561328 -0.451910
H 3.856082 3.169779 -1.504845
H 4.307591 3.098967 0.214723
O 0.336291 1.843395 -0.633824
C -3.515739 -1.383165 -0.143238
H -3.948682 -1.726248 0.800273
H -4.194319 -1.663620 -0.957191
H -2.561365 -1.879866 -0.307075
C 1.608172 -2.825721 0.612609
H 1.997793 -3.503440 -0.154939
H 1.806624 -3.264682 1.594549
H 0.534602 -2.725077 0.474030
C 2.135543 1.583163 -2.209628
H 2.226369 2.375670 -2.962377
H 3.129088 1.162417 -2.035823
H 1.478490 0.800691 -2.591224

3FeBr2_cis_4sv
Opt Eel: -1302.346025
SP Eel B3LYP: -7637.60649743
SP Eel M06L: -7563.58042255
SP Eel MN15: -7563.40925979
Gcorr: 0.468764
Fe 0.114268 -0.300850 0.223622
Br 0.640429 -2.067800 2.260134
H 1.682362 1.097572 -2.309807
C 2.640846 0.896033 -2.784132
N 3.286689 -0.232290 -2.119296
H 3.278802 1.787065 -2.735848
H 2.484271 0.637446 -3.836418
C 2.861088 -0.639784 -0.918764
C 4.327064 -0.911549 -2.882041
O 2.029342 0.064408 -0.280098
H 4.925168 -0.159261 -3.404657
H 4.987339 -1.479174 -2.227784
H 3.885126 -1.586145 -3.626177
H -3.415240 1.405982 0.689811
C -4.349563 0.861071 0.792666
N -4.098789 -0.570912 0.662245
H -5.051302 1.181923 0.016603
H -4.793993 1.071596 1.773499
C -2.842448 -1.054597 0.615890
C -5.281221 -1.419587 0.764849
O -1.876835 -0.249034 0.583172
H -5.585079 -1.544924 1.812054
H -6.100116 -0.940790 0.220618
H -5.103474 -2.398794 0.323457
H 1.222654 2.598172 -0.266987
C 2.026663 3.155324 0.205285
N 2.241367 2.663562 1.562161
H 1.784068 4.225283 0.233913
H 2.948909 3.025278 -0.370743
C 3.442416 3.169157 2.216060
C 1.401005 1.774789 2.120273
H 4.337074 2.672892 1.818643
H 3.402276 3.023250 3.293872
H 3.526307 4.242577 2.017674
O 0.350698 1.406338 1.537070
Br 0.004021 -2.134923 -1.742068
H -0.888741 3.093685 0.362949
C -1.525422 3.677746 -0.300811
N -2.229140 2.779167 -1.210069
H -0.910825 4.400936 -0.852938
H -2.267154 4.228255 0.284907
C -3.497513 3.269458 -1.730750
C -1.622007 1.641776 -1.612644
H -4.183678 3.479444 -0.903084
H -3.960005 2.540990 -2.392983
H -3.337905 4.199403 -2.291432
O -0.446239 1.393235 -1.263043
C -2.385043 0.679739 -2.493199
H -3.378658 0.457059 -2.092891
H -2.512602 1.095543 -3.500164
H -1.803772 -0.241151 -2.553908
C -2.646296 -2.546649 0.618353
H -3.172171 -3.000881 1.465079
H -3.038255 -2.987562 -0.304231
H -1.582906 -2.759997 0.689662
C 3.427841 -1.897078 -0.316415
H 3.465888 -2.714774 -1.040387
H 4.447125 -1.712850 0.047730
H 2.791520 -2.180185 0.523259
C 1.717197 1.248129 3.501421
H 2.748062 0.889146 3.576949
H 1.576444 2.032957 4.254977
H 1.041533 0.417285 3.699978

3FeBr2_trans_1sv
Opt Eel: -438.697767
SP Eel B3LYP: -6773.22990500
SP Eel M06L: -6699.79949145
SP Eel MN15: -6700.55340573
Gcorr: 0.095111
C 4.560792 -0.195406 0.703331
H 5.021809 -1.175591 0.863723
C 2.137272 -0.242652 0.292978
N 3.380292 -0.335475 -0.150964
C 3.657933 -0.552144 -1.573489
H 2.812332 -1.043976 -2.050319
H 3.850879 0.407013 -2.066254
H 4.545753 -1.182738 -1.656751
Fe -0.713453 -0.019228 -0.339129
O 1.175841 -0.316063 -0.553988
H 4.305655 0.251728 1.661372
H 5.276368 0.455250 0.193591
Br -1.260353 2.297059 -0.003244
Br -2.137879 -1.899652 0.114845
C 1.855790 -0.052101 1.756481
H 2.440893 -0.739608 2.372233
H 2.099100 0.973921 2.055748
H 0.795648 -0.224669 1.950790

3FeBr2_trans_3sv
Opt Eel: -1014.481045
SP Eel B3LYP: -7349.49743262
SP Eel M06L: -7275.67087462
SP Eel MN15: -7275.80509056
Gcorr: 0.343289
C -5.760461 0.332008 -0.269746
H -6.295055 0.520155 0.669596
N -4.399369 0.850818 -0.187821
H -5.762642 -0.737386 -0.468360
H -6.291052 0.839346 -1.081282
C -3.305748 0.082397 -0.066559
C -4.269854 2.300241 -0.049653
O -2.196682 0.647973 0.133284
H -3.363012 2.642665 -0.549185
H -5.140912 2.771316 -0.509140
H -4.223208 2.591267 1.007030
Br -0.518383 -0.720546 -2.373893
Fe -0.348487 -0.055356 0.111809
Br -0.618910 -1.346624 2.325657
H 4.473357 0.132679 0.719113
C 4.215330 -0.114623 -0.317897
N 3.580387 -1.428077 -0.401419
H 5.130210 -0.132174 -0.914725
H 3.539080 0.646087 -0.704657
C 2.257018 -1.534002 -0.192372
C 4.482962 -2.563195 -0.552863
O 1.607163 -0.491009 0.077249
H 5.167371 -2.612395 0.302853
H 3.932967 -3.499380 -0.614100
H 5.074985 -2.441273 -1.466011

H 1.218350 2.358681 -1.761349
C 1.905715 3.135347 -1.427628
N 2.293384 2.886683 -0.041539
H 1.421987 4.114913 -1.527960
H 2.805846 3.122840 -2.047912
C 3.574432 3.449971 0.367458
C 1.455652 2.231516 0.774080
H 4.391473 2.954039 -0.168559
H 3.729503 3.336838 1.437935
H 3.593994 4.517926 0.123458
O 0.304723 1.911705 0.369839
C -3.438433 -1.414392 -0.168045
H -4.085910 -1.795877 0.628431
H -3.868516 -1.704563 -1.131511
H -2.456651 -1.870680 -0.064832
C 1.598485 -2.885382 -0.284250
H 1.815930 -3.365736 -1.242700
H 1.955341 -3.539149 0.519107
H 0.522958 -2.762515 -0.182033
C 1.884207 1.901745 2.182336
H 2.876101 1.443276 2.212155
H 1.908636 2.808954 2.798044
H 1.156504 1.205222 2.601090

4FeBr_1sv
Opt Eel: -425.218689
SP Eel B3LYP: -6773.22990500
SP Eel M06L: -6699.79949145
SP Eel MN15: -6700.55340573
Gcorr: 0.096360
C -4.475154 0.716093 -0.035685
Fe 0.808234 -0.175339 0.058367
C -2.054690 0.252824 -0.010035
N -3.316113 -0.173951 -0.017122
C -3.632634 -1.601220 0.002776
H -4.953866 0.730488 0.949913
H -3.983607 -1.920506 -0.984927
H -2.750018 -2.173902 0.279503
H -4.428069 -1.773375 0.733750
O -1.102226 -0.593721 -0.038231
H -4.193433 1.728502 -0.316161
H -5.192439 0.337985 -0.770190
Br 3.231608 0.019824 -0.027380
C -1.762255 1.730980 0.024510
H -2.063110 2.206713 -0.915583
H -2.291493 2.227277 0.843349
H -0.685325 1.877147 0.157426

4FeBr_2sv
Opt Eel: -713.147798
SP Eel B3LYP: -4455.13760489
SP Eel M06L: -4413.62117313
SP Eel MN15: -4413.62677952
Gcorr: 0.219147
C 3.123555 2.409906 0.273262
H 3.198053 3.454012 -0.055765
C 1.361810 1.232758 -0.994126
N 1.763612 1.905805 0.101304
C 0.825749 2.335220 1.131636
H 0.838628 3.429431 1.200348
H -0.184898 2.008561 0.885642
H 1.114342 1.916500 2.100692
Fe -1.322520 -0.084171 0.023545
O 0.188616 0.811144 -1.140179
H 3.842738 1.807122 -0.278510
H 3.378631 2.361456 1.335336
Br -3.723789 0.014483 -0.017386
O 0.213377 -0.945216 1.159123
C 1.424592 -1.238323 0.999547
N 1.883396 -1.858128 -0.103340
C 3.291286 -2.200854 -0.292252
C 0.983468 -2.378097 -1.126030
H 3.505074 -3.208476 0.085466
H 3.942073 -1.483470 0.205890
H 3.511222 -2.176110 -1.362523
H -0.053583 -2.189690 -0.847839
H 1.190834 -1.901108 -2.088763
H 1.136413 -3.459118 -1.224544
C 2.411504 -0.892926 2.089772
H 3.124581 -0.135710 1.747720
H 1.857687 -0.495299 2.940680
H 2.983662 -1.770741 2.407257
C 2.367869 0.984390 -2.094055
H 2.820489 1.918905 -2.441777
H 3.175513 0.329509 -1.751541
H 1.852669 0.502165 -2.925261

4FeBr_3sv
Opt Eel: -1001.015664
SP Eel B3LYP: -7349.49614855
SP Eel M06L: -7275.66852842
SP Eel MN15: -7275.80222243
Gcorr: 0.342867
C -3.865159 -0.967263 -1.903803
H -4.556005 -1.265801 -1.107938
N -2.717419 -0.293050 -1.313154
H -3.562487 -1.856707 -2.452499
H -4.396539 -0.292298 -2.587133
C -1.432559 -0.554215 -1.635881
C -3.040036 0.810991 -0.416600
O -0.503876 0.127667 -1.143758
H -2.127304 1.191468 0.035184
H -3.534994 1.617239 -0.973049
H -3.721333 0.458127 0.364277
Fe 1.328086 -0.276832 -0.179185
Br 3.785362 -0.967127 -0.100724
H 0.690444 2.387916 2.217031
C -0.054798 3.160730 2.043249
N -0.287613 3.295792 0.610582
H 0.303336 4.112847 2.456142
H -0.988936 2.893812 2.546879
C 0.528734 2.686087 -0.278882
C -1.310369 4.266252 0.241731
O 1.429071 1.901139 0.098412
H -0.954794 5.292336 0.404181
H -1.605501 4.152589 -0.799508
H -2.192773 4.103306 0.868729
H -0.116602 0.096870 1.886194
C -1.008964 -0.189131 2.443437
N -1.613842 -1.366314 1.837766
H -1.726714 0.634707 2.426218
H -0.728339 -0.389290 3.486997
C -2.929186 -1.727658 2.353888
C -0.890043 -2.183709 1.035756
H -2.850310 -2.260134 3.311486
H -3.474567 -2.350066 1.645604
H -3.503314 -0.811635 2.515794
O 0.279192 -1.912121 0.679157
C 0.339776 2.992897 -1.747427
H -0.657231 2.703136 -2.090496
H 0.472614 4.062343 -1.946913
H 1.081911 2.427314 -2.311177
C -1.128161 -1.670660 -2.606375
H -1.501242 -2.634760 -2.248394
H -1.581696 -1.477086 -3.585081
H -0.044410 -1.731834 -2.719777
C -1.536223 -3.464627 0.558270
H -1.841789 -4.098439 1.398146
H -2.427617 -3.259810 -0.044922
H -0.812785 -4.005700 -0.052826

5FeBr2_cis_2sv
Opt Eel: -726.641610
SP Eel B3LYP: -7061.37347213
SP Eel M06L: -6987.74533825
SP Eel MN15: -6988.18640877
Gcorr: 0.217435
C 5.138040 -1.564372 -0.128781
H 5.581663 -2.254399 0.594337
C 2.820215 -0.722425 -0.148218
N 3.686430 -1.734209 -0.095054
C 3.219933 -3.114990 0.021467
H 2.176227 -3.181009 -0.279411
H 3.831443 -3.745884 -0.629476
H 3.325186 -3.463141 1.055374
C -5.138031 -1.564329 0.128828
Fe 0.000002 0.306922 -0.000007
C -2.820197 -0.722439 0.148229
N -3.686428 -1.734209 0.095050
C -3.219969 -3.115002 -0.021479
H -5.527393 -1.799325 1.125952
H -3.325359 -3.463184 -1.055361
H -2.176227 -3.181027 0.279270
H -3.831407 -3.745866 0.629561
O -1.577035 -0.958782 0.040219
O 1.577053 -0.958761 -0.040185
H -5.423325 -0.550556 -0.144852
H -5.581704 -2.254407 -0.594210
H 5.423356 -0.550586 0.144819
H 5.527436 -1.799472 -1.125867
Br -0.282933 1.599590 -2.115024
Br 0.282928 1.599612 2.115005
C -3.326948 0.684444 0.328084
H -3.760090 1.051891 -0.609105
H -4.090833 0.745304 1.107613
H -2.494396 1.334785 0.600954
C 3.326962 0.684462 -0.328065
H 3.760094 1.051906 0.609130
H 4.090847 0.745337 -1.107592
H 2.494405 1.334797 -0.600933

5FeBr2_cis_3sv
Opt Eel: -1014.517348
SP Eel B3LYP: -7349.49614855
SP Eel M06L: -7275.66852842
SP Eel MN15: -7275.80222243
Gcorr: 0.341848
Fe -0.018727 -0.923956 -0.018935
Br 0.304584 -1.920388 2.322416
H -2.177390 2.346812 -0.535237
C -1.790433 3.343485 -0.339772
N -0.642302 3.244004 0.553741
H -2.573281 3.957620 0.121710
H -1.485947 3.815827 -1.280368
C -0.282228 2.050713 1.069247
C -0.008816 4.512585 0.888231
O -0.917919 1.011792 0.774797
H 0.201656 5.062141 -0.035368
H -0.678649 5.121522 1.508298
H 0.926693 4.361260 1.422054
H 2.523769 2.807048 -2.655891
C 2.339731 2.808229 -1.575212
N 3.140386 1.772823 -0.924587
H 1.283138 2.632501 -1.386056
H 2.629063 3.782119 -1.169718
C 4.557417 2.088013 -0.768336
C 2.575532 0.635995 -0.500401
H 4.927731 2.511136 -1.707002
H 5.138162 1.196885 -0.539751
H 4.696366 2.827365 0.029133
O 1.348276 0.434794 -0.720808
Br 0.964884 -2.786872 -1.582132
H -2.145308 0.320269 -2.483402
C -3.222941 0.465973 -2.429047
N -3.688498 0.230582 -1.064111
H -3.716234 -0.220837 -3.127127
H -3.469826 1.493186 -2.709856
C -4.954615 0.867152 -0.713906
C -2.980990 -0.539578 -0.231847
H -4.813442 1.946911 -0.587858
H -5.365872 0.448062 0.201932
H -5.670473 0.698801 -1.524365
O -1.949845 -1.141374 -0.653513
C 3.406868 -0.371239 0.249461
H 4.151268 -0.824559 -0.414213
H 3.935264 0.097912 1.085056
H 2.756756 -1.159214 0.628991
C -3.436868 -0.721915 1.192047
H -3.668664 0.233648 1.668995
H -4.335532 -1.349687 1.225882
H -2.636852 -1.214941 1.745690
C 0.892247 1.992536 2.018917
H 1.807830 2.375597 1.558039
H 0.695495 2.591798 2.915031
H 1.039127 0.952512 2.312385

5FeBr2_cis_4sv
Opt Eel: -1302.388059
SP Eel B3LYP: -7637.60649743
SP Eel M06L: -7563.58042255
SP Eel MN15: -7563.40925979
Gcorr: 0.466360
Fe 0.108547 -0.312425 0.263039
Br 0.579361 -1.993150 2.333626
H 1.650435 0.987739 -2.342055
C 2.595162 0.768466 -2.835999
N 3.259313 -0.338545 -2.153950
H 3.235117 1.659533 -2.835512
H 2.407837 0.475725 -3.874074
C 2.887289 -0.687445 -0.918226
C 4.269678 -1.048286 -2.928556
O 2.075948 0.033188 -0.273667
H 4.880735 -0.315072 -3.463986
H 4.923033 -1.631473 -2.281682
H 3.798240 -1.713198 -3.663016
H -3.408329 1.522101 0.659745
C -4.367194 1.020382 0.759191
N -4.176023 -0.424005 0.670918
H -5.040187 1.348892 -0.038630
H -4.819529 1.276751 1.725293
C -2.941120 -0.959775 0.673398
C -5.397127 -1.218546 0.750956
O -1.936040 -0.204674 0.657299
H -5.747269 -1.294913 1.788262
H -6.172337 -0.724759 0.158123
H -5.244043 -2.218805 0.349594
H 1.321850 2.589861 -0.327365
C 2.139015 3.143946 0.125689
N 2.342644 2.689700 1.497005
H 1.920442 4.219587 0.117083
H 3.056912 2.972862 -0.446660
C 3.571240 3.156950 2.126562
C 1.465575 1.854898 2.085834
H 4.438215 2.597633 1.751601
H 3.525846 3.060783 3.209945
H 3.711968 4.214994 1.882842
O 0.399644 1.519775 1.515664
Br -0.008310 -2.266499 -1.662439
H -0.802004 3.135434 0.207959
C -1.424982 3.693768 -0.490042
N -2.149772 2.758947 -1.345133
H -0.794257 4.367767 -1.084496
H -2.153581 4.295744 0.060678
C -3.397209 3.253804 -1.910454
C -1.583576 1.573591 -1.653677
H -4.087731 3.529243 -1.105946
H -3.871380 2.503191 -2.538904
H -3.202163 4.145946 -2.518898
O -0.420487 1.311279 -1.269577
C -2.371082 0.576635 -2.471199
H -3.375015 0.416094 -2.066965
H -2.476778 0.925510 -3.505742
H -1.819618 -0.364673 -2.464276
C -2.802893 -2.459396 0.704519
H -3.365521 -2.883006 1.543429
H -3.186605 -2.900835 -0.221283
H -1.749146 -2.710082 0.805487
C 3.478218 -1.914825 -0.275836
H 3.485120 -2.768908 -0.957340
H 4.510481 -1.718226 0.041212
H 2.870143 -2.152620 0.598554
C 1.772317 1.349633 3.477491
H 2.783604 0.937586 3.549118
H 1.684861 2.160207 4.211532
H 1.056117 0.562120 3.708285

5FeBr2_trans_1sv
Opt Eel: -438.746567
SP Eel B3LYP: -6773.22990500
SP Eel M06L: -6699.79949145
SP Eel MN15: -6700.55340573
Gcorr: 0.094291
C 4.724406 -0.040389 0.405016
H 5.179901 -0.917585 0.876383
C 2.270852 -0.116429 0.340107
N 3.442708 -0.408246 -0.199561
C 3.534359 -1.121795 -1.475750
H 2.604729 -1.650009 -1.677194
H 3.737343 -0.411036 -2.283961
H 4.358555 -1.836251 -1.411205
Fe -0.680953 -0.050830 -0.092788

O 1.201275 -0.435402 -0.290630
H 4.600460 0.751071 1.140783
H 5.384010 0.319982 -0.388470
Br -1.338897 2.264876 -0.210585
Br -2.223471 -1.883934 0.159878
C 2.190175 0.577793 1.670555
H 2.843213 0.106990 2.410142
H 2.489306 1.627228 1.566943
H 1.162226 0.544060 2.036195

5FeBr2_trans_3sv
Opt Eel: -1014.513687
SP Eel B3LYP: -7349.49743262
SP Eel M06L: -7275.67087462
SP Eel MN15: -7275.80509056
Gcorr: 0.341000
C 4.677139 -1.682154 -1.804743
O 0.112260 1.392121 1.646660
C 1.879781 -2.330529 -1.405868
H 1.699083 -1.951146 -2.417002
H 2.467394 -3.250060 -1.475758
H 0.918873 -2.564323 -0.945606
C -2.382157 -1.937478 -1.359769
H -3.137648 -2.721806 -1.456026
H -2.109514 -1.584807 -2.360000
H -1.494894 -2.362496 -0.888042
C -1.468238 3.101429 1.054685
H -1.692978 3.846954 1.826859
H -1.608233 3.568819 0.076122
H -2.158264 2.264211 1.152697

5FeBr2_trans_4sv
Opt Eel: -1302.387224
SP Eel B3LYP: -7637.61168208
SP Eel M06L: -7563.58658769
SP Eel MN15: -7563.41393537
Gcorr: 0.465880
C -5.091020 -1.254514 1.514581
H -5.487943 -1.248399 2.537741
N -3.759479 -0.665457 1.490028
H -5.080597 -2.278213 1.147966
H -5.760648 -0.661908 0.881838
C -2.624136 -1.355433 1.260391
C -3.705507 0.742009 1.868194
O -1.509024 -0.791118 1.335309
H 5.300584 -0.917573 -2.277944
N 3.875733 -1.047827 -0.761795
H 4.045834 -2.129214 -2.569981
H 5.330017 -2.450890 -1.374918
C 2.572423 -1.282638 -0.573545
C 4.584880 -0.081833 0.074667
O 1.941293 -0.632438 0.305744
H 4.058798 0.048252 1.018632
H 5.592521 -0.460888 0.266658
H 4.661291 0.885331 -0.435567
Br -0.253057 -2.492591 2.042394
Fe -0.076804 -0.334049 0.518229
Br 0.023715 0.949417 -1.898256
H -4.462079 1.740550 -0.345606
C -4.608622 0.771178 0.145130
N -4.105265 -0.312349 -0.696687
H -5.677953 0.615815 0.311039
H -2.686294 1.113510 1.768760
H -4.380015 1.317672 1.226621
H -4.036222 0.858023 2.908808
Br -0.001674 2.313664 1.632456
Fe 0.013764 -0.011909 0.042312
Br -0.013571 -2.332393 -1.558432
H -2.605493 -1.091598 -1.780004
C -3.607974 -0.705314 -1.959018
N -3.673045 0.704552 -1.588701
H -4.339875 -1.268802 -1.371989
H -3.857480 -0.816513 -3.022077
C -2.562204 1.371497 -1.231439
C -4.983706 1.320014 -1.750889
O -1.452161 0.787222 -1.193850
H -5.728646 0.726955 -1.210059
H -4.997676 2.335820 -1.363121
H -5.260958 1.340285 -2.812194
H 2.072398 -3.001908 0.327398
C 3.033882 -3.152660 0.817394
N 3.545475 -1.873505 1.301341
H 3.749477 -3.568942 0.100815
H 2.923785 -3.858477 1.650449
C 2.729286 -0.812653 1.407307
C 4.967821 -1.846092 1.618848
O 1.499233 -0.942503 1.180542
H 5.217703 -2.737527 2.203248
H 5.565741 -1.854241 0.699094
H 5.226098 -0.967005 2.205759
H -4.088388 0.769607 1.101550
C -2.865876 -0.783571 -0.520393
C -5.017717 -0.781824 -1.735749
O -2.119327 -0.261815 0.353701
H -5.491381 0.087329 -2.201980
H -4.485223 -1.334376 -2.507272
H -5.799108 -1.418288 -1.304146
H 2.291069 1.728928 0.841011
C 2.330338 2.809643 0.954300
N 0.974936 3.353875 0.934289
H 2.890555 3.243627 0.121288
H 2.836715 3.068755 1.892489
C 0.854587 4.746793 0.520434
C -0.067236 2.569374 1.217418
H 1.634977 5.330013 1.018546
H -0.113620 5.158350 0.799879
H 0.987958 4.836538 -0.564601
H 2.135716 2.984599 -0.327475
C 3.081267 3.142713 -0.846269
N 3.584232 1.866832 -1.344014
H 3.815413 3.566352 -0.152630
H 2.937074 3.849567 -1.673789
C 4.994804 1.844164 -1.705798
C 2.760063 0.802534 -1.424623
H 5.220213 2.719184 -2.325084
H 5.243611 0.949892 -2.273806
H 5.623931 1.884929 -0.807546
O 1.542769 0.930382 -1.164603
C -2.712633 -2.832593 0.954304
H -3.112685 -3.381849 1.814688
H -3.359740 -3.031836 0.095237
H -1.709147 -3.183774 0.718378
C 3.305287 0.519560 1.820378
H 3.628691 0.481560 2.867722
H 4.172238 0.793579 1.212694
H 2.523059 1.272783 1.723342
C 3.331131 -0.533239 -1.841773
H 3.635393 -0.502633 -2.895064
H 4.209065 -0.806227 -1.249051
H 2.549583 -1.285157 -1.726785
C -2.650150 2.846556 -0.922640
H -2.929202 3.409316 -1.821196
H -3.391863 3.058046 -0.147195
H -1.673057 3.169978 -0.565902

Structure coordinate of iodine study:

01withI
Opt Eel: -724.679006
SP Eel B3LYP: -11568.9869769
SP Eel M06L: -4711.64337079
SP Eel MN15: -4710.78424778
Gcorr: 0.217264
C 5.347482 0.994209 -0.954490
H 5.617536 0.797793 -1.998346
C 2.962855 0.535315 -0.556781
N 3.942079 1.387503 -0.852629
C 3.662870 2.797083 -1.123365
H 2.593376 2.943333 -1.258087
H 4.016685 3.414740 -0.290592
H 4.193572 3.090867 -2.033912
C -4.865658 2.132748 -0.216655
Fe 0.124383 -0.012133 0.230944
C -2.578575 1.309813 0.196089
N -3.420029 2.127148 -0.433879
C -2.936223 3.086425 -1.426404
H -5.360427 2.206285 -1.189296
H -3.457126 4.036148 -1.276965
H -1.864491 3.233105 -1.310192
H -3.148747 2.719297 -2.436833
O -1.340160 1.345454 -0.092856
O 1.770776 0.963413 -0.438144
H -5.195661 1.217271 0.269563
H -5.153907 2.996896 0.392341
H 5.554050 0.112228 -0.350524
H 5.960311 1.818406 -0.580956
Br 0.654564 -0.349434 2.667264
I -0.906670 -2.213503 -1.102048
C 3.280707 -0.923645 -0.363661
H 3.951836 -1.299190 -1.140368
H 3.759895 -1.079841 0.609569
H 2.355598 -1.503149 -0.391555
C -3.097405 0.358782 1.241859
H -3.755851 0.863635 1.954215
H -3.659152 -0.455266 0.770516
H -2.253287 -0.069117 1.785192

04withI
Opt Eel: -825.921094
SP Eel B3LYP: -16599.7349666
SP Eel M06L: -2951.12522244
SP Eel MN15: -2949.15609755
Gcorr: 0.217653
C -5.046201 1.759215 -0.839991
H -5.515280 2.584909 -0.297573
C -2.744740 0.911781 -0.567054
N -3.595793 1.921191 -0.763071
C -3.112808 3.290724 -0.931211
H -2.039278 3.284889 -1.106524
H -3.623655 3.743116 -1.786498
H -3.335019 3.879389 -0.034020
C 4.872310 2.223484 0.070440
Zn -0.011509 -0.136553 -0.023996
C 2.626372 1.201231 0.135233
N 3.419589 2.250728 -0.088799
C 2.864994 3.533367 -0.518854
H 5.162046 2.711905 1.007873
H 3.063044 3.689349 -1.585469
H 1.791785 3.550868 -0.341725
H 3.346038 4.333588 0.050978
O 1.377559 1.313092 -0.064185
O -1.502656 1.154654 -0.476346
H 5.253136 1.204358 0.058701
H 5.321432 2.769469 -0.763937
H -5.364825 0.824033 -0.384005
H -5.378889 1.789810 -1.883890
I 0.596392 -1.923576 -1.911217
C -3.276300 -0.493324 -0.455712
H -2.444771 -1.198258 -0.484265
H -3.810022 -0.623680 0.492306
H -3.966161 -0.726361 -1.271488
C 3.230177 -0.090550 0.622301
H 2.435327 -0.780226 0.905859
H 3.828796 -0.554577 -0.169167
H 3.878215 0.074901 1.487811
I -0.454982 -0.895705 2.515393

09withI
Opt Eel: -745.237289
SP Eel B3LYP: -11589.5359192
SP Eel M06L:
SP Eel MN15:
Gcorr: 0.197241
Fe 0.993017 0.291308 -0.324099
C -1.557290 1.188508 1.097558
O -0.464437 0.540339 1.045387
N -2.574667 0.690431 1.795603
C -3.839731 1.388960 2.007323
H -4.631673 0.908872 1.422699
H -4.097651 1.330462 3.068999
H -3.765317 2.436923 1.726271
C -2.466307 -0.615955 2.445798
H -3.428450 -1.126065 2.362163
H -1.695343 -1.209811 1.960495
H -2.219425 -0.488318 3.506094
C -0.684232 0.062676 -2.133358
C 0.335998 0.603856 -2.539056
H 1.131280 1.042201 -3.108764
C -1.903303 -0.526227 -1.675587
C -1.903491 -1.813520 -1.107256
C -3.104109 0.201148 -1.774307
C -3.094746 -2.358080 -0.637397
H -0.971747 -2.364494 -1.029797
C -4.289230 -0.355963 -1.300924
H -3.094556 1.192495 -2.214399
C -4.286018 -1.631450 -0.729435
H -3.093772 -3.348639 -0.193190
H -5.214608 0.206785 -1.375841
H -5.211634 -2.059784 -0.356577
I 2.423175 -1.870083 0.439399
Br 2.280698 2.436655 -0.191299
C -1.690623 2.521515 0.411613
H -2.612992 2.591437 -0.168529
H -1.694288 3.324731 1.158097
H -0.834299 2.672124 -0.245972

10withI
Opt Eel: -731.784196
SP Eel B3LYP: -8983.29785517
SP Eel M06L:
SP Eel MN15:
Gcorr: 0.199351
Fe -0.964765 -0.589683 -0.047092
C 1.087695 1.480879 0.725021
O -0.069446 1.185091 0.290549
N 1.854961 2.334815 0.050521
C 3.170153 2.774713 0.510433
H 3.956519 2.183635 0.027624
H 3.296656 3.825699 0.238106
H 3.260024 2.684879 1.591451
C 1.448436 2.840281 -1.258839
H 2.294143 2.751735 -1.946941
H 0.607081 2.261380 -1.633330
H 1.162319 3.895054 -1.182067
C 0.608697 -1.810523 -0.200031
C -0.454041 -2.494191 -0.027422
H -0.905832 -3.476955 -0.003344
C 2.031107 -1.571608 -0.290747
C 2.541613 -0.654988 -1.228527
C 2.917741 -2.201539 0.603507
C 3.907558 -0.385313 -1.278523
H 1.858424 -0.157458 -1.909735
C 4.280714 -1.913812 0.559389
H 2.526261 -2.901655 1.335375
C 4.780206 -1.006460 -0.379959
H 4.290349 0.317371 -2.013072
H 4.955136 -2.399154 1.259302
H 5.843017 -0.784497 -0.411283
I -3.641869 0.063113 -0.044806
C 1.584812 0.894322 2.019407
H 2.592330 0.484371 1.916290
H 1.606835 1.664824 2.799270
H 0.902398 0.102547 2.331155

11withI
Opt Eel: -672.061330
SP Eel B3LYP: -11516.2922983
SP Eel M06L: -4658.99896264
SP Eel MN15: -4658.15737878
Gcorr: 0.246934
Fe 0.003957 0.192109 0.303618
Br -0.148627 0.375200 2.782903
I 1.114026 2.297379 -1.035159
C 3.487359 -2.945635 -1.026631
C 3.491922 -2.517272 0.444446
C 2.062838 -3.170884 -1.543250
H 4.076479 -3.863417 -1.149217

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 H 4.511555 -2.307526 0.789383
 H 3.098634 -3.331967 1.067129
 H 1.603918 -4.013596 -1.009307
 H 2.066721 -3.424051 -2.610261
 C 2.617979 -1.250010 0.660825
 C 1.186810 -1.903291 -1.333137
 C 1.241526 -1.528521 0.123235
 H 0.615085 -2.146725 0.775389
 H 2.585336 -0.987724 1.722063
 H 3.075167 -0.414408 0.116170
 H 0.161064 -2.097651 -1.661036
 H 1.597322 -1.093103 -1.949111
 O -1.698454 -0.782095 -0.179609
 C -2.840277 -0.293113 -0.460002
 N -3.860683 -1.121999 -0.663273
 C -3.041612 1.195940 -0.562427
 C -5.195586 -0.695703 -1.077516
 C -3.667451 -2.568280 -0.545594
 H -3.294493 1.481769 -1.589182
 H -3.848136 1.533504 0.095325
 H -2.118906 1.709039 -0.285175
 H -5.476687 -1.243331 -1.982756
 H -5.222039 0.369941 -1.291361
 H -5.917755 -0.924421 -0.286892
 H -2.902534 -2.783274 0.199327
 H -4.614476 -3.017978 -0.240166
 H -3.363951 -2.992480 -1.509565
 H 3.974715 -2.169171 -1.632933
```

```
12withI
Opt Eel: -946.508187
SP Eel B3LYP: -9198.18213659
SP Eel M06L:
SP Eel MN15:
Gcorr: 0.371234
 C -3.079903 3.427465 -1.371431
 H -3.300553 3.911388 -2.328382
 C -0.953067 2.276118 -0.860342
 N -2.070306 2.394991 -1.583657
 C -2.337373 1.474078 -2.687067
 H -1.779921 0.550319 -2.540114
 H -3.408975 1.258817 -2.709137
 H -2.046986 1.926890 -3.642438
 Fe 0.788456 0.070991 0.174362
 O -0.090322 1.404693 -1.173857
 H -2.729907 4.184079 -0.673200
 H -4.001045 2.976408 -0.985328
 I 0.275026 -2.371598 -1.338802
 C 2.410296 0.017365 1.444150
 C 3.647089 -0.553269 0.731181
 C 2.737090 1.401365 2.028408
 H 2.126688 -0.661042 2.267932
 H 3.432013 -1.543101 0.304615
 H 4.481401 -0.700598 1.444716
 H 3.528420 1.325408 2.799598
 H 1.861214 1.831316 2.536421
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 C 4.137184 0.392931 -0.374438
 C 3.231867 2.369448 0.943218
 C 4.436409 1.790282 0.187130
 H 4.743996 2.469790 -0.619078
 H 5.289094 1.717496 0.879342
 H 5.031313 -0.014481 -0.865898
 H 3.357426 0.473561 -1.148288
 H 3.496013 3.340848 1.383623
 H 2.416827 2.555697 0.228796
 C -0.722165 3.195255 0.312488
 H -0.551636 4.221331 -0.033174
 H -1.576030 3.201630 0.994572
 H 0.164018 2.860907 0.852604
 O -1.089973 0.165413 1.197685
 C -1.773265 -0.731315 1.761794
 N -3.109792 -0.641987 1.744860
 C -1.105306 -1.892419 2.454858
 C -4.006692 -1.533463 2.472340
 C -3.735204 0.477820 1.041432
 H -1.293124 -1.860139 3.533899
 H -1.471497 -2.850168 2.073234
 H -0.030355 -1.828421 2.283354
 H -4.587575 -0.956900 3.201372
 H -3.449473 -2.303551 3.000906
 H -4.699552 -2.012859 1.772738
 H -3.214979 0.662168 0.101610
 H -4.776479 0.220389 0.838333
 H -3.705251 1.389874 1.649115
```

Structures coordinate for the aromatic main reaction mechanism:

```
01
Opt Eel: -726.641610
SP Eel B3LYP: -7061.45988691
SP Eel M06L: -6987.83137736
SP Eel MN15: -6988.28422722
Gcorr: 0.217435
 C 5.138040 -1.564372 -0.128781
 H 5.581663 -2.254399 0.594337
 C 2.820215 -0.722425 -0.148218
 N 3.686430 -1.734209 -0.095054
 C 3.219933 -3.114990 0.021467
 H 2.176227 -3.181009 -0.279411
 H 3.831443 -3.745884 -0.629476
 H 3.325186 -3.463141 1.055374
 C -5.138031 -1.564329 0.128828
 Fe 0.000002 0.306922 -0.000007
 C -2.820197 -0.722439 0.148229
 N -3.686428 -1.734209 0.095050
 C -3.219969 -3.115002 -0.021479
 H -5.527393 -1.799325 1.125952
 H -3.325359 -3.463184 -1.055361
 H -2.176227 -3.181027 0.279270
 H -3.831407 -3.745866 0.629561
 O -1.577035 -0.958782 0.040219
 O 1.577053 -0.958761 -0.040185
 H -5.423325 -0.550556 -0.144852
 H -5.581704 -2.254407 -0.594210
 H 5.423356 -0.550586 0.144819
 H 5.527436 -1.799472 -1.125867
 Br -0.282933 1.599590 -2.115024
 Br 0.282928 1.599612 2.115005
 C -3.326948 0.684444 0.328084
 H -3.760090 1.051891 -0.609105
 H -4.090833 0.745304 1.107613
 H -2.494396 1.334785 0.600954
 C 3.326962 0.684462 -0.328065
 H 3.760094 1.051906 0.609130
 H 4.090847 0.745337 -1.107592
 H 2.494405 1.334797 -0.600933

03
Opt Eel: -713.147798
SP Eel B3LYP: -4455.15899755
SP Eel M06L: -4413.65276050
SP Eel MN15: -4413.69239967
Gcorr: 0.219147
 C 3.123555 2.409906 0.273262
 H 3.198053 3.454012 -0.055765
 C 1.361810 1.232758 -0.994126
 N 1.763612 1.905805 0.101304
 C 0.825749 2.335220 1.131636
 H 0.838628 3.429431 1.200348
 H -0.184898 2.008561 0.885642
 H 1.114342 1.916500 2.100692
 Fe -1.322520 -0.084171 0.023545
 O 0.188616 0.811144 -1.140179
 H 3.842738 1.807122 -0.278510
 H 3.378631 2.361456 1.335336
 Br -3.723789 0.014483 -0.017386
 O 0.213377 -0.945216 1.159123
 C 1.424592 -1.238323 0.999547
 N 1.883396 -1.858128 -0.103340
 C 3.291286 -2.200854 -0.292252
 C 0.983468 -2.378097 -1.126030
 H 3.505074 -3.208476 0.085466
 H 3.942073 -1.483470 0.205890
 H 3.511222 -2.176110 -1.362523
 H -0.053583 -2.189690 -0.847839
 H 1.190834 -1.901108 -2.088763
 H 1.136413 -3.459118 -1.224544
 C 2.411504 -0.892926 2.089772
 H 3.124581 -0.135710 1.747720
 H 1.857687 -0.495299 2.940680
 H 2.983662 -1.770741 2.407257
 C 2.367869 0.984390 -2.094055
 H 2.820489 1.918905 -2.441777
 H 3.175513 0.329509 -1.751541
 H 1.852669 0.502165 -2.925261

04
Opt Eel: -829.840572
SP Eel B3LYP: -7584.67399963
SP Eel M06L: -7503.49618356
SP Eel MN15: -7504.15187815
Gcorr: 0.219295
 C -5.038093 1.647765 -0.069417
 H -5.443259 2.352232 0.662294
 C -2.741602 0.752543 -0.182408
 N -3.582949 1.784361 -0.082335
 C -3.084968 3.154912 0.017195
 H -2.031568 3.186313 -0.252617
 H -3.659427 3.788939 -0.664791
 H -3.212745 3.527522 1.039854
 C 5.038159 1.647930 0.068258
 Zn 0.000037 -0.363942 0.000000
 C 2.741700 0.752635 0.181512
 N 3.583012 1.784456 0.081276
 C 3.084903 3.154916 -0.018930
 H 5.454991 1.886761 1.053571
 H 3.211234 3.526577 -1.042119
 H 2.031878 3.186618 0.252329
 H 3.660334 3.789554 0.661650
 O 1.491868 0.961736 0.140854
 O -1.491764 0.961681 -0.142179
 H 5.339009 0.642738 -0.220276
 H 5.443194 2.351798 -0.664106
 H -5.338940 0.642802 0.219923
 H -5.454804 1.885747 -1.054989
 Br 0.271412 -1.619194 -2.065667
 Br -0.271519 -1.616736 2.067138
 C -3.296659 -0.638859 -0.342122
 H -2.494368 -1.316618 -0.634572
 H -3.719508 -0.988957 0.606152
 H -4.082310 -0.674597 -1.101688
 C 3.296762 -0.638685 0.341907
 H 2.494515 -1.316263 0.634900
 H 3.719375 -0.989316 -0.606277
 H 4.082575 -0.674035 1.101320

05
Opt Eel: -246.722213
SP Eel B3LYP: -7349.15744525
SP Eel M06L: -533.181254194
SP Eel MN15: -532.011029008
Gcorr: 0.130387
 C 0.524897 -0.031190 -0.324878
 H 0.564352 -0.208080 -1.399114
 I -1.716949 -0.008010 -0.012940
 C 1.158549 -1.177290 0.439114
 H 1.106716 -0.964949 1.513003
 H 0.627193 -2.116306 0.264420
 C 1.111257 1.329382 0.055360
 H 0.936187 2.034515 -0.764087
 H 0.608037 1.728046 0.940895
 C 2.638340 -1.309345 -0.017375
 C 2.628790 1.196763 0.353382
 H 2.774276 1.014221 1.425581
 H 3.125864 2.146261 0.125198
 C 3.256487 0.043987 -0.435834
 H 3.211764 -1.744031 0.809846
 H 2.700047 -2.015424 -0.853313
 H 3.091833 0.214621 -1.507958
 H 4.342124 0.021828 -0.287274

06
Opt Eel: -308.419514
SP Eel B3LYP: -308.648320666
SP Eel M06L: -308.459171027
SP Eel MN15: -308.110721120
Gcorr: 0.082280
 C -0.118924 1.215305 -0.000001
 C 0.592141 0.000001 -0.000003
 C -0.118922 -1.215305 -0.000001
 C -1.511980 -1.209930 0.000005
 C -2.211725 -0.000001 0.000007
 C -1.511981 1.209929 0.000004
 H 0.428529 2.152673 -0.000003
 H 0.428532 -2.152672 -0.000003
 H -2.052705 -2.151978 0.000006
 H -3.297983 -0.000002 0.000011
 H -2.052708 2.151976 0.000006
 C 2.021990 0.000002 -0.000010
 C 3.233316 0.000001 -0.000009
 H 4.302850 -0.000009 0.000031

07
Opt Eel: -959.896293
SP Eel B3LYP: -11804.3601944
SP Eel M06L: -4946.86739363
SP Eel MN15: -4945.71431326
Gcorr: 0.372546
 C 0.598650 4.632364 -0.674259
 H 1.663751 4.592206 -0.419760
 C -0.819533 2.596867 -0.747388
 N 0.180028 3.354667 -1.235769
 C 0.864089 2.954751 -2.460989
 H 0.783257 1.876789 -2.591553
 H 0.426206 3.456442 -3.333424
 H 1.916832 3.239679 -2.385245
 Fe -2.162764 -0.180627 -0.844095
 O -1.172662 1.561087 -1.364973
 H 0.032119 4.876038 0.221471
 H 0.447925 5.429102 -1.412570
 Br -4.249733 -0.855230 0.166103
 I 0.301033 -0.079848 2.350524
 C 2.378894 0.191289 1.497825
 C 2.283473 0.962752 0.193615
 C 3.047010 -1.163513 1.345403
 H 2.850549 0.784877 2.282455
 H 1.807936 1.933705 0.353435
 H 1.666025 0.404498 -0.518458
 H 2.461519 -1.782639 0.657122
 H 3.094454 -1.683060 2.307604
 C 3.699360 1.153040 -0.386175
 C 4.464203 -0.960877 0.772178
 C 4.427338 -0.185767 -0.549429
 H 5.446972 -0.018821 -0.918085
 H 3.909237 -0.788854 -1.305904
 H 3.622095 1.671746 -1.349371
 H 4.277950 1.805189 0.282697
 H 4.936279 -1.941263 0.634103
 H 5.074289 -0.412005 1.502876
 O -0.552594 -1.152279 -1.729411
 C 0.200571 -2.094047 -1.375613
 N 1.386961 -2.257283 -1.992792
 C 2.261478 -3.406186 -1.784995
 C 1.725242 -1.377974 -3.109462
 H 2.162410 -4.121371 -2.611650
 H 2.027112 -3.912156 -0.850546
 H 3.298811 -3.062157 -1.742914
 H 1.413110 -0.357271 -2.887787
 H 2.805632 -1.405529 -3.261156
 H 1.228781 -1.706125 -4.031567
 C -0.205848 -3.054691 -0.285828
 H 0.520447 -3.072342 0.531456
 H -1.172205 -2.737848 0.110082
 H -0.295810 -4.072182 -0.683023
 C -1.507164 3.013926 0.529744
 H -0.795160 3.144099 1.349585
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 H -2.043334 3.959525 0.388674
 H -2.222884 2.237257 0.803756

08
Opt Eel: -235.231904
SP Eel B3LYP: -235.389155911
SP Eel M06L: -235.241698393
SP Eel MN15: -234.954238253
Gcorr: 0.128424
 C 0.398470 1.368371 -0.279334
 H 0.635382 2.352651 -0.676312
 C -0.944801 1.088493 0.311039
 H -0.876251 1.133864 1.414341
 H -1.669254 1.860956 0.029189
 C 1.488936 0.355630 -0.112407
 H 1.990901 0.177589 -1.078927
 H 2.283966 0.732826 0.555897
 C -1.481474 -0.319833 -0.074190
 C 0.934572 -0.975913 0.424021
 H 0.718908 -0.886461 1.497699
 H 1.686713 -1.766772 0.318609
 C -0.349972 -1.343815 -0.329160
 H -2.136811 -0.677175 0.729670
 H -2.104750 -0.239085 -0.972540
 H -0.116551 -1.375181 -1.402493
 H -0.686638 -2.350813 -0.054958

09
Opt Eel: -747.197582
SP Eel B3LYP: -7082.00768054
SP Eel M06L: -7008.39245857
SP Eel MN15: -7008.79814679
Gcorr: 0.198217
 Fe 1.288957 -0.078351 -0.092812
 C -1.271031 1.177382 1.013428
 O -0.249464 0.425247 1.090385
 N -2.365309 0.858493 1.701344
 C -3.552612 1.703923 1.798884
 H -4.396900 1.212206 1.305073
 H -3.795464 1.849025 2.856313
 H -3.385507 2.677692 1.344839
 C -2.406126 -0.364115 2.503645
 H -3.419519 -0.769520 2.466159
 H -1.705290 -1.094362 2.105368
 H -2.148799 -0.139009 3.545359
 C -0.185982 -0.586227 -1.920404
 C 0.989545 -0.469191 -2.254948
 H 1.906888 -0.469563 -2.812307
 C -1.572152 -0.707115 -1.596612
 C -2.030719 -1.780730 -0.810546
 C -2.478634 0.267882 -2.053923
 C -3.380186 -1.868091 -0.483207
 H -1.326974 -2.527287 -0.457802
 C -3.826586 0.167947 -1.719932
 H -2.116547 1.092379 -2.658771
 C -4.278337 -0.895352 -0.933219
 H -3.731612 -2.693309 0.128320
 H -4.524238 0.921822 -2.071519
 H -5.329764 -0.966900 -0.671136
 Br 2.242116 -2.183660 0.715716
 Br 2.727738 1.919478 -0.306215
 C -1.227879 2.436695 0.189337
 H -2.131752 2.576560 -0.405409
 H -1.113171 3.303774 0.851086
 H -0.362038 2.400515 -0.472501

10
Opt Eel: -733.742735
SP Eel B3LYP: -4475.76022958
SP Eel M06L: -4434.26397249
SP Eel MN15: -4434.23825628
Gcorr: 0.199942
 Fe -1.446185 -0.410929 -0.035397
 C 0.725104 1.523517 0.677302
 O -0.430959 1.294976 0.199676
 N 1.565783 2.331477 0.034776
 C 2.888747 2.681992 0.547627
 H 3.646785 2.006609 0.134968
 H 3.117033 3.705046 0.239118
 H 2.913468 2.636184 1.635113
 C 1.244911 2.856778 -1.290376
 H 2.098775 2.685980 -1.952693
 H 0.366653 2.350779 -1.685086
 H 1.052332 3.933488 -1.230001
 C 0.040496 -1.729796 -0.247626
 C -1.075769 -2.334045 -0.130779
 H -1.617012 -3.270027 -0.152482
 C 1.478488 -1.602011 -0.302959
 C 2.085361 -0.712016 -1.208159
 C 2.287115 -2.315419 0.602532
 C 3.469279 -0.549624 -1.214426
 H 1.463860 -0.151056 -1.899151
 C 3.668783 -2.133931 0.602961
 H 1.821114 -2.996288 1.308470
 C 4.264558 -1.252232 -0.303951
 H 3.927087 0.133627 -1.923979
 H 4.282218 -2.682978 1.311897
 H 5.341766 -1.112948 -0.300904
 Br -3.867468 0.069446 -0.048109
 C 1.142765 0.909406 1.987178
 H 2.131903 0.449889 1.921075
 H 1.173955 1.676883 2.769805
 H 0.410423 0.152515 2.271197

11
Opt Eel: -674.018188
SP Eel B3LYP: -7008.76104649
SP Eel M06L: -6935.18342307
SP Eel MN15: -6935.65392191
Gcorr: 0.246542
 Fe 0.204957 0.470046 0.004650
 C 1.373636 -0.590309 1.489218
 C 1.041926 -2.059409 1.381380
 C 2.830562 -0.215426 1.376991
 H 0.832244 -0.069911 2.286612
 H -0.035913 -2.209022 1.265613
 H 1.300114 -2.487564 2.368135
 H 3.280168 -0.467037 2.355965
 H 2.949775 0.867533 1.265155
 C 1.832931 -2.806848 0.299392
 C 3.583507 -0.978697 0.279147
 C 3.331374 -2.488978 0.373125
 H 3.865619 -3.010165 -0.430885
 H 3.738106 -2.866299 1.323012
 H 1.663362 -3.884334 0.412477
 H 1.451883 -2.522876 -0.688825
 H 4.655368 -0.762718 0.361444
 H 3.256245 -0.616199 -0.703349
 O -1.522772 -0.422957 0.518745
 C -2.699159 -0.199106 0.086847
 N -3.683810 -1.005526 0.473062
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 C -5.055126 -0.924797 -0.026754
 C -3.404066 -2.100719 1.404309
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 H -3.854603 1.523968 -0.525936
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 H -5.725339 -0.587565 0.771206
 H -2.649823 -1.792777 2.128014
 H -4.329159 -2.352714 1.926213
 H -3.045077 -2.983088 0.862588
 Br 0.504460 2.769487 0.771093
 Br 0.693284 -0.173225 -2.300423

12
Opt Eel: -948.463465
SP Eel B3LYP: -4690.64688270
SP Eel M06L: -4648.98071065
SP Eel MN15: -4648.71845182
Gcorr: 0.372111
 C 2.960813 3.480546 0.099706
 H 3.179165 4.287173 0.807648
 C 0.754850 2.362932 0.013496
 N 1.900135 2.640297 0.645916
 C 2.131595 2.141098 2.000835
 H 1.533106 1.247527 2.174517
 H 3.192535 1.897050 2.103024
 H 1.872985 2.908711 2.740306
 Fe -0.792917 -0.217049 0.193718
 O -0.157535 1.719016 0.607018
 H 2.667785 3.920598 -0.850592
 H 3.869182 2.885134 -0.044283
 Br 0.303124 -1.531548 2.150312
 C -2.547599 -1.019365 -0.546855
 C -3.711612 -0.919475 0.452818
 C -2.962546 -0.390384 -1.887402
 H -2.315218 -2.086398 -0.711260
 H -3.434965 -1.361988 1.420149
 H -4.589390 -1.491306 0.092259
 H -3.813213 -0.940180 -2.336170
 H -2.144631 -0.448189 -2.620283
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 H -2.529355 1.661648 -1.365941
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 H 0.491004 3.929240 -1.444217
 H 1.367281 2.513933 -2.054829
 H -0.387583 2.420286 -1.773802
 O 0.829766 -0.386428 -1.194194
 C 1.544078 -1.414703 -1.350543
 N 2.879599 -1.308547 -1.351006
 C 0.907728 -2.767376 -1.555067
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 H 1.108580 -3.141560 -2.565340
 H 1.286835 -3.500066 -0.836884
 H -0.170161 -2.667677 -1.425425
 H 4.460405 -2.113630 -2.463213
 H 3.254045 -3.302784 -1.938288
 H 4.404446 -2.629831 -0.760929
 H 2.858168 0.591179 -0.470137
 H 4.460609 -0.178482 -0.595483
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13
Opt Eel: -1682.235409
SP Eel B3LYP: -9166.43604377
SP Eel M06L: -9083.25940742
SP Eel MN15: -9082.97496836
Gcorr: 0.598704
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 C 1.543534 -1.373805 -2.243616
 C 1.736053 -2.271823 -3.481319
 C 0.988845 -3.601848 -3.318884
 C 1.396549 -4.325284 -2.028627
 C 1.211766 -3.414415 -0.798566
 H 1.390815 -1.748934 -4.383725
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 C -0.464681 0.194148 0.446961
 Fe 2.225140 -0.929232 0.640956
 Br 3.017038 -1.569236 2.979851
 O 3.795589 0.195292 -0.058527
 C 4.234238 1.359302 0.175768
 N 4.534279 2.172282 -0.841441
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 C 4.289977 1.759532 -2.220775
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 H 4.330277 4.225771 -1.183061
 H 5.104397 3.813859 0.360682
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 H 5.134754 2.073704 -2.840740
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 H 1.557215 4.681935 -1.762989
 Fe -2.514207 0.145801 0.685229
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 O -3.393882 1.721000 -0.318466
 N -3.113182 3.713714 -1.342964
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 Br -3.682055 -0.036189 2.918223
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 H -2.783699 -2.607453 1.539615
 H -3.403961 -5.199925 -2.065977
 H -1.732191 -4.919222 -2.609396
 H -2.077759 -5.099001 -0.882750
 H -3.940483 -2.333369 -3.141757
 H -2.328587 -1.596945 -2.995407
 H -2.518469 -3.165411 -3.818699

14e
Opt Eel: -1798.943048
SP Eel B3LYP: -12295.9449066
SP Eel M06L: -12173.1027321
SP Eel MN15: -12173.4637023
Gcorr: 0.603302
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 C -1.373550 4.649479 2.168545
 C -1.895565 4.704753 0.727302
 C -0.750567 4.606923 -0.288269
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Fe 1.649645 0.637072 -1.006948
C 4.463253 -0.407920 -1.222924
O 3.251011 -0.631224 -1.493418
N 5.289928 -1.431593 -0.971916
C 6.715804 -1.292241 -0.700562
H 6.921844 -1.543093 0.346145
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H -1.978404 0.681256 -1.567185
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H 5.538605 1.219307 -0.274333
H 5.698750 1.151520 -2.039694
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14
Opt Eel: -969.020405
SP Eel B3LYP: -4711.19644613
SP Eel M06L: -4669.54403273
SP Eel MN15: -4669.23445718
Gcorr: 0.350982
Fe -0.568155 -0.002817 -0.768156
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14z
Opt Eel: -1798.946366
SP Eel B3LYP: -12295.9487464
SP Eel M06L: -12173.1022177
SP Eel MN15: -12173.4671185
Gcorr: 0.603156
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C -2.715892 -1.971949 -2.967329
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Fe -0.950285 -0.892373 1.307532
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Zn 2.162418 0.342817 -0.823821
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Br 1.483788 0.966744 -3.039119
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H 4.186258 -2.802457 -1.733146
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H -4.748608 -1.753409 1.356535
H -4.517811 -2.919297 2.673398
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15e
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SP Eel B3LYP: -12007.8384354
SP Eel M06L: -11885.1967342
SP Eel MN15: -11885.8664667
Gcorr: 0.478821
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H -1.319155 2.465376 -0.767005
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C 2.697136 -2.312799 2.805211
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C 3.696582 -0.122218 2.888748
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H 2.727509 -3.376264 3.027323
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C 3.948592 0.069353 -0.590280
O 2.794626 0.257025 -1.086707
N 4.399221 -1.173168 -0.439861
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H 3.739929 -3.119138 -0.081310
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Zn -0.754944 -1.123925 -0.056251
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Br -0.300663 -3.423457 -0.699334
C 4.812033 1.249132 -0.231302
H 5.231123 1.158246 0.773162
H 5.642184 1.336147 -0.942265
H 4.205066 2.153325 -0.290860
O -2.703486 -1.196821 0.445923
C -3.787772 -1.267188 -0.205738
N -4.952039 -1.221530 0.446612
C -3.785216 -1.388888 -1.705433
C -6.249782 -1.202772 -0.227728
C -5.003440 -1.218065 1.907567
H -4.539520 -2.095906 -2.059351
H -3.988944 -0.412418 -2.160805
H -2.800696 -1.723172 -2.032104
H -6.930266 -0.583643 0.361995
H -6.169014 -0.767672 -1.222692
H -6.665065 -2.214599 -0.300223
H -4.025800 -1.470149 2.312158
H -5.308550 -0.231887 2.272504
H -5.738884 -1.960025 2.233518

15z
Opt Eel: -1511.074280
SP Eel B3LYP: -12007.8434488
SP Eel M06L: -11885.2003944
SP Eel MN15: -11885.8687242
Gcorr: 0.479255
C -0.381724 2.866513 0.948855
C -1.140435 2.978528 2.295913
C -1.035654 4.393590 2.877425
C -1.532946 5.448887 1.881908
C -0.791674 5.339378 0.543308
C -0.892863 3.926026 -0.041918
H -1.604957 4.451936 3.813894
H -2.197535 2.724504 2.131951
H -0.738034 2.240904 3.000749
H 0.675187 3.059604 1.155707
H -2.609663 5.302669 1.710536
H -1.412595 6.454902 2.303587
H -1.188790 6.069510 -0.173347
H 0.268383 5.590802 0.695681
H -1.943812 3.704406 -0.282270
H -0.329781 3.854370 -0.979273
H 0.014534 4.599674 3.130058
C -0.565008 1.466538 0.423893
H -1.483158 1.339010 -0.156253
C 0.153042 0.339578 0.720572
C 1.374874 0.379122 1.570435
C 1.487673 -0.482405 2.674690
C 2.462462 1.225495 1.283589
C 2.630333 -0.484191 3.475263
H 0.670871 -1.161128 2.903497
C 3.610849 1.217129 2.074903
H 2.418210 1.884623 0.420908
C 3.699951 0.364344 3.178136
H 2.688007 -1.157430 4.326399
H 4.438897 1.874585 1.824553
H 4.594348 0.356604 3.794609
Fe 0.697120 0.216088 -1.459085
C 3.551914 -0.746408 -0.914383
O 2.360095 -0.877153 -1.340456
N 4.044301 -1.637743 -0.059559
C 5.429150 -1.649953 0.403006
H 6.040862 -0.948360 -0.159181
H 5.464501 -1.393349 1.466643
H 5.835607 -2.657072 0.267159
C 3.206308 -2.720631 0.453816
H 2.156161 -2.459963 0.360514
H 3.403384 -3.644311 -0.103175
H 3.450139 -2.879396 1.506531

Br -1.175590 -1.316732 -2.224978
Zn -0.924196 -1.379126 0.498393
Br 1.198247 2.124373 -2.945663
Br -0.531044 -3.644405 1.202153
C 4.410145 0.384899 -1.413469
H 4.901648 0.913242 -0.593355
H 5.185672 -0.000727 -2.085780
H 3.781248 1.080578 -1.969844
O -2.830469 -0.833104 0.882676
C -3.915650 -1.125141 0.296621
N -4.877890 -0.203938 0.201047
C -4.140730 -2.502727 -0.270774
C -6.171221 -0.430629 -0.437140
C -4.688683 1.138916 0.747524
H -5.022971 -2.968569 0.180484
H -4.295002 -2.463120 -1.353507
H -3.266798 -3.118866 -0.059287
H -6.359503 0.377318 -1.151434
H -6.190676 -1.378498 -0.969481
H -6.965495 -0.423732 0.317896
H -3.798373 1.161474 1.371185
H -4.582713 1.861125 -0.070025
H -5.566098 1.407638 1.343997

16e
Opt Eel: -1798.950135
SP Eel B3LYP: -12295.9525158
SP Eel M06L: -12173.1053351
SP Eel MN15: -12173.4688251
Gcorr: 0.602671
C 2.115395 0.280044 2.871434
C 3.554184 0.833740 2.758614
C 4.598276 -0.169884 3.266177
C 4.464408 -1.530244 2.568631
C 3.037864 -2.079027 2.697437
C 2.008048 -1.079346 2.157175
H 5.608847 0.234691 3.120858
H 3.748417 1.063800 1.705516
H 3.632952 1.776549 3.316586
H 1.932250 0.089141 3.940057
H 4.706163 -1.417524 1.502834
H 5.189628 -2.242168 2.984647
H 2.949804 -3.035432 2.163948
H 2.824842 -2.288874 3.756855
H 2.179671 -0.945679 1.085787
H 0.990397 -1.467622 2.265690
H 4.468616 -0.309612 4.349886
C 1.087445 1.304719 2.433889
H 0.571808 1.787252 3.272851
C 0.767797 1.720416 1.191178
C -0.300310 2.745345 1.075721
C -0.117462 3.910023 0.305583
C -1.536017 2.586274 1.734877
C -1.107657 4.889445 0.227733
H 0.815169 4.042874 -0.234872
C -2.532469 3.561179 1.649177
H -1.712796 1.677933 2.303485
C -2.322474 4.721965 0.901266
H -0.932366 5.786022 -0.362184
H -3.478911 3.408086 2.161883
H -3.096123 5.481946 0.835773
Zn 1.484968 1.035986 -0.530912
C 4.082792 -0.394869 -1.372591
O 3.408428 0.360886 -0.619639
N 5.410779 -0.477930 -1.215274
C 6.255174 -1.373886 -2.003349
H 6.627703 -0.871768 -2.904278
H 7.108933 -1.667450 -1.387682
H 5.713454 -2.275677 -2.286446
C 6.119739 0.396491 -0.283834
H 5.428223 1.122407 0.136533
H 6.565277 -0.194876 0.522515
H 6.918805 0.918063 -0.821825
Br 1.387859 2.153789 -2.741539
Fe -2.071968 -1.045937 0.451473
Br -0.017754 -1.198827 -1.038736
Br -1.957826 -1.303582 2.898140
O -2.957888 -2.740793 -0.261020
C -2.417997 -3.849776 -0.557612
N -2.736053 -4.447347 -1.707009
C -2.279908 -5.778685 -2.097411
C -3.645751 -3.789398 -2.644329
H -3.149921 -6.395317 -2.346131
H -1.635743 -5.706029 -2.980343
H -1.730380 -6.259737 -1.291695
H -3.545696 -2.707855 -2.559867
H -3.385186 -4.103910 -3.657501
H -4.684451 -4.073674 -2.438662
O -3.311740 0.343328 -0.194130
C -3.411470 1.443105 -0.821006
N -4.482386 2.204824 -0.607825
C -4.767243 3.435217 -1.338335
C -5.495591 1.787185 0.360076
H -5.680784 3.306248 -1.929665
H -4.919677 4.250437 -0.625570
H -3.947247 3.696714 -2.002082
H -5.989913 2.679287 0.749567
H -6.244284 1.144487 -0.117962
H -5.026651 1.242052 1.178505
C -1.436910 -4.500183 0.383890
H -1.846166 -5.435856 0.781206
H -0.492225 -4.728318 -0.118577
H -1.246770 -3.824309 1.218477
C -2.353832 1.867440 -1.799432
H -2.771474 1.939796 -2.809760
H -1.935272 2.840225 -1.531005
H -1.550855 1.132860 -1.805196
C 3.420726 -1.222975 -2.442055
H 4.002460 -1.238951 -3.367008
H 3.299734 -2.256123 -2.094574
H 2.434800 -0.807711 -2.645151

16z
Opt Eel: -1798.953664
SP Eel B3LYP: -12295.9570449
SP Eel M06L: -12173.1066527
SP Eel MN15: -12173.4753380
Gcorr: 0.602177
C 3.675342 -1.377702 0.859965
C 4.981781 -1.402174 0.037498
C 6.117513 -2.120177 0.776606
C 5.708929 -3.541717 1.183110
C 4.417997 -3.529566 2.011590
C 3.283124 -2.812795 1.269031
H 7.017612 -2.146196 0.148423
H 4.787029 -1.913863 -0.916885
H 5.277765 -0.374867 -0.211567
H 3.862228 -0.803966 1.776680
H 5.548827 -4.144034 0.276461
H 6.518563 -4.024901 1.745235
H 4.115621 -4.554954 2.261573
H 4.606339 -3.014370 2.965066
H 3.026539 -3.380644 0.361551
H 2.376610 -2.783813 1.886473
H 6.378490 -1.548458 1.679309
C 2.579404 -0.713880 0.063498
H 2.410453 -1.191665 -0.905370
C 1.854500 0.381565 0.370820
C 1.983568 1.067330 1.674145
C 2.314952 2.434241 1.739641
C 1.735993 0.396079 2.888603
C 2.426191 3.093895 2.963480
H 2.485933 2.977669 0.814449
C 1.829379 1.059476 4.113738
H 1.456512 -0.653649 2.862393
C 2.179624 2.411602 4.159398
H 2.695858 4.147116 2.984370
H 1.629150 0.517442 5.034903
H 2.254991 2.928232 5.112329
Zn 0.677050 1.112134 -1.056634
C 3.019069 0.935852 -2.809963
O 1.760880 0.833869 -2.828593
N 3.781171 -0.038886 -3.325259
C 5.231316 0.032071 -3.461947
H 5.685110 -0.835383 -2.972390
H 5.503345 0.016959 -4.523947
H 5.627152 0.938151 -3.009629
C 3.163310 -1.244024 -3.870303
H 2.146363 -1.334401 -3.492662
H 3.142557 -1.202338 -4.966171
H 3.752442 -2.112810 -3.562740
Br -0.341831 3.337558 -1.188449
Fe -2.058497 -1.075461 0.607814
Br -1.223251 -0.609902 -1.760480
Br -1.222014 -3.056685 1.799311
O -4.050567 -1.393997 0.307879
C -4.659197 -1.958243 -0.651374
N -5.878089 -1.541925 -1.001048
C -6.664911 -2.142583 -2.075513
C -6.546119 -0.464288 -0.273137
H -7.433476 -2.804352 -1.659463
H -7.156304 -1.341068 -2.634204
H -6.034096 -2.704963 -2.760663
H -5.963547 -0.196986 0.605007
H -6.655756 0.409775 -0.923861
H -7.540944 -0.804305 0.032478
O -2.017714 0.713959 1.452521
C -2.595278 1.825871 1.216258
N -2.272787 2.893679 1.937196
C -2.889840 4.202551 1.735200
C -1.165255 2.858814 2.889897
H -2.867360 4.740380 2.685549
H -2.329068 4.773930 0.986685
H -3.927956 4.104817 1.419738
H -0.495335 3.694746 2.675698
H -1.548468 2.959724 3.911121
H -0.620766 1.924346 2.789558
C -4.025292 -3.109173 -1.389077
H -4.685902 -3.981621 -1.403904
H -3.802660 -2.832221 -2.424883
H -3.093750 -3.379072 -0.890719
C -3.652262 1.946388 0.152744
H -4.635402 2.101334 0.611389
H -3.441462 2.789938 -0.508609
H -3.684482 1.032729 -0.437327
C 3.679611 2.154856 -2.211898
H 4.368454 1.881417 -1.406904
H 4.244184 2.705833 -2.972158
H 2.902835 2.807996 -1.812666

Cy_dimer
Opt Eel: -470.615466
SP Eel B3LYP: -470.923234319
SP Eel M06L: -470.623355272
SP Eel MN15: -470.05896316
Gcorr: 0.290024
C 0.221808 2.971452 -1.257357
C -0.221102 1.501853 -1.257701
C 0.238423 0.737658 0.000239
C -0.221441 1.502182 1.257863
C 0.221441 2.971793 1.257230
C -0.252221 3.706205 -0.000233
H -1.319811 1.455449 -1.315150
H 0.160240 1.016567 -2.161996
H 1.320073 3.015623 -1.305652
H -0.152200 3.472619 -2.159764
H -1.320164 1.455766 1.315061
H 0.159699 1.017186 2.162390
H -0.152827 3.473206 2.159391
H 1.319692 3.015988 1.305827
H -1.351314 3.754710 -0.000401
H 0.110935 4.742260 -0.000321
H 1.341383 0.727602 0.000374
C -0.238423 -0.737658 0.000239
C 0.221102 -1.501853 -1.257701
C 0.221441 -1.502182 1.257863
H -1.341383 -0.727602 0.000374
C -0.221808 -2.971452 -1.257357
H 1.319811 -1.455449 -1.315150
H -0.160240 -1.016567 -2.161996
C -0.221441 -2.971793 1.257230
H 1.320164 -1.455766 1.315061
H -0.159699 -1.017186 2.162390
C 0.252221 -3.706205 -0.000233
H 0.152200 -3.472619 -2.159764
H -1.320073 -3.015623 -1.305652
H 0.152827 -3.473206 2.159391
H -1.319692 -3.015988 1.305827
H -0.110935 -4.742260 -0.000321
H 1.351314 -3.754710 -0.000401

DMA
Opt Eel: -287.854060
SP Eel B3LYP: -288.093611871
SP Eel M06L: -287.896739094
SP Eel MN15: -287.587510784
Gcorr: 0.102454
H 1.152780 -1.922947 -0.000502
C 1.625289 -0.941887 0.000036
N 0.589152 0.077732 -0.000057
H 2.261696 -0.840766 -0.888813
H 2.260970 -0.841422 0.889486
C -0.727555 -0.291801 -0.000023
C 1.077337 1.446632 0.000120
O -1.075233 -1.477027 -0.000030
H 1.697020 1.628218 0.888327
H 1.697307 1.628328 -0.887861
H 0.258522 2.163127 0.000033
C -1.765926 0.818577 -0.000087
H -1.676706 1.458533 0.884910
H -1.676529 1.458616 -0.885007
H -2.752125 0.351280 -0.000203

P0
Opt Eel: -543.720612
SP Eel B3LYP: -544.098191474
SP Eel M06L: -543.757734876
SP Eel MN15: -543.124379273
Gcorr: 0.236130
C 1.584700 0.000092 0.172088
C 2.448040 -1.265894 0.337276
C 3.642282 -1.265230 -0.625627
C 4.494471 -0.000153 -0.461985
C 3.642438 1.264995 -0.625889
C 2.448194 1.266009 0.337013
H 4.253687 -2.161795 -0.461671
H 2.813594 -1.312856 1.373764
H 1.828233 -2.157220 0.178506
H 1.161920 0.000011 -0.841321
H 4.950822 -0.000077 0.538861
H 5.318886 -0.000278 -1.186391
H 4.253952 2.161519 -0.462120
H 3.271444 1.319578 -1.659689
H 2.813754 1.313143 1.373491
H 1.828497 2.157377 0.178055
H 3.271281 -1.319981 -1.659415
C 0.437530 0.000266 1.170792
H 0.745355 0.000343 2.223390
C -0.827996 0.000284 0.858553
C -2.110726 0.000123 0.364468
C -2.806415 -1.227706 0.105445
C -2.806666 1.227781 0.105317
C -4.101409 -1.213606 -0.385074
H -2.296559 -2.166867 0.297493
C -4.101658 1.213363 -0.385200
H -2.297004 2.167067 0.297269
C -4.762898 -0.000202 -0.635985
H -4.609149 -2.155018 -0.578442
H -4.609592 2.154650 -0.578663
H -5.778445 -0.000327 -1.020258

P1e
Opt Eel: -1256.975166
SP Eel B3LYP: -4999.37769452
SP Eel M06L: -4957.51522548
SP Eel MN15: -4956.91499328
Gcorr: 0.482547
Fe -0.183311 -0.798825 -0.479839
C 2.446961 -1.627524 0.875151
O 1.186143 -1.515365 0.855795
N 3.107143 -1.491770 2.030046
C 2.397808 -1.193978 3.271498
H 2.455985 -2.054445 3.948102
H 2.870087 -0.333310 3.755276
H 1.355661 -0.970867 3.056731
C 4.542764 -1.704950 2.183256
H 4.983232 -0.837350 2.683880
H 4.718268 -2.593278 2.800989
H 5.028465 -1.840350 1.220441
C -2.437173 -0.835116 1.490657
O -1.848193 -1.501878 0.592070

N -3.773802 -0.836361 1.555990
C -4.549003 -0.187220 2.608146
H -5.100845 0.664314 2.195554
H -5.266171 -0.906946 3.016882
H -3.909132 0.158030 3.416804
C -4.561885 -1.561275 0.562935
H -5.445034 -0.967375 0.313807
H -3.965582 -1.724256 -0.332021
H -4.886452 -2.527962 0.967085
C -0.522433 1.227397 -0.634398
C 0.466906 2.143552 -0.572139
C -1.934800 1.670921 -0.579631
C -2.903545 1.079683 -1.415378
C -2.382527 2.628478 0.353878
C -4.248699 1.438710 -1.337160
H -2.586597 0.322436 -2.129038
C -3.730435 2.979599 0.444924
H -1.661254 3.080592 1.029571
C -4.672628 2.388001 -0.401369
H -4.971177 0.968297 -1.999496
H -4.047142 3.713174 1.182573
H -5.722801 2.657392 -0.328588
Br -0.094097 -2.216560 -2.613158
C 1.942016 1.839450 -0.544146
C 2.705961 2.632458 -1.622957
C 2.544820 2.117051 0.850596
H 2.078607 0.769232 -0.756502
C 4.214753 2.360822 -1.580420
H 2.525991 3.706839 -1.467397
H 2.301801 2.385382 -2.613521
C 4.055796 1.853919 0.890006
H 2.348594 3.165619 1.120746
H 2.033121 1.497091 1.597573
C 4.795316 2.651448 -0.190828
H 4.727538 2.962310 -2.342169
H 4.398593 1.306345 -1.834782
H 4.453646 2.093904 1.884752
H 4.235702 0.783335 0.727449
H 5.867636 2.417741 -0.168941
H 4.700280 3.726480 0.022229
H 0.233706 3.217800 -0.529058
C 3.208892 -1.923904 -0.391286
H 3.955205 -1.150195 -0.595496
H 3.729327 -2.884704 -0.313946
H 2.503308 -1.973320 -1.221692
C -1.646076 -0.052514 2.511316
H -2.028935 0.961983 2.638707
H -1.680380 -0.559533 3.482988
H -0.607499 -0.000528 2.185773

P1z
Opt Eel: -1256.971323
SP Eel B3LYP: -4999.37090506
SP Eel M06L: -4957.51003890
SP Eel MN15: -4956.90665643
Gcorr: 0.481907
Fe 0.563826 -1.283182 0.003331
C 3.109094 -0.971421 1.520704
O 1.899525 -1.331738 1.607924
N 3.577782 0.028943 2.277503
C 2.717229 0.717381 3.234713
H 3.199152 0.713878 4.218211
H 2.566643 1.755950 2.920641
H 1.757849 0.209280 3.295013
C 4.959258 0.497960 2.249292
H 4.958441 1.591579 2.202708
H 5.484118 0.187249 3.160392
H 5.490022 0.114489 1.381168
C 1.725796 0.929094 -1.766177
O 1.943660 0.052674 -0.885519
N 2.290936 2.136849 -1.644677
C 2.203998 3.195194 -2.643831
H 1.705606 4.069704 -2.212735
H 3.213637 3.483287 -2.957496
H 1.649014 2.865104 -3.518921
C 3.132493 2.427263 -0.485277
H 3.037467 3.487854 -0.241759
H 2.810793 1.825454 0.361589
H 4.183636 2.206060 -0.707931
C -1.154637 -0.184648 0.223030
C -2.367151 -0.770355 0.333254
C -0.993581 1.286843 0.163401
C -0.198845 1.961420 1.110815
C -1.539657 2.051049 -0.887763
C 0.033007 3.333340 1.019930
H 0.243658 1.392642 1.923023
C -1.299231 3.422696 -0.988067
H -2.146376 1.552712 -1.638883
C -0.510257 4.073444 -0.035160
H 0.647365 3.825821 1.769766
H -1.729699 3.984559 -1.813462
H -0.321107 5.140541 -0.113420
Br 0.666589 -3.483661 -1.222309
C -3.714179 -0.107032 0.489816
C -4.618591 -0.391114 -0.728327
C -4.411761 -0.575297 1.784559
H -3.573598 0.979690 0.556215
C -6.009747 0.235018 -0.568641
H -4.719776 -1.480348 -0.848976
H -4.134962 -0.016856 -1.639690
C -5.802487 0.051311 1.946452
H -4.506225 -1.671496 1.760330
H -3.781097 -0.331949 2.649655
C -6.688625 -0.229373 0.726222
H -6.635195 -0.010803 -1.436724
H -5.910409 1.330351 -0.550504
H -6.280794 -0.325267 2.859989
H -5.694674 1.138826 2.071292
H -7.663670 0.261285 0.842520
H -6.883183 -1.310320 0.663606
H -2.420110 -1.864469 0.330765
C 4.048109 -1.690759 0.584493
H 4.453529 -1.007907 -0.167264
H 4.886043 -2.133489 1.133573
H 3.491316 -2.480057 0.077915
C 0.857772 0.619360 -2.960445
H 0.072178 1.365453 -3.099401
H 1.464772 0.586148 -3.872736
H 0.400978 -0.360375 -2.811253

P2e
Opt Eel: -1360.180009
SP Eel B3LYP: -5522.59837750
SP Eel M06L: -5473.18335129
SP Eel MN15: -5472.78516113
Gcorr: 0.485148
Zn 0.216636 -0.882230 -0.229456
C 3.093510 -0.980546 0.813186
O 1.858371 -1.081498 1.056145
N 3.832579 -0.108226 1.508496
C 3.174631 0.767464 2.477132
H 2.943173 0.225926 3.401563
H 3.847503 1.595163 2.707031
H 2.251542 1.164479 2.055177
C 5.279815 0.028916 1.388546
H 5.527700 1.014386 0.980140
H 5.736441 -0.068863 2.379176
H 5.693850 -0.739218 0.739397
C -1.671614 -0.721509 2.039483
O -1.216288 -1.467479 1.125305
N -2.963323 -0.817495 2.376438
C -3.585618 -0.065420 3.461392
H -4.515118 0.381457 3.097321
H -3.819624 -0.731674 4.300209
H -2.932088 0.730569 3.810930
C -3.800039 -1.822505 1.719999
H -4.845888 -1.533403 1.834251
H -3.550185 -1.883021 0.660840
H -3.650578 -2.808121 2.176843
C 0.178266 1.051258 -0.732881
C -0.943977 1.768538 -0.931370
C 1.493683 1.728170 -0.804900
C 1.745144 2.938582 -0.129031
C 2.560773 1.148260 -1.518716
C 3.002988 3.543210 -0.170127
H 0.945407 3.391775 0.450941
C 3.814447 1.755656 -1.572254
H 2.395690 0.207688 -2.038921
C 4.045319 2.956263 -0.892692
H 3.171298 4.472108 0.369464
H 4.616450 1.287138 -2.137161
H 5.025515 3.424210 -0.922132
Br 0.255095 -2.786461 -1.816096
C -2.358814 1.257287 -0.882991
C -3.210754 2.064894 0.118669
C -3.009868 1.293429 -2.281828
H -2.343442 0.210530 -0.551758
C -4.671057 1.596369 0.146783
H -3.175056 3.127800 -0.164333
H -2.769348 1.991823 1.120108
C -4.467831 0.817610 -2.250019
H -2.970479 2.323683 -2.666765
H -2.420978 0.675778 -2.972333
C -5.299600 1.632056 -1.251528
H -5.251436 2.216077 0.842846
H -4.710526 0.568125 0.530635
H -4.907016 0.881125 -3.254110
H -4.493866 -0.243443 -1.960442
H -6.329604 1.254242 -1.215435
H -5.356185 2.675256 -1.596164
H -0.868792 2.835301 -1.184544
C 3.747326 -1.857607 -0.225126
H 4.350954 -1.277015 -0.927670
H 4.401606 -2.593457 0.257156
H 2.964603 -2.386039 -0.770747
C -0.777453 0.260410 2.754179
H -1.072501 1.292381 2.537716
H -0.819984 0.115003 3.838097
H 0.246421 0.102398 2.418151

P2z
Opt Eel: -1360.175318
SP Eel B3LYP: -5522.59362593
SP Eel M06L: -5473.17889012
SP Eel MN15: -5472.77907720
Gcorr: 0.483816
Zn 0.532235 -1.116447 -0.405820
C 2.596979 -1.311149 1.712296
O 1.383357 -1.540469 1.452104
N 2.929403 -0.511679 2.738279
C 1.902520 0.109057 3.569692
H 1.987969 -0.258616 4.598865
H 2.044083 1.194913 3.573264
H 0.918493 -0.133512 3.175990
C 4.299658 -0.232110 3.153107
H 4.433952 0.851623 3.236137
H 4.493784 -0.683516 4.133294
H 5.018845 -0.618521 2.435195
C 2.134221 1.243133 -1.425291
O 2.137388 0.149592 -0.796111
N 2.871768 2.268424 -0.980888
C 2.984558 3.550909 -1.667049
H 2.358731 4.303352 -1.173230
H 4.027568 3.879455 -1.630154
H 2.688161 3.466882 -2.710829
C 3.567798 2.171227 0.299547
H 3.481386 3.129262 0.819620
H 3.116381 1.386328 0.901901
H 4.630154 1.946473 0.147220
C -1.170589 -0.114773 -0.167119
C -2.343892 -0.751828 0.027373
C -1.066013 1.363509 -0.157642
C -0.145147 2.012954 0.687123
C -1.809460 2.165481 -1.046780
C 0.015675 3.397742 0.658744
H 0.457202 1.415568 1.365018
C -1.643408 3.550965 -1.084991
H -2.509652 1.687556 -1.726519
C -0.729114 4.176647 -0.232540
H 0.732104 3.869339 1.326768
H -2.227081 4.143135 -1.785646
H -0.596252 5.254607 -0.263925
Br 0.857178 -3.133878 -1.795790
C -3.685456 -0.156758 0.382201
C -4.729830 -0.404825 -0.726192
C -4.188608 -0.737279 1.720800
H -3.579150 0.928454 0.505503
C -6.112522 0.140892 -0.344427
H -4.803025 -1.487431 -0.910077
H -4.386122 0.050899 -1.663695
C -5.570245 -0.191426 2.103396
H -4.241050 -1.833151 1.634513
H -3.459593 -0.518157 2.511820
C -6.596270 -0.438651 0.990613
H -6.836225 -0.078281 -1.140320
H -6.055916 1.236393 -0.262022
H -5.908446 -0.647692 3.042888
H -5.491760 0.890197 2.287626
H -7.567228 -0.005665 1.263948
H -6.752404 -1.521786 0.878230
H -2.357052 -1.845039 -0.025592
C 3.690275 -1.947304 0.889675
H 4.333933 -1.190420 0.433323
H 4.313315 -2.600532 1.510375
H 3.224458 -2.538032 0.100547
C 1.328475 1.406682 -2.689257
H 0.705387 2.303651 -2.656873
H 1.993440 1.481870 -3.557579
H 0.691545 0.530762 -2.817690

TS1
Opt Eel: -959.894226
SP Eel B3LYP: -11804.3595838
SP Eel M06L: -4946.87115824
SP Eel MN15: -4945.72604579
Gcorr: 0.372267
C -0.458150 4.654091 0.614231
H -1.546542 4.716220 0.524600
C 0.983033 2.649122 0.749517
N -0.105123 3.339253 1.137853
C -0.891234 2.887198 2.281109
H -0.677655 1.838710 2.475209
H -0.645059 3.478299 3.172709
H -1.954056 3.015034 2.058195
Fe 2.059855 -0.206141 0.635564
O 1.297766 1.583449 1.338855
H -0.021202 4.815763 -0.369287
H -0.118317 5.446430 1.293415
Br 4.107155 -1.075708 -0.320794
I -0.027761 0.053427 -1.737104
C -2.356580 0.201398 -1.591807
C -2.670554 1.034481 -0.364954
C -2.921480 -1.202234 -1.531884
H -2.600198 0.714881 -2.523419
H -2.254514 2.042535 -0.464156
H -2.206398 0.573104 0.514943
H -2.467375 -1.740719 -0.691840
H -2.686754 -1.755881 -2.447262
C -4.197801 1.094376 -0.154996
C -4.448714 -1.136883 -1.318871
C -4.802128 -0.312406 -0.075513
H -5.891383 -0.250550 0.040485
H -4.414445 -0.821997 0.818244
H -4.413754 1.661337 0.759506
H -4.658037 1.643550 -0.988069
H -4.843261 -2.157155 -1.232200
H -4.919798 -0.685355 -2.203025
O 0.554520 -1.205215 1.719067
C -0.246021 -2.111369 1.378236
N -1.489035 -2.149732 1.897867
C -2.419648 -3.256023 1.703298
C -1.900047 -1.165805 2.893691
H -2.433263 -3.903474 2.589513
H -2.151267 -3.851698 0.833561
H -3.424811 -2.851872 1.552250
H -1.216547 -0.320261 2.871135
H -2.915729 -0.828817 2.666911
H -1.892740 -1.611435 3.896770
C 0.164390 -3.175141 0.389432
H -0.512866 -3.211356 -0.469029
H 1.169849 -2.945506 0.033721
H 0.167952 -4.163332 0.863028
C 1.819674 3.180920 -0.388537
H 1.234640 3.274764 -1.308151
H 2.228606 4.167391 -0.142511
H 2.641995 2.486334 -0.566724

TS2
Opt Eel: -543.658665
SP Eel B3LYP: -544.041302725
SP Eel M06L: -543.703122602

SP Eel MN15: -543.064658482
Gcorr: 0.231047
C -1.821318 -0.090164 -0.168840
C -2.444934 1.220369 0.205804
C -3.810488 1.381949 -0.508819
C -4.714299 0.169670 -0.244027
C -4.033586 -1.145937 -0.646981
C -2.667606 -1.304311 0.067606
H -4.299410 2.306619 -0.174833
H -2.627747 1.249366 1.291791
H -1.784471 2.061752 -0.034036
H -1.152969 -0.101743 -1.027587
H -4.961777 0.133159 0.827275
H -5.663377 0.282704 -0.783759
H -4.679707 -2.001675 -0.410545
H -3.872664 -1.154512 -1.733957
H -2.863590 -1.418349 1.145868
H -2.163273 -2.217707 -0.268650
H -3.640367 1.480082 -1.590043
C -0.065858 -0.313003 1.544409
H -0.873055 -0.432665 2.237287
C 1.076761 -0.219147 1.116287
C 2.337918 -0.091974 0.475259
C 2.922999 1.179529 0.287915
C 3.029074 -1.235407 0.018260
C 4.159649 1.297322 -0.340356
H 2.396503 2.062489 0.637062
C 4.265127 -1.104573 -0.608560
H 2.584691 -2.215825 0.159864
C 4.836008 0.159118 -0.791021
H 4.598046 2.281607 -0.479841
H 4.785832 -1.992272 -0.956824
H 5.800658 0.256315 -1.280695

TS3
Opt Eel: -968.985896
SP Eel B3LYP: -4711.16008283
SP Eel M06L: -4669.51395609
SP Eel MN15: -4669.19892829
Gcorr: 0.351929
C -0.590983 2.454488 -0.227364
C -0.530837 1.975697 1.191320
C -1.587837 2.706704 2.054594
C -2.981143 2.604084 1.418883
C -2.987633 3.148164 -0.015904
C -1.936124 2.416379 -0.886257
H -1.595070 2.284564 3.068261
H -0.749834 0.898723 1.231051
H 0.472053 2.110105 1.613104
H 0.087189 3.256816 -0.513068
H -3.294458 1.550454 1.402503
H -3.715189 3.143744 2.030871
H -3.983355 3.036768 -0.465516
H -2.760575 4.223206 0.000980
H -2.262228 1.374736 -0.997362
H -1.901074 2.852905 -1.891445
H -1.309409 3.765614 2.149003
C 0.678504 0.794444 -1.562202
H 0.286564 1.350155 -2.401010
C 1.735246 0.401085 -0.927923
C 3.075556 0.726792 -0.493333
C 3.870173 -0.189583 0.220317
C 3.603746 2.004279 -0.778721
C 5.156786 0.158289 0.627494
H 3.461349 -1.168504 0.449471
C 4.888070 2.347358 -0.364690
H 2.993707 2.717722 -1.325450
C 5.671175 1.425643 0.338473
H 5.760009 -0.561010 1.175086
H 5.280622 3.335225 -0.590689
H 6.673485 1.694794 0.659791
Fe 0.313811 -0.915428 -0.658337
C -2.642680 -1.158278 -0.024870
O -1.670765 -1.228390 -0.836241
N -3.859848 -0.842726 -0.475742
C -5.052224 -0.763679 0.363030
H -5.494192 0.233112 0.263811
H -5.783819 -1.506790 0.027101
H -4.817491 -0.944185 1.408591
C -4.097568 -0.580851 -1.893563
H -4.591397 0.389814 -2.001462
H -3.153299 -0.576832 -2.432332
H -4.752778 -1.357239 -2.304246
Br 1.187061 -2.919598 0.521929
C -2.440608 -1.442876 1.441706
H -2.702842 -0.575287 2.054459
H -3.064196 -2.284718 1.761091
H -1.394654 -1.699436 1.610819

TS4
Opt Eel: -968.996545
SP Eel B3LYP: -4711.17513191
SP Eel M06L: -4669.52698766
SP Eel MN15: -4669.21555898
Gcorr: 0.354898
C 2.212464 -0.875571 0.027527
C 3.446237 -0.484651 -0.773940
C 4.714146 -1.142786 -0.195713
C 4.553861 -2.663119 -0.073545
C 3.310467 -3.027340 0.747429
C 2.044831 -2.388120 0.146740
H 5.579106 -0.897395 -0.825996
H 3.321940 -0.814323 -1.816410
H 3.566622 0.604357 -0.796804
H 2.293884 -0.474433 1.052681
H 4.459366 -3.097844 -1.079726
H 5.451634 -3.103968 0.378480
H 3.187909 -4.117404 0.795500
H 3.439744 -2.674453 1.780866
H 1.872089 -2.829168 -0.845215
H 1.169658 -2.628731 0.760238
H 4.915334 -0.719037 0.798804
C 0.596551 -0.669569 -1.362308
H 1.181956 -1.097974 -2.171089
C -0.628729 -0.388866 -1.036958
C -2.019370 -0.596653 -1.334933
C -2.523755 -1.900556 -1.537570
C -2.931295 0.480804 -1.339490
C -3.888564 -2.112115 -1.727570
H -1.834858 -2.740668 -1.529123
C -4.289691 0.263221 -1.554726
H -2.556983 1.486537 -1.169887
C -4.779748 -1.034323 -1.741433
H -4.257109 -3.124339 -1.873523
H -4.972528 1.108875 -1.563103
H -5.842028 -1.203053 -1.892985
Fe 0.650035 0.742050 0.035736
C -1.471430 0.668545 1.987478
O -0.202518 0.751870 1.867954
N -2.074173 -0.513171 2.071383
C -3.524027 -0.688511 2.125775
H -4.043463 0.239657 1.902443
H -3.809910 -1.437295 1.381607
H -3.819290 -1.043723 3.119106
C -1.308033 -1.756365 2.070431
H -0.256259 -1.541712 2.241416
H -1.688406 -2.401404 2.868422
H -1.430125 -2.266243 1.110094
Br 1.524777 2.987769 -0.514523
C -2.283118 1.935648 2.047435
H -1.596200 2.781499 2.092316
H -2.903100 2.032251 1.149640
H -2.942495 1.953979 2.920348

TS5
Opt Eel: -1682.215060
SP Eel B3LYP: -9166.41671997
SP Eel M06L: -9083.24685486
SP Eel MN15: -9082.91122772
Gcorr: 0.596538
C 2.150061 -2.380819 -1.613024
C 1.084776 -1.915329 -2.620753
C 0.575259 -3.047245 -3.532907
C 0.081687 -4.246423 -2.713451
C 1.165682 -4.744882 -1.750190
C 1.649975 -3.608861 -0.830832
H -0.228083 -2.678770 -4.187537
H 0.223677 -1.501846 -2.074481
H 1.474162 -1.096282 -3.242385
H 3.048575 -2.688628 -2.182904
H -0.799629 -3.944354 -2.128893
H -0.245359 -5.056327 -3.379622
H 0.785309 -5.586451 -1.153519
H 2.018979 -5.127439 -2.330801
H 0.806172 -3.318941 -0.183047
H 2.435196 -3.979906 -0.159206
H 1.393544 -3.375204 -4.191843
C 0.637953 -0.551834 0.697434
H 0.958249 -1.457050 1.176493
C 0.106574 0.548124 0.324609
Fe 2.821128 -0.906654 -0.351168
Br 4.019836 -1.750365 1.789527
O 3.572025 0.982603 -0.559903
C 3.415983 2.072804 0.067770
N 3.574538 3.230352 -0.579076
C 3.516594 4.539375 0.063952
C 3.969698 3.242485 -1.986089
H 4.521918 4.973633 0.117870
H 2.878654 5.197817 -0.531910
H 3.104074 4.469431 1.067353
H 3.477533 4.081830 -2.481516
H 5.056476 3.364183 -2.072378
H 3.671108 2.311253 -2.461854
C 3.078975 2.074095 1.536362
H 3.870922 2.568463 2.109504
H 2.140630 2.601573 1.727839
H 2.992917 1.043319 1.879435
C 0.200742 1.775333 -0.440499
C -0.143210 3.002447 0.155737
C 0.560298 1.753801 -1.799761
C -0.106313 4.181853 -0.585524
H -0.440409 3.020199 1.199339
C 0.579898 2.934691 -2.539764
H 0.811028 0.808888 -2.267824
C 0.249040 4.152624 -1.938002
H -0.362152 5.123810 -0.108852
H 0.857963 2.904283 -3.589555
H 0.267412 5.071067 -2.517533
Fe -1.424569 -0.397888 1.177826
C -3.679189 -1.703283 -0.414965
O -2.453697 -1.685755 -0.116881
N -4.059903 -1.863940 -1.691066
C -5.447089 -1.929063 -2.135405
H -5.654185 -1.096022 -2.816875
H -5.613578 -2.868535 -2.674230
H -6.136721 -1.878899 -1.296226
C -3.069135 -1.987558 -2.756902
H -2.075350 -1.808195 -2.354931
H -3.112897 -2.992352 -3.191972
H -3.289770 -1.255628 -3.541194
Br -1.758734 -1.238201 3.541057
C -4.726512 -1.544523 0.659518
H -5.361548 -0.674208 0.466297
H -5.370266 -2.428971 0.714246
H -4.220669 -1.413661 1.616687
O -2.831121 1.167466 0.992504
C -3.103062 1.925188 0.024040
N -3.536964 3.176836 0.245376
C -2.977409 1.453490 -1.404304
C -3.890279 4.102843 -0.826347
C -3.547235 3.735992 1.592874
H -3.971833 1.256897 -1.822537
H -2.482563 2.193712 -2.036962
H -2.402825 0.530301 -1.422803
H -4.650923 4.791842 -0.450374
H -3.015381 4.683020 -1.144991
H -4.304808 3.573678 -1.683838
H -4.574763 3.957256 1.903020
H -3.104310 3.023015 2.285068
H -2.969513 4.666914 1.602014

TS6
Opt Eel: -1682.221869
SP Eel B3LYP: -9166.42021902
SP Eel M06L: -9083.24712556
SP Eel MN15: -9082.96454137
Gcorr: 0.599404
C -1.535241 -1.714393 1.069166
C -1.256542 -0.832971 2.279000
C -1.727903 -1.519126 3.573264
C -1.096613 -2.909046 3.729048
C -1.361180 -3.785493 2.497782
C -0.885982 -3.088977 1.211027
H -1.481590 -0.889407 4.438604
H -0.176748 -0.651482 2.341974
H -1.737799 0.142261 2.170198
H -2.634195 -1.899989 1.024900
H -0.010632 -2.794701 3.859203
H -1.474365 -3.400819 4.634695
H -0.857172 -4.755200 2.603106
H -2.438672 -3.992678 2.422282
H 0.201895 -2.971027 1.257135
H -1.108966 -3.711074 0.334965
H -2.823286 -1.617325 3.554028
C -0.409980 -0.999629 -0.477370
H 0.009741 -1.929409 -0.869339
C 0.414166 0.080151 -0.306501
Fe -2.358392 -0.880907 -0.723637
Br -3.366297 -2.049203 -2.696857
O -3.769353 0.313604 0.232626
C -4.189845 1.468175 -0.064084
N -4.404479 2.370087 0.900232
C -4.856857 3.736669 0.666552
C -4.086231 2.063392 2.291763
H -5.815101 3.898995 1.172374
H -4.120328 4.433829 1.079987
H -4.976054 3.941293 -0.394435
H -3.159384 2.573486 2.579888
H -4.900231 2.419205 2.930667
H -3.963595 0.990015 2.414748
C -4.466523 1.830740 -1.501924
H -5.505197 2.148782 -1.638600
H -3.815562 2.646282 -1.832470
H -4.280740 0.953099 -2.123360
C -0.053898 1.386541 0.197595
C -1.011293 2.141062 -0.512385
C 0.507518 1.979337 1.348950
C -1.403946 3.410889 -0.085075
H -1.430953 1.724646 -1.424543
C 0.105724 3.239528 1.786886
H 1.262017 1.432911 1.907441
C -0.852389 3.968617 1.071309
H -2.139785 3.966544 -0.660133
H 0.546989 3.660060 2.687045
H -1.153348 4.957992 1.404422
Fe 2.369181 -0.051805 -0.800774
C 3.137255 2.787362 -0.250358
O 3.478773 1.576211 -0.131246
N 3.439397 3.670266 0.710072
C 3.083937 5.084140 0.646210
H 2.146279 5.268646 1.183538
H 3.881804 5.664598 1.117679
H 2.978799 5.417567 -0.384634
C 4.028789 3.232475 1.971116
H 4.121788 2.148815 1.973161
H 5.017112 3.687378 2.099896
H 3.385339 3.549592 2.799207
Br 3.268749 -0.601708 -3.116355
C 2.402422 3.268690 -1.476476
H 1.484991 3.799660 -1.208931
H 3.033105 3.948255 -2.061265
H 2.151790 2.409941 -2.100969
O 3.200104 -1.315273 0.663425
C 2.896505 -2.526381 0.851311
N 2.729999 -2.972189 2.104321
C 2.719788 -3.472707 -0.310348
C 2.515367 -4.371093 2.460175
C 2.893858 -2.038733 3.217821
H 3.473916 -4.267101 -0.279148
H 1.732459 -3.943842 -0.298381
H 2.840225 -2.911492 -1.238453
H 3.397285 -4.764803 2.979376
H 1.652273 -4.445016 3.128171
H 2.327621 -4.975452 1.575815
H 3.954962 -1.885140 3.447829
H 2.444143 -1.077421 2.967328
H 2.396771 -2.456844 4.094566

TS7e
Opt Eel: -1798.930571
SP Eel B3LYP: -12295.9328462

SP Eel M06L: -12173.0901411
SP Eel MN15: -12173.4549054
Gcorr: 0.603337
C -0.240787 2.181020 1.934315
C -0.060670 2.938484 0.619678
C -0.814358 4.272879 0.634782
C -0.356120 5.148688 1.808422
C -0.474296 4.400948 3.143385
C 0.261735 3.054881 3.107562
H -0.661507 4.799134 -0.315995
H 1.007824 3.133972 0.461103
H -0.390615 2.332951 -0.229709
H -1.316470 2.030056 2.100775
H 0.693575 5.436404 1.649012
H -0.937632 6.078977 1.841968
H -0.085372 5.020109 3.961875
H -1.536818 4.217633 3.361273
H 1.342302 3.225242 2.990266
H 0.123667 2.521670 4.056851
H -1.893761 4.079563 0.722014
C 0.415528 0.829175 1.997823
H 0.333309 0.377110 2.994731
C 1.134459 0.164530 1.051058
C 1.911224 -1.026087 1.512613
C 1.986045 -2.222303 0.774117
C 2.689010 -0.940395 2.685440
C 2.777523 -3.287876 1.198770
H 1.416316 -2.318660 -0.142306
C 3.489752 -2.002667 3.109273
H 2.680286 -0.015770 3.255883
C 3.536922 -3.186098 2.368394
H 2.807141 -4.200348 0.608935
H 4.082999 -1.901050 4.014584
H 4.162384 -4.013593 2.692021
Fe 1.804852 0.767525 -0.844883
C 4.533476 -0.279985 -0.365116
O 3.580266 -0.221481 -1.197305
N 5.331820 -1.349831 -0.345955
C 6.498317 -1.490770 0.519774
H 6.308200 -2.258549 1.277754
H 7.355629 -1.798750 -0.087473
H 6.743195 -0.552665 1.012626
C 5.089886 -2.473650 -1.247639
H 4.067457 -2.435497 -1.615981
H 5.787089 -2.434825 -2.093250
H 5.249473 -3.405131 -0.698723
Br 2.070011 2.724829 -2.414522
Zn -1.066846 -0.652373 0.036200
Br 0.052108 -0.815557 -2.167705
Br -1.595802 -2.606181 1.326580
O -3.389249 -1.115550 -1.590328
C -3.791929 -2.267747 -1.363463
N -4.803189 -2.505265 -0.484900
C -5.139382 -3.832611 0.008102
C -5.306897 -1.393828 0.311010
H -4.585848 -4.060490 0.930063
H -6.211134 -3.873582 0.226572
H -4.913987 -4.597069 -0.734386
H -5.234965 -0.472903 -0.265297
H -6.352244 -1.585198 0.571171
H -4.724125 -1.279051 1.233701
O -2.376369 0.754671 0.415667
C -3.099551 1.522906 -0.283515
N -4.168067 2.088922 0.286714
C -5.022313 3.073455 -0.369629
C -4.491519 1.836784 1.689539
H -6.066374 2.756876 -0.280301
H -4.907650 4.046688 0.121253
H -4.774734 3.175880 -1.423120
H -4.256545 2.723320 2.290195
H -5.561535 1.625959 1.775618
H -3.917839 0.988182 2.052820
C -3.180729 -3.452956 -2.083596
H -2.675632 -4.118267 -1.375677
H -3.932937 -4.037715 -2.624215
H -2.443755 -3.069997 -2.791037
C -2.759350 1.847108 -1.711636
H -3.584446 1.584741 -2.378390
H -2.551469 2.916655 -1.820613
H -1.881495 1.278345 -2.011092
C 4.794012 0.859530 0.589495
H 4.900639 0.513579 1.619486
H 5.710923 1.388082 0.303698
H 3.963561 1.566886 0.540835

TS7z
Opt Eel: -1798.935853
SP Eel B3LYP: -12295.9374467
SP Eel M06L: -12173.0975302
SP Eel MN15: -12173.4586748
Gcorr: 0.602443
C -0.810932 3.227952 -0.037113
C 0.574204 3.885664 -0.232863
C 0.443792 5.346411 -0.680031
C -0.401653 6.161345 0.306776
C -1.775192 5.514327 0.526549
C -1.644827 4.051345 0.969024
H 1.440103 5.794177 -0.789012
H 1.125144 3.840755 0.718232
H 1.150867 3.306207 -0.963265
H -1.332514 3.234948 -1.001277
H 0.127105 6.220922 1.269558
H -0.520726 7.191304 -0.053257
H -2.348322 6.079742 1.272520
H -2.348553 5.555177 -0.411022
H -1.155669 4.007562 1.953325
H -2.637653 3.599827 1.088485
H -0.027738 5.377752 -1.673178
C -0.631340 1.814315 0.437429
H -0.013849 1.738063 1.331913
C -1.062455 0.652123 -0.126048
C -1.997817 0.625679 -1.283538
C -1.821685 -0.272355 -2.353755
C -3.164803 1.417619 -1.288034
C -2.745888 -0.348800 -3.395729
H -0.948182 -0.913556 -2.370401
C -4.093355 1.339198 -2.326368
H -3.352446 2.087632 -0.455803
C -3.887986 0.457000 -3.390172
H -2.577163 -1.048057 -4.210790
H -4.982304 1.964113 -2.299125
H -4.611333 0.391651 -4.198223
Fe -1.479734 -1.008652 1.082819
C -4.366721 -1.218960 0.465812
O -3.275954 -1.841539 0.659371
N -5.170586 -1.598159 -0.526223
C -6.488010 -1.023347 -0.780635
H -6.463805 -0.436352 -1.704741
H -7.211093 -1.836883 -0.895969
H -6.808252 -0.388603 0.042416
C -4.771082 -2.672055 -1.434859
H -3.688785 -2.780915 -1.422891
H -5.239093 -3.616418 -1.132872
H -5.104525 -2.415902 -2.443139
Br -1.244420 -0.959798 3.561740
Zn 1.012720 -0.341864 -0.350035
Br 0.117446 -2.738245 -0.119446
Br 1.823135 0.531868 -2.460541
O 3.390531 -1.607864 -0.193430
C 3.999188 -1.756972 -1.267122
N 5.090445 -1.007957 -1.572084
C 5.693622 -0.984976 -2.896691
C 5.448149 0.099720 -0.696351
H 5.215533 -0.227943 -3.534656
H 6.754772 -0.736799 -2.800142
H 5.614703 -1.957034 -3.382493
H 5.105390 -0.116164 0.313502
H 6.535049 0.226567 -0.699671
H 4.980747 1.032673 -1.038446
O 1.875123 0.385728 1.281361
C 2.734197 -0.074954 2.089726
N 3.741790 0.714770 2.471158
C 4.720445 0.361804 3.494379
C 3.890656 2.049902 1.894250
H 5.706973 0.224655 3.037356
H 4.781933 1.175959 4.223933
H 4.435531 -0.549619 4.014848
H 3.441864 2.802916 2.553040
H 4.956573 2.266252 1.784604
H 3.405120 2.086802 0.921394
C 3.554950 -2.806288 -2.264431
H 3.281744 -2.348770 -3.220368
H 4.343402 -3.543915 -2.452553
H 2.679653 -3.309068 -1.851253
C 2.600383 -1.455327 2.668626
H 3.535105 -2.014171 2.587166
H 2.319101 -1.390943 3.725674
H 1.816217 -1.983861 2.130905
C -4.764924 -0.080282 1.369105
H -5.091519 0.796215 0.805915
H -5.585687 -0.392401 2.025880
H -3.912208 0.190808 1.994307

TSiso
Opt Eel: -1256.929716
SP Eel B3LYP: -4999.33741763
SP Eel M06L: -4957.49309233
SP Eel MN15: -4956.87044055
Gcorr: 0.481052
Fe 0.052557 -0.974636 0.031121
C -2.813164 -1.887440 -0.301370
O -1.592098 -2.096887 -0.549190
N -3.682234 -1.665405 -1.295747
C -3.222671 -1.514818 -2.673211
H -2.143220 -1.640873 -2.711943
H -3.705980 -2.264663 -3.308467
H -3.491274 -0.517186 -3.038213
C -5.102381 -1.404857 -1.077978
H -5.665621 -1.830964 -1.912386
H -5.449883 -1.866452 -0.155289
H -5.293620 -0.325347 -1.038909
C 2.448395 -1.273867 -1.613348
O 1.527609 -1.957757 -1.070849
N 3.690074 -1.297764 -1.122311
C 4.816475 -0.575533 -1.704494
H 4.585458 -0.222337 -2.706946
H 5.076945 0.280108 -1.071185
H 5.677595 -1.248674 -1.761725
C 3.996634 -2.052859 0.090516
H 4.511526 -2.986163 -0.167351
H 4.654991 -1.450084 0.721999
H 3.077518 -2.276411 0.628978
C 0.578352 0.857093 -0.195654
C -0.640119 0.805837 -0.842845
C 1.733065 1.605060 0.078126
C 2.776555 1.123135 0.926792
C 1.932007 2.886485 -0.527303
C 3.931608 1.862889 1.135997
H 2.640806 0.165637 1.418177
C 3.096801 3.610717 -0.310365
H 1.152954 3.281763 -1.173607
C 4.112252 3.111752 0.518910
H 4.705416 1.467318 1.790365
H 3.218878 4.578632 -0.791726
H 5.020010 3.684257 0.685960
Br 0.521093 -1.699905 2.426509
C -1.944023 1.414204 -0.337305
C -1.996912 1.588183 1.185585
C -2.197120 2.767085 -1.034657
H -2.769062 0.748234 -0.630513
C -3.331075 2.198529 1.632777
H -1.170646 2.242317 1.497948
H -1.831605 0.623745 1.680528
C -3.531091 3.386147 -0.595559
H -1.373716 3.451308 -0.783245
H -2.178830 2.632771 -2.124275
C -3.600376 3.535425 0.929709
H -3.337404 2.333749 2.722084
H -4.145073 1.496250 1.397635
H -3.673765 4.360140 -1.081417
H -4.355098 2.740287 -0.933644
H -4.578367 3.933605 1.229439
H -2.846810 4.268308 1.253754
H -0.671328 0.575433 -1.918863
C -3.311791 -1.899805 1.122067
H -3.867376 -0.987897 1.360893
H -3.978591 -2.753645 1.289107
H -2.451261 -1.987535 1.786693
C 2.151621 -0.440041 -2.835160
H 2.443031 0.603823 -2.686503
H 2.690171 -0.824164 -3.708993
H 1.081268 -0.488669 -3.035973

Structures coordinate for the non-aromatic system:

06 - Non aromatic system
Opt Eel: -195.297364
SP Eel: -195.438378583
Gcorr: 0.087396
C 2.641991 -0.243622 -0.000226
H 3.650641 -0.598230 -0.000329
C 1.502800 0.163823 -0.000016
C 0.114986 0.627427 0.000215
H -0.056111 1.263716 -0.878815
H -0.055829 1.263754 0.879280
C -0.905174 -0.529110 0.000353
H -0.729236 -1.159527 -0.879885
H -0.729871 -1.158703 0.881305
C -2.343620 -0.013624 -0.000328
H -2.543578 0.602164 0.885525
H -2.542854 0.601516 -0.886773
H -3.059054 -0.844052 -0.000300

09 - Non aromatic system
Opt Eel: -634.073033
SP Eel: -6968.83493487
Gcorr: 0.202604
Fe 0.988349 0.069332 0.041087
C -1.546401 -1.335654 -0.685382
O -0.520561 -0.664195 -1.037380
N -2.727764 -1.054380 -1.225986
C -3.959294 -1.781131 -0.926018
H -4.676153 -1.098331 -0.458679
H -4.387840 -2.157785 -1.860338
H -3.774317 -2.618603 -0.258353
C -2.874089 0.022105 -2.206328
H -3.759442 0.610691 -1.951960
H -1.991828 0.657998 -2.195774
H -3.006088 -0.405472 -3.206426
C -0.485865 0.827710 1.687944
C 0.436000 0.211812 2.209738
H 1.145902 -0.270548 2.852014
C -1.669748 1.558622 1.222245
Br 1.845722 2.201945 -0.803005
Br 2.642779 -1.766289 0.341694
C -1.416795 -2.440194 0.329545
H -2.040500 -2.243188 1.206906
H -1.724679 -3.399190 -0.099589
H -0.374093 -2.516189 0.639958
H -1.707604 1.556044 0.128041
H -1.566115 2.607632 1.527696
C -2.976511 0.965844 1.789636
H -3.027300 -0.098237 1.535331
H -2.953750 1.033766 2.883506
C -4.199025 1.694479 1.235062
H -5.122952 1.269317 1.643022
H -4.175931 2.760598 1.492184
H -4.242700 1.613598 0.142382

10 - Non aromatic system
Opt Eel: -620.609931
SP Eel: -4362.57119957
Gcorr: 0.204733
C 0.806597 2.428154 -0.112208
H 1.420682 3.263431 -0.422752
C -0.346715 1.988956 0.230118
C -1.811553 2.148631 0.420542
Fe 0.977755 0.530758 0.255203
C -1.213824 -1.425742 0.803923
O 0.011238 -1.129077 0.943016
N -1.669302 -1.844780 -0.377743
C -3.063412 -2.183213 -0.653769
H -3.457285 -1.514108 -1.425856
H -3.122845 -3.214711 -1.015155
H -3.672973 -2.086429 0.241260
C -0.741799 -1.910637 -1.508034
H 0.176835 -2.422327 -1.214599
H -1.221840 -2.459325 -2.319018
H -0.489153 -0.903021 -1.860735
Br 3.349757 -0.260820 -0.196749
C -2.141103 -1.326085 1.987359
H -2.953156 -0.618902 1.789491
H -2.588943 -2.296461 2.226201
H -1.565749 -0.975293 2.844947
H -2.133289 1.597492 1.312353
H -2.056604 3.207029 0.588900
C -2.597350 1.626266 -0.798324
H -2.342904 2.237401 -1.673614
H -2.266504 0.606443 -1.020147
C -4.107470 1.640809 -0.566475
H -4.644199 1.270164 -1.447659
H -4.381543 1.005526 0.285124
H -4.468695 2.655319 -0.356515

13 - Non aromatic system
Opt Eel: -1569.101677
SP Eel: -9053.25807103
Gcorr: 0.602669
C 3.226693 0.236037 -1.067310
C 2.718010 0.055568 -2.499547
C 3.739942 -0.694417 -3.375672
C 4.127483 -2.038211 -2.745055
C 4.644484 -1.858872 -1.311339
C 3.620155 -1.103288 -0.444221
H 3.333315 -0.850298 -4.384645
H 1.782467 -0.520330 -2.481931
H 2.480933 1.025987 -2.956517
H 4.113450 0.905489 -1.079870
H 3.241126 -2.689874 -2.726968
H 4.879859 -2.547121 -3.362147
H 4.873279 -2.836245 -0.864962
H 5.587598 -1.292682 -1.334649
H 2.721430 -1.727514 -0.344484
H 4.017331 -0.958729 0.569270
H 4.641530 -0.074078 -3.488305
C 0.786093 0.083972 0.410352
H 1.091551 -0.486282 1.295805
C -0.398444 -0.031767 -0.179030
Fe 2.145405 1.501729 0.055499
Br 3.337305 2.237339 2.216536
O 1.102132 3.203254 -0.451088
C -0.073564 3.512390 -0.095219
N -0.929321 4.024016 -0.987018
C -2.304052 4.406567 -0.684608
C -0.550047 4.191362 -2.386815
H -2.453641 5.460264 -0.943853
H -2.989993 3.798683 -1.285406
H -2.535516 4.265296 0.367833
H -1.202921 3.577590 -3.017052
H -0.670333 5.241685 -2.673215
H 0.484659 3.888345 -2.526327
C -0.515225 3.313385 1.333171
H -0.854197 4.255616 1.775834
H -1.337624 2.593706 1.391556
H 0.329743 2.935037 1.909599
C -0.831248 0.628151 -1.465407
Fe -1.589065 -1.259824 0.954405
C -4.048855 -0.192474 -0.231943
O -3.493165 -1.274769 0.123269
N -4.714181 -0.118831 -1.389640
C -5.391609 1.096134 -1.840190
H -5.423098 1.084326 -2.931796
H -6.418817 1.137217 -1.458850
H -4.850896 1.987417 -1.522071
C -4.896166 -1.297041 -2.234188
H -4.390055 -2.148310 -1.785070
H -5.965988 -1.513734 -2.330635
H -4.483821 -1.102934 -3.229015
Br -1.880241 -1.112520 3.459187
C -3.972863 1.035410 0.641173
H -3.358570 1.809371 0.170789
H -4.966737 1.458264 0.819188
H -3.525561 0.763051 1.598380
O -0.911416 -3.135361 0.356722
C 0.274303 -3.551799 0.509573
N 0.964619 -4.029112 -0.533670
C 0.929671 -3.521216 1.867129
C 2.274502 -4.664430 -0.403187
C 0.363463 -4.093220 -1.863019
H 1.219697 -4.528948 2.183720
H 1.831362 -2.900037 1.854691
H 0.223059 -3.107738 2.587919
H 2.164072 -5.748390 -0.276102
H 2.843855 -4.474321 -1.314950
H 2.827272 -4.256817 0.441162
H 0.176970 -5.137720 -2.140103
H -0.573812 -3.542230 -1.865056
H 1.054081 -3.653269 -2.588623
H -0.027572 1.255231 -1.875989
H -1.678522 1.299298 -1.265506
C -1.272996 -0.375215 -2.542719
H -0.421687 -1.014879 -2.810150
H -2.040145 -1.038850 -2.129163
C -1.813077 0.322209 -3.791397
H -1.051374 0.969738 -4.244622
H -2.128963 -0.401786 -4.552097
H -2.678994 0.950415 -3.545536

14e - Non aromatic system
Opt Eel: -1685.809556
SP Eel: -12182.7888507
Gcorr: 0.607541
C 0.771567 3.366069 1.522399
C -0.525595 3.423606 2.360770
C -1.374963 4.649846 2.000315
C -1.692822 4.693465 0.499664
C -0.417850 4.595552 -0.347891
C 0.430277 3.374413 0.031770
H -2.305183 4.650329 2.583902
H -1.101289 2.507769 2.173557
H -0.277712 3.437055 3.430732
H 1.314484 4.304889 1.736613
H -2.352865 3.854257 0.249722
H -2.243735 5.610941 0.253869
H -0.674316 4.557578 -1.414840
H 0.182634 5.505683 -0.201204
H -0.117632 2.456375 -0.220571
H 1.346324 3.363711 -0.567560
H -0.826839 5.561680 2.280731
C 1.669757 2.243030 1.983441
H 1.933924 2.357501 3.047027
C 2.184221 1.188902 1.314782
C 3.119115 0.281102 2.112031
Fe 1.949033 0.613160 -0.649405
C 4.766987 -0.520547 -0.785824
O 3.541850 -0.721061 -1.005513
N 5.567774 -1.558136 -0.501813
C 7.014111 -1.464898 -0.338223
H 7.292662 -1.754043 0.681383
H 7.501830 -2.149775 -1.040919
H 7.370791 -0.456113 -0.532675
C 5.018884 -2.909653 -0.421575
H 3.946992 -2.860071 -0.241478
H 5.206350 -3.453809 -1.355625
H 5.508846 -3.440820 0.398822
Br 1.734593 1.628629 -2.955258
Zn -1.527107 -1.209625 0.740394
Br 0.300933 -1.586360 -0.844846
Br -1.346818 -2.094520 2.956566
O -3.240048 -1.740712 -0.178220
C -3.519897 -2.577703 -1.086846
N -4.571952 -2.361050 -1.879830
C -4.984575 -3.274422 -2.943292
C -5.442339 -1.202277 -1.682114
H -5.805643 -3.915282 -2.601192
H -5.333406 -2.679214 -3.791435
H -4.154082 -3.894095 -3.276006
H -5.148290 -0.668996 -0.781626
H -5.373000 -0.534482 -2.547077
H -6.477221 -1.546715 -1.585042
O -2.106516 0.702458 0.751163
C -2.828939 1.213780 -0.160664
N -3.943898 1.867573 0.171522
C -4.793202 2.580473 -0.778351
C -4.356707 1.984670 1.568649
H -5.811372 2.182426 -0.720298
H -4.815734 3.643881 -0.516620
H -4.427696 2.475215 -1.796487
H -4.181123 3.006404 1.923249
H -5.425660 1.763580 1.640271
H -3.791134 1.284604 2.179091
C -2.692721 -3.822987 -1.271737
H -3.322729 -4.717184 -1.291006
H -2.131858 -3.780840 -2.211604
H -1.984225 -3.905342 -0.447290
C -2.417675 1.124127 -1.606503
H -3.202091 0.672969 -2.220595
H -2.205867 2.122517 -2.003538
H -1.511017 0.525924 -1.683893
C 5.347395 0.872073 -0.843392
H 5.915834 1.115820 0.058660
H 6.016984 0.971814 -1.705380
H 4.531722 1.588007 -0.955851
H 4.116335 0.280097 1.646150
H 3.266921 0.682392 3.130109
C 2.661778 -1.180122 2.226356
H 2.496569 -1.587588 1.223899
H 1.687058 -1.217192 2.729785
C 3.672683 -2.051737 2.973933
H 3.343137 -3.097179 3.026071
H 4.650595 -2.035569 2.475072
H 3.822619 -1.698470 4.002827

14 - Non aromatic system
Opt Eel: -855.895658
SP Eel: -4598.00571338
Gcorr: 0.355158
Fe 0.196149 -0.618461 0.384933
H -3.748708 1.894656 -0.271255
C -2.944045 2.271535 -0.912371
N -1.901138 2.917561 -0.113952
H -3.354555 3.008743 -1.604135
H -2.523226 1.438523 -1.477197
C -1.919815 4.377152 -0.079731
C -1.056150 2.156861 0.586877
H -1.769464 4.770259 -1.090485
H -1.139139 4.764050 0.570853
H -2.891359 4.721231 0.291422
O -1.201905 0.898251 0.561087
C 0.039839 2.794845 1.400853
H 0.664908 3.448956 0.785608
H -0.384672 3.396848 2.212190
H 0.656322 2.008284 1.837562
C 3.497400 -1.179132 -2.492464
C 4.047561 0.253455 -2.501938
C 2.915155 1.289193 -2.499859
C 1.958427 1.065430 -1.313002
C 1.401991 -0.366710 -1.262947
C 2.540199 -1.397484 -1.305047
H 3.331306 2.306575 -2.473744
H 4.670302 0.403401 -1.606617
H 4.703753 0.406177 -3.369398
H 2.951748 -1.361090 -3.430824
H 4.324549 -1.902775 -2.461390
H 2.508855 1.280206 -0.382726
H 1.139378 1.797543 -1.360939
H 0.764412 -0.520039 -2.154498
H 3.124384 -1.333542 -0.373245
H 2.134238 -2.419173 -1.342409
H 2.346473 1.202902 -3.438167
Br 1.397487 -0.672277 2.657075
C -0.680090 -2.663004 0.683946
H -0.054571 -3.326598 1.246813
C -1.558864 -2.111293 0.029359
C -2.699755 -1.615921 -0.746371
H -3.085979 -0.709351 -0.268451
H -2.349736 -1.317077 -1.742990
C -3.819441 -2.666907 -0.878629
H -4.153435 -2.960828 0.123816
H -3.414038 -3.566046 -1.357980
C -4.996105 -2.122249 -1.687292
H -5.426138 -1.233333 -1.209149
H -4.682437 -1.839779 -2.699891
H -5.789739 -2.872613 -1.777984

14z - Non aromatic system
Opt Eel: -1685.811907
SP Eel: -12182.7914244
Gcorr: 0.607051
C -2.980932 2.595525 -0.836973
C -1.926642 3.612258 -1.325699
C -2.566032 4.798148 -2.059041
C -3.615514 5.495482 -1.183914
C -4.673558 4.500044 -0.690955
C -4.031624 3.312192 0.037563
H -1.791448 5.512577 -2.367654
H -1.365862 3.985436 -0.456458
H -1.200241 3.105762 -1.974148
H -3.499718 2.206166 -1.722035
H -3.115465 5.949153 -0.315281
H -4.092228 6.314595 -1.737919
H -5.392683 5.003441 -0.031517
H -5.244382 4.125465 -1.553465
H -3.543428 3.668931 0.957364
H -4.802985 2.595085 0.348278
H -3.047006 4.436499 -2.979911
C -2.325749 1.462379 -0.079789
H -1.803567 1.810694 0.818009
C -2.295263 0.138939 -0.357078
C -2.979346 -0.461234 -1.572254
Fe -1.285337 -1.059661 0.935306
C -3.156819 -3.309686 0.510195
O -1.940749 -3.047053 0.734646
N -3.492180 -4.181706 -0.450391
C -4.863857 -4.598883 -0.724733
H -4.989506 -4.693479 -1.807087
H -5.069271 -5.571983 -0.262121
H -5.580251 -3.867112 -0.356651
C -2.464119 -4.888229 -1.210475
H -1.486140 -4.482584 -0.962375
H -2.492863 -5.956754 -0.965840
H -2.656672 -4.766980 -2.280531
Br -1.090216 -0.572574 3.389484
Zn 2.055184 0.430032 -0.696021
Br 1.135387 -1.767874 -0.030459
Br 1.643339 1.234578 -2.921966
O 4.023147 0.235360 -0.342406
C 4.835843 -0.651364 -0.748155
N 6.008118 -0.792428 -0.128190
C 6.998987 -1.808183 -0.476732
C 6.376316 0.083351 0.983964
H 7.828937 -1.355254 -1.030790
H 7.388562 -2.242870 0.448218
H 6.556425 -2.604248 -1.071699
H 5.767578 0.984950 0.963894
H 6.229830 -0.435756 1.938027
H 7.432215 0.349217 0.883679
O 1.549902 1.749265 0.691683
C 1.655435 1.673924 1.957367
N 1.001709 2.549444 2.719426
C 1.020610 2.523353 4.179773
C 0.194497 3.614410 2.129597
H 1.721030 3.272767 4.566766
H 0.015642 2.759105 4.538696
H 1.290165 1.538743 4.553584
H -0.866323 3.425272 2.324101
H 0.474383 4.568271 2.588491
H 0.366060 3.656223 1.057268
C 4.502375 -1.536565 -1.920694
H 5.313895 -1.546954 -2.654238
H 4.330405 -2.566417 -1.588994
H 3.596798 -1.168526 -2.403644
C 2.514925 0.623835 2.608299
H 3.125963 1.045236 3.410567
H 1.876958 -0.161119 3.028844
H 3.171163 0.181734 1.859954
C -4.245261 -2.652143 1.323855
H -4.893209 -2.031610 0.696346
H -4.871184 -3.401786 1.819259
H -3.780057 -2.021653 2.083314
H -3.804553 -1.108712 -1.235062
H -3.442920 0.299211 -2.218688
C -2.041700 -1.322520 -2.434440
H -1.573568 -2.087751 -1.804720
H -1.219236 -0.696862 -2.806529
C -2.766358 -1.989848 -3.604111
H -3.206981 -1.243834 -4.278507
H -2.086163 -2.613506 -4.197534
H -3.581892 -2.631946 -3.246354

15e - Non aromatic system
Opt Eel: -1397.940985
SP Eel: -11894.6860138
Gcorr: 0.482811
C -0.783844 2.149945 1.257532
C -1.824721 1.995958 2.394015
C -2.906173 3.081728 2.329798
C -3.593820 3.108429 0.959528
C -2.565764 3.254968 -0.167812
C -1.489359 2.162079 -0.107013
H -3.644803 2.918143 3.125399
H -2.289547 1.006668 2.298609
H -1.318145 2.022730 3.367659
H -0.309965 3.133583 1.373955
H -4.154980 2.175556 0.814986
H -4.324022 3.926788 0.916615
H -3.064898 3.226406 -1.145012
H -2.081700 4.239752 -0.089602
H -1.953597 1.193321 -0.299211
H -0.758107 2.331715 -0.902830
H -2.446216 4.062077 2.522194
C 0.315974 1.122772 1.484763
H 1.095185 1.508004 2.156699
C 0.338449 -0.228383 1.248155
C 1.362197 -1.045402 2.033142
Fe 1.501575 0.836942 -0.587999
C 4.267530 0.097870 0.426867
O 3.306113 0.038834 -0.404540
N 5.215631 -0.835336 0.392420
C 6.367443 -0.856146 1.291280
H 6.218316 -0.195972 2.142138
H 6.503444 -1.877618 1.657457
H 7.269414 -0.552524 0.748360
C 5.191393 -1.912032 -0.597101
H 4.372993 -1.756565 -1.295562
H 6.143090 -1.918771 -1.138029
H 5.066354 -2.872198 -0.086851
Br 0.131134 -0.287720 -2.345769
Zn -1.021956 -1.283979 0.220844
Br 2.040899 3.243332 -1.018487
Br -1.326407 -3.601935 -0.449278
C 4.346300 1.213730 1.434469
H 4.308699 0.823392 2.456090
H 5.280738 1.772682 1.319318
H 3.510759 1.896101 1.280438
O -2.964895 -0.784010 0.523588
C -3.966176 -0.554900 -0.214112
N -5.151389 -0.294851 0.347013
C -3.837507 -0.549663 -1.714463
C -6.350981 0.056060 -0.408374
C -5.325539 -0.345365 1.796925
H -4.604553 -1.171012 -2.185391
H -3.939591 0.470181 -2.102460
H -2.853667 -0.928465 -1.990076
H -6.840358 0.898708 0.088889
H -6.104650 0.352595 -1.425476
H -7.046514 -0.790684 -0.432969
H -4.465623 -0.827603 2.256105
H -5.434533 0.668353 2.198102
H -6.232424 -0.914412 2.023785
H 2.195075 -0.403226 2.356288
H 0.855378 -1.355570 2.961316
C 1.912647 -2.309691 1.363033
H 1.091389 -3.012548 1.182353
H 2.323400 -2.059755 0.379313
C 2.988138 -2.985063 2.215626
H 3.836988 -2.312343 2.389097
H 2.590007 -3.274607 3.196996
H 3.370938 -3.891329 1.731697

15z - Non aromatic system
Opt Eel: -1397.943325
SP Eel: -11894.6900485
Gcorr: 0.482413
C -1.152414 2.629525 1.139438
C -1.943139 2.522566 2.466961
C -2.267794 3.907072 3.040890
C -3.026511 4.772543 2.027220
C -2.256352 4.878718 0.705014
C -1.930998 3.494225 0.132494
H -2.850970 3.799765 3.964456
H -2.877597 1.976067 2.273705
H -1.372358 1.930392 3.192066
H -0.197082 3.125063 1.355540
H -4.011378 4.321833 1.835014
H -3.210710 5.771337 2.443212
H -2.832491 5.459924 -0.026299
H -1.318222 5.427359 0.875832
H -2.868342 2.976176 -0.121866
H -1.355315 3.585568 -0.794963
H -1.328857 4.409963 3.315059
C -0.897064 1.240341 0.602578
H -1.692331 0.874798 -0.053741
C 0.098101 0.369201 0.951864
C 1.163124 0.749697 1.971746
Fe 0.757224 0.681871 -1.205030
C 3.691236 0.608838 -0.377365
O 2.678370 0.146871 -0.993164
N 4.454240 -0.211272 0.341635
C 5.682661 0.201605 1.017483
H 6.034776 1.162313 0.648418
H 5.510292 0.265364 2.097614
H 6.454207 -0.550061 0.827059
C 4.094665 -1.619241 0.507428
H 3.049641 -1.772857 0.252614
H 4.723848 -2.244788 -0.136348
H 4.263702 -1.901820 1.549825
Br -0.529304 -1.225115 -2.262475
Zn -0.286298 -1.575230 0.491641
Br 0.789200 2.719018 -2.617762
Br 0.770383 -3.727508 0.760821
C 4.034491 2.071955 -0.468397
H 4.197361 2.508888 0.520870
H 4.948564 2.211406 -1.057213
H 3.218222 2.594071 -0.968905
O -2.282364 -1.782568 0.809737
C -3.192619 -2.234122 0.053624
N -4.350601 -1.573965 -0.050976
C -2.994903 -3.523265 -0.702038
C -5.489447 -2.027103 -0.843195
C -4.568879 -0.321631 0.670520
H -3.720071 -4.275301 -0.371781
H -3.121658 -3.381032 -1.779229
H -1.987556 -3.891168 -0.507581
H -5.810197 -1.214309 -1.502892
H -5.233608 -2.891615 -1.450759
H -6.321688 -2.288079 -0.179562
H -3.715438 -0.113689 1.310676
H -4.701268 0.496324 -0.046215
H -5.476276 -0.407417 1.277640
H 2.099986 1.003707 1.462746
H 0.870866 1.650350 2.526169
C 1.475913 -0.370590 2.971693
H 0.561292 -0.632785 3.522772
H 1.775001 -1.270299 2.420008
C 2.584046 0.018065 3.950852
H 3.510937 0.262913 3.415031
H 2.301784 0.897350 4.544444
H 2.806059 -0.799439 4.647621

16e - Non aromatic system
Opt Eel: -1685.821099
SP Eel: -12182.8003698
Gcorr: 0.606640
C 2.628326 -0.615099 2.652956
C 4.114308 -0.358889 2.310164
C 4.965367 -1.630868 2.424306
C 4.388684 -2.775621 1.581024
C 2.918618 -3.034620 1.933499
C 2.080421 -1.759166 1.783152
H 5.999546 -1.418600 2.121493
H 4.160389 0.022369 1.283233
H 4.517281 0.426356 2.964070
H 2.598204 -0.967704 3.695934
H 4.456909 -2.511713 0.516210
H 4.984472 -3.687369 1.720492
H 2.510104 -3.829779 1.294910
H 2.852536 -3.398463 2.970292
H 2.094479 -1.459258 0.731263
H 1.032190 -1.952072 2.037200
H 5.004884 -1.947028 3.477449
C 1.828062 0.673651 2.597884
H 1.701352 1.145961 3.583090
C 1.331487 1.327325 1.530840
C 0.670617 2.673723 1.773483
Zn 1.424470 0.798510 -0.378913
C 3.501980 -0.670297 -2.121511
O 3.140640 -0.050702 -1.082317
N 4.786003 -1.022452 -2.271260
C 5.282560 -1.792726 -3.409487
H 5.690899 -1.129073 -4.181220
H 6.080592 -2.451395 -3.056467
H 4.496642 -2.410821 -3.840613
C 5.805733 -0.595009 -1.316063
H 5.381597 0.127696 -0.623318
H 6.185767 -1.457056 -0.758036
H 6.635212 -0.136747 -1.865087
Br 0.944603 2.429463 -2.216914
Fe -2.161236 -0.790897 0.847241
Br -0.424625 -1.116292 -0.974562
Br -1.962640 -2.271306 2.798289
O -3.871774 -1.219966 -0.189800
C -4.085839 -2.077434 -1.098669
N -4.907551 -1.785021 -2.109238
C -5.228139 -2.708994 -3.194021
C -5.586072 -0.491948 -2.180704
H -6.243783 -3.101343 -3.067653
H -5.177375 -2.164827 -4.141873
H -4.522990 -3.536375 -3.231066
H -5.454134 0.046879 -1.245366
H -5.175900 0.098355 -3.007234
H -6.652118 -0.660913 -2.362517
O -2.527125 1.135778 1.142929
C -2.702614 2.120694 0.354641
N -2.794780 3.352189 0.851905
C -2.964154 4.530441 -0.002309
C -2.794008 3.597728 2.293571
H -4.011383 4.650613 -0.301014
H -2.657965 5.408090 0.568519
H -2.335559 4.460242 -0.891078
H -1.967824 4.266831 2.548396
H -3.739092 4.073307 2.576763
H -2.681339 2.656769 2.826528
C -3.436338 -3.436239 -1.031809
H -4.184471 -4.233924 -1.079857
H -2.735376 -3.576818 -1.861132
H -2.889634 -3.519591 -0.091456
C -2.786424 1.917323 -1.131215
H -3.567172 2.534056 -1.583372
H -1.822858 2.176792 -1.588749
H -2.990783 0.868490 -1.340174
C 2.516328 -1.031591 -3.202212
H 2.921922 -0.842096 -4.199457
H 2.256009 -2.094517 -3.134981
H 1.611694 -0.441135 -3.067117
H -0.238976 2.767177 1.169145
H 0.360310 2.770830 2.827280
C 1.584945 3.859879 1.424235
H 2.468629 3.832993 2.077497
H 1.947745 3.738292 0.395673
C 0.876516 5.209221 1.559368
H 1.546285 6.043322 1.315188
H 0.013162 5.266558 0.883855
H 0.509290 5.366632 2.581899

16z - Non aromatic system
Opt Eel: -1685.821403
SP Eel: -12182.7971662
Gcorr: 0.607288
C -3.792410 -1.459795 -0.983035
C -5.177028 -1.280360 -0.325518
C -6.251521 -2.153483 -0.985565
C -5.844763 -3.632584 -0.988722
C -4.475735 -3.827806 -1.652615
C -3.402965 -2.953381 -0.990555

H -7.212173 -2.023010 -0.470135
H -5.097091 -1.546163 0.739534
H -5.468033 -0.222236 -0.362763
H -3.874002 -1.131392 -2.027070
H -5.796042 -3.994429 0.049118
H -6.606288 -4.236420 -1.499118
H -4.179500 -4.884264 -1.611889
H -4.550392 -3.561667 -2.717432
H -3.254647 -3.284013 0.049097
H -2.438180 -3.076220 -1.499341
H -6.401935 -1.818805 -2.022640
C -2.758801 -0.633606 -0.252748
H -2.762305 -0.835146 0.822008
C -1.881073 0.270988 -0.732424
C -1.784351 0.608313 -2.204456
Zn -0.789122 1.223784 0.625217
C -3.218681 1.458039 2.267239
O -1.977809 1.251304 2.362630
N -4.088244 0.667512 2.914574
C -5.533653 0.858215 2.919725
H -6.021125 -0.022442 2.487507
H -5.883017 0.979278 3.951473
H -5.820604 1.736776 2.347169
C -3.616078 -0.473682 3.691955
H -2.564055 -0.649461 3.476628
H -3.743771 -0.280567 4.763826
H -4.202872 -1.357608 3.422369
Br 0.268824 3.452196 0.585262
Fe 2.030269 -1.098710 -0.537943
Br 1.092430 -0.364257 1.709175
Br 1.180059 -3.162564 -1.569830
O 3.987756 -1.451024 -0.089637
C 4.512046 -1.974646 0.940339
N 5.708202 -1.558118 1.359927
C 6.395155 -2.102758 2.528746
C 6.446427 -0.526821 0.632081
H 7.189396 -2.790399 2.216037
H 6.845389 -1.274394 3.083021
H 5.702859 -2.623222 3.187179
H 5.981027 -0.353520 -0.335271
H 6.454984 0.404195 1.209135
H 7.477690 -0.864621 0.490528
O 2.099214 0.594959 -1.577242
C 2.705934 1.703329 -1.409330
N 2.475505 2.709366 -2.248928
C 3.060688 4.036836 -2.075916
C 1.427098 2.619952 -3.262202
H 3.172195 4.493634 -3.061927
H 2.399748 4.660747 -1.463307
H 4.042291 3.978640 -1.608488
H 0.576173 3.237107 -2.955644
H 1.816296 2.990782 -4.214582
H 1.105990 1.587577 -3.370348
C 3.805998 -3.079851 1.682601
H 4.450490 -3.958095 1.788862
H 3.512288 -2.751387 2.685216
H 2.909933 -3.363310 1.129313
C 3.693139 1.890687 -0.289799
H 4.692864 2.098589 -0.685532
H 3.390133 2.728294 0.344618
H 3.739411 0.987115 0.313668
C -3.745469 2.599379 1.429556
H -4.421758 2.239116 0.648582
H -4.291509 3.319812 2.048502
H -2.901271 3.109775 0.964841
H -2.371575 -0.082437 -2.827670
H -0.739972 0.498816 -2.530296
C -2.231090 2.046302 -2.517144
H -3.255442 2.189166 -2.144811
H -1.598432 2.745228 -1.954563
C -2.181976 2.374055 -4.010631
H -1.175364 2.222769 -4.419234
H -2.866244 1.729943 -4.577947
H -2.467704 3.415512 -4.203922

I08 - Non aromatic system
Opt Eel: -1569.090396
SP Eel: -9053.24087530
Gcorr: 0.602792
C 1.615516 2.665176 0.947718
C 0.966645 2.082747 2.214869
C 0.199414 3.133593 3.037758
C -0.836690 3.868472 2.176628
C -0.194443 4.483711 0.926868
C 0.572330 3.426649 0.111028
H -0.293323 2.659839 3.899270
H 0.260299 1.290296 1.928461
H 1.722019 1.599580 2.850963
H 2.398604 3.382438 1.258400
H -1.612300 3.155956 1.863682
H -1.343726 4.643703 2.767026
H -0.962422 4.966370 0.305301
H 0.506635 5.274560 1.234270
H -0.155736 2.711382 -0.301579
H 1.049541 3.904358 -0.755493
H 0.914748 3.864217 3.445164
C 0.980407 -0.838465 -0.948931
H 1.654392 -0.756293 -1.790596
C 0.766140 -1.155223 0.276357
Fe 2.548929 1.239016 -0.178455
Br 3.260458 1.742396 -2.586217
O 4.023018 -0.022398 0.498020
C 4.324868 -1.239927 0.323235
N 4.657297 -2.004143 1.367877
C 5.007240 -3.418046 1.262495
C 4.718232 -1.455688 2.720096
H 6.091129 -3.550843 1.358134
H 4.514596 -3.957554 2.076685
H 4.672551 -3.839575 0.317087
H 3.963411 -1.939148 3.348849
H 5.709193 -1.652710 3.142909
H 4.538954 -0.383551 2.691803
C 4.327668 -1.832147 -1.062477
H 5.277636 -2.330131 -1.280179
H 3.525054 -2.569927 -1.170195
H 4.169818 -1.028595 -1.782744
C 1.267044 -1.511344 1.633859
Fe -0.958213 -0.993304 -0.739609
C -3.503907 0.705217 -1.357891
O -2.249248 0.584049 -1.327357
N -4.072113 1.897103 -1.114278
C -5.509250 2.144569 -1.158937
H -5.690065 3.081334 -1.695485
H -6.034652 1.344866 -1.676063
H -5.909512 2.241705 -0.142359
C -3.257188 3.053613 -0.754636
H -2.253195 2.727046 -0.500306
H -3.210186 3.759034 -1.592886
H -3.710903 3.557950 0.103792
Br -1.424135 -2.732024 -2.632242
C -4.392131 -0.474627 -1.669517
H -5.147337 -0.622076 -0.891618
H -4.915104 -0.317728 -2.619878
H -3.771716 -1.365508 -1.756316
O -2.407303 -1.543900 0.679784
C -3.142418 -0.867545 1.443320
N -4.316067 -1.365815 1.869048
C -2.733515 0.511048 1.902699
C -5.235841 -0.642326 2.740368
C -4.799915 -2.655149 1.385970
H -3.511392 1.249396 1.688531
H -2.545332 0.522750 2.981639
H -1.819752 0.794868 1.385742
H -6.031302 -0.167331 2.152462
H -5.692916 -1.353261 3.434725
H -4.716699 0.117710 3.321527
H -5.795620 -2.528974 0.946843
H -4.115017 -3.042251 0.634829
H -4.871665 -3.363374 2.219372
H 1.964584 -0.733970 1.967354
H 1.862954 -2.430718 1.539141
C 0.192934 -1.713977 2.707334
H -0.496762 -2.503144 2.387921
H -0.401800 -0.798376 2.793852
C 0.809535 -2.061240 4.062130
H 1.473897 -1.260347 4.411208
H 0.035611 -2.208078 4.824932
H 1.401302 -2.983969 4.005357

P0 - Non aromatic system
Opt Eel: -430.587278
SP Eel: -430.876597577
Gcorr: 0.240806
C -0.931976 0.000364 0.347524
C -1.628685 -1.264669 -0.193722
C -3.132744 -1.264751 0.109574
C -3.813373 -0.000440 -0.429718
C -3.133257 1.264358 0.109027
C -1.629154 1.264761 -0.194250
H -3.600826 -2.161788 -0.315996
H -1.475920 -1.312628 -1.282352
H -1.151923 -2.156867 0.231653
H -1.025657 0.000524 1.442502
H -3.756548 -0.000651 -1.528313
H -4.879310 -0.000595 -0.168023
H -3.601684 2.161030 -0.316927
H -3.281147 1.317342 1.197577
H -1.476465 1.312443 -1.282910
H -1.152875 2.157433 0.230709
H -3.280640 -1.317323 1.198145
C 0.539253 0.000374 -0.006680
H 0.753584 0.000223 -1.086209
C 1.541092 0.000544 0.847257
C 3.016476 0.000478 0.863916
C 3.645885 -0.000391 -0.548451
H 3.289090 0.879900 -1.097402
H 3.289117 -0.881388 -1.096290
C 5.173565 -0.000336 -0.492790
H 5.605129 -0.001016 -1.500916
H 5.550276 0.886123 0.032700
H 5.550267 -0.886068 0.033917
H 3.381484 -0.876187 1.419519
H 3.381557 0.877742 1.418495

P1e - Non aromatic system
Opt Eel: -1143.842818
SP Eel: -4886.17908755
Gcorr: 0.486562
Fe -0.192496 0.576707 -0.192177
C 1.227977 -1.009914 -2.286800
O 0.097802 -0.761727 -1.779020
N 1.833658 -2.184201 -2.060700
C 1.192064 -3.206872 -1.239063
H 0.823747 -4.021521 -1.874800
H 1.925378 -3.613551 -0.536842
H 0.361368 -2.769056 -0.691338
C 3.079795 -2.597595 -2.697248
H 3.748503 -3.011485 -1.936219
H 2.880531 -3.373176 -3.446532
H 3.575709 -1.757733 -3.177848
C 2.671341 1.256138 0.727703
O 1.925369 0.750667 -0.153566
N 3.874888 0.714852 0.969325
C 4.862465 1.281490 1.880417
H 5.221076 0.497744 2.555192
H 5.715921 1.670042 1.311798
H 4.436852 2.087387 2.473555
C 4.329475 -0.439434 0.197194
H 4.850343 -1.130320 0.865851
H 3.474646 -0.936534 -0.254713
H 5.023529 -0.121261 -0.590515
C -0.711734 -0.321150 1.582912
C -1.982944 -0.705900 1.807584
C 0.346077 -0.634624 2.626606
Br -1.033818 2.759790 -1.163039
C -3.138575 -0.536812 0.853609
C -3.612957 -1.898232 0.302800
C -4.316636 0.210779 1.509313
H -2.796361 0.066054 -0.003618
C -4.808477 -1.753681 -0.647492
H -3.894614 -2.544955 1.147789
H -2.776978 -2.393778 -0.208263
C -5.514322 0.352470 0.561243
H -4.628331 -0.341635 2.408942
H -3.979715 1.199417 1.848256
C -5.969450 -1.010546 0.024650
H -5.137155 -2.742081 -0.994437
H -4.492115 -1.194226 -1.540602
H -6.343589 0.857175 1.073994
H -5.229434 0.994781 -0.285332
H -6.800937 -0.883971 -0.680752
H -6.350724 -1.618227 0.858788
H -2.253071 -1.215925 2.746579
C 1.893742 0.010564 -3.176107
H 2.890449 0.270485 -2.809798
H 1.992119 -0.369314 -4.199152
H 1.274942 0.908339 -3.184966
C 2.225902 2.469286 1.506532
H 2.250525 2.291231 2.585585
H 2.874532 3.325478 1.290093
H 1.206926 2.717993 1.205824
H 0.937560 0.265529 2.850421
H -0.114455 -0.945808 3.580744
C 1.320216 -1.735600 2.171906
H 0.762451 -2.675440 2.056623
H 1.703274 -1.482859 1.177438
C 2.492536 -1.939292 3.132836
H 2.144021 -2.221547 4.134830
H 3.167865 -2.729157 2.781192
H 3.079609 -1.017652 3.233942

P1z - Non aromatic system
Opt Eel: -1143.837760
SP Eel: -4886.17361696
Gcorr: 0.486392
Fe -0.311129 1.017403 -0.053862
C -2.695459 0.784050 1.747489
O -1.448558 0.982635 1.710999
N -3.201468 -0.249321 2.436382
C -2.333374 -1.155502 3.182413
H -2.612098 -1.135613 4.242180
H -2.456305 -2.176681 2.806805
H -1.298016 -0.844860 3.069282
C -4.627562 -0.528498 2.565171
H -4.801752 -1.587955 2.350774
H -4.961786 -0.319581 3.588379
H -5.212678 0.067592 1.869204
C -2.005678 -0.753857 -1.931923
O -1.978403 0.041616 -0.954697
N -2.804969 -1.829907 -1.889283
C -3.004287 -2.753777 -3.000227
H -2.660336 -3.754953 -2.717748
H -4.071960 -2.805657 -3.240729
H -2.464214 -2.427933 -3.886106
C -3.619446 -2.091823 -0.704131
H -3.666602 -3.171976 -0.542458
H -3.174217 -1.609919 0.162917
H -4.638262 -1.711124 -0.846229
C 1.254992 -0.303172 -0.114886
C 2.490319 0.189585 0.129587
C 0.998867 -1.775901 -0.382369
Br -0.252813 3.440734 -0.790481
C 3.823166 -0.521701 0.211524
C 4.762137 -0.071291 -0.928199
C 4.491061 -0.263319 1.578383
H 3.677891 -1.604975 0.112179
C 6.147776 -0.722982 -0.827607
H 4.870739 1.023189 -0.885637
H 4.299799 -0.304178 -1.896350
C 5.876057 -0.915234 1.680480
H 4.589727 0.823251 1.723758
H 3.836887 -0.629424 2.380635
C 6.793000 -0.459105 0.538629
H 6.796819 -0.355062 -1.633082
H 6.046833 -1.808474 -0.974840
H 6.331722 -0.682512 2.651819
H 5.764185 -2.008770 1.638243
H 7.765071 -0.964809 0.604794
H 6.988453 0.618533 0.642449
H 2.590116 1.268512 0.303483
C -3.635155 1.726308 1.036202
H -4.225792 1.199957 0.281319
H -4.324408 2.199856 1.743720
H -3.040121 2.496181 0.543636
C -1.155044 -0.501626 -3.152941
H -0.577278 -1.383309 -3.442303
H -1.785156 -0.214526 -4.002783
H -0.470896 0.319432 -2.933811
H 0.585708 -1.885004 -1.396804
H 1.917113 -2.382306 -0.369383
C -0.010838 -2.397815 0.596868

H 0.417772 -2.387120 1.608913
H -0.904342 -1.765457 0.637370
C -0.413790 -3.823150 0.217080
H 0.454810 -4.494225 0.202445
H -1.142785 -4.237870 0.924256
H -0.866527 -3.846969 -0.782428

P2e - Non aromatic system
Opt Eel: -1247.044995
SP Eel: -5409.40176925
Gcorr: 0.487781
Zn 0.476875 0.689394 0.370855
C 3.435566 0.654915 -0.235582
O 2.301184 1.051028 -0.616951
N 4.276013 0.082622 -1.112060
C 3.844461 -0.157457 -2.486406
H 3.064465 0.551684 -2.756649
H 4.702457 -0.033375 -3.152599
H 3.457982 -1.178807 -2.594531
C 5.558422 -0.509504 -0.748755
H 5.493017 -1.603187 -0.803509
H 6.325761 -0.169754 -1.451420
H 5.855172 -0.224427 0.257855
C -1.126847 0.844833 -2.113553
O -0.724517 1.500262 -1.112425
N -2.351823 1.075947 -2.608099
C -2.883483 0.435566 -3.806279
H -3.913573 0.122683 -3.612201
H -2.883302 1.138390 -4.648515
H -2.300679 -0.442829 -4.074345
C -3.183371 2.128612 -2.028098
H -4.232183 1.836276 -2.112827
H -2.922863 2.266889 -0.980331
H -3.034634 3.074396 -2.564063
C 0.321942 -1.286466 0.584481
C -0.867029 -1.901878 0.704845
C 1.622900 -2.071687 0.542233
Br 0.299633 2.429621 2.138534
C -2.217934 -1.231204 0.740741
C -3.130946 -1.743135 -0.393303
C -2.910151 -1.430665 2.104577
H -2.076115 -0.150688 0.595610
C -4.521149 -1.096265 -0.353045
H -3.235313 -2.834807 -0.298031
H -2.653946 -1.557113 -1.363229
C -4.301947 -0.786107 2.147073
H -3.001975 -2.509610 2.302322
H -2.274519 -1.018030 2.899083
C -5.193150 -1.301881 1.010082
H -5.151058 -1.502551 -1.155490
H -4.421130 -0.018819 -0.544570
H -4.776733 -0.973754 3.119054
H -4.195538 0.304946 2.053310
H -6.169297 -0.800174 1.033541
H -5.384350 -2.374902 1.159914
H -0.928002 -2.994252 0.787733
C 3.872769 0.836511 1.197772
H 4.084850 -0.127326 1.671099
H 4.779199 1.448609 1.256840
H 3.071288 1.335425 1.744262
C -0.244832 -0.191452 -2.767317
H -0.670949 -1.194207 -2.660206
H -0.120438 0.014568 -3.835367
H 0.733270 -0.169884 -2.288236
H 2.285134 -1.699129 1.340295
C 1.560649 -3.600267 0.645396
H 1.074217 -3.888603 1.587089
H 0.930267 -3.998466 -0.161400
C 2.950567 -4.235681 0.570233
H 2.900620 -5.329099 0.642759
H 3.447489 -3.987025 -0.376796
H 3.593799 -3.876644 1.384173
H 2.152917 -1.815977 -0.389419

P2z - Non aromatic system
Opt Eel: -1247.041366
SP Eel: -5409.39762054
Gcorr: 0.488197
Zn 0.714569 -0.092866 0.841834
C 1.474542 2.725962 0.453790
O 1.961796 1.580320 0.650735
N 1.958122 3.511677 -0.520991
C 3.081335 3.074511 -1.344759
H 2.770668 3.013737 -2.393157
H 3.898694 3.799826 -1.261676
H 3.421627 2.098807 -1.005683
C 1.466021 4.855043 -0.806470
H 2.160189 5.610244 -0.418193
H 1.390029 4.976333 -1.891348
H 0.480814 5.015384 -0.373302
C 2.101365 -2.370545 -0.565862
O 2.213401 -1.304448 0.097701
N 3.157360 -2.838532 -1.247445
C 3.179054 -4.114619 -1.955404
H 3.170085 -3.950146 -3.039330
H 4.096987 -4.649577 -1.691035
H 2.329408 -4.735242 -1.678896
C 4.406332 -2.082497 -1.280113
H 4.844192 -2.172052 -2.278354
H 4.207898 -1.035077 -1.059105
H 5.117339 -2.479222 -0.545240
C -0.914049 0.186010 -0.265051
C -2.103864 -0.293179 0.150634
C -0.745164 0.954389 -1.562792
Br 0.628367 -0.686637 3.257444
C -3.464118 -0.200187 -0.502948
C -4.092827 -1.599491 -0.668206
C -4.405631 0.705740 0.320011
H -3.374296 0.241813 -1.503678
C -5.501658 -1.532256 -1.271829
H -4.143326 -2.083670 0.319045
H -3.439510 -2.224607 -1.291223
C -5.815608 0.774460 -0.280665
H -4.466186 0.312468 1.346315
H -3.971714 1.711450 0.394054
C -6.421879 -0.624970 -0.445197
H -5.928741 -2.540841 -1.347773
H -5.435728 -1.139498 -2.297338
H -6.463714 1.399657 0.347475
H -5.764305 1.262465 -1.265282
H -7.412620 -0.558686 -0.913342
H -6.570281 -1.072483 0.548768
H -2.136574 -0.826239 1.107415
C 0.340745 3.231553 1.314350
H 0.574766 4.205555 1.755095
H -0.579163 3.335200 0.728946
H 0.168835 2.510106 2.114184
C 0.803444 -3.139753 -0.605335
H 0.532827 -3.429992 -1.624188
H 0.886148 -4.051787 -0.002521
H 0.006435 -2.520433 -0.193150
H -1.675507 1.011062 -2.146872
H -0.475630 1.997225 -1.331138
C 0.361706 0.387344 -2.467350
H 1.302178 0.346240 -1.904572
H 0.115582 -0.651377 -2.730072
C 0.563482 1.210570 -3.740184
H 0.813317 2.251429 -3.496983
H 1.376055 0.807280 -4.356930
H -0.346049 1.225401 -4.354610

TS2 - Non aromatic system
Opt Eel: -430.532713
SP Eel: -430.826600277
Gcorr: 0.235499
C -0.861086 -0.310694 0.321733
C -2.058083 -1.159327 0.642075
C -3.293110 -0.263027 0.906516
C -3.525770 0.711731 -0.256252
C -2.278643 1.559070 -0.545477
C -1.049194 0.656977 -0.811424
H -4.181735 -0.888068 1.066988
H -2.291068 -1.812705 -0.214108
H -1.868367 -1.811248 1.503387
H -0.282077 0.047774 1.172028
H -3.788237 0.139283 -1.158298
H -4.381718 1.362521 -0.035384
H -2.453885 2.219548 -1.405175
H -2.069450 2.205089 0.318856
H -1.226957 0.103754 -1.746755
H -0.151720 1.267971 -0.965095
H -3.131115 0.307008 1.832140
C 0.700777 -1.814106 -0.526446
H -0.092052 -2.500001 -0.753727
C 1.875738 -1.451543 -0.511590
C 3.140237 -0.737098 -0.341688
H 3.607967 -0.580597 -1.324116
C 2.978676 0.626639 0.366022
H 2.515505 0.464949 1.347045
H 2.284531 1.247299 -0.213756
C 4.317010 1.346469 0.528693
H 4.786460 1.533567 -0.445299
H 4.186200 2.313057 1.029127
H 5.016736 0.750379 1.127841
H 3.841683 -1.360127 0.231322

TS3 - Non aromatic system
Opt Eel: -855.857727
SP Eel: -4597.96851963
Gcorr: 0.357035
C -2.041587 1.693493 -0.638605
C -1.547937 1.717554 0.777546
C -2.589956 2.407878 1.690919
C -3.968000 1.748220 1.540584
C -4.434621 1.736781 0.078003
C -3.384923 1.055335 -0.833723
H -2.255455 2.365346 2.736169
H -1.410983 0.686953 1.136351
H -0.576374 2.218063 0.859718
H -1.825430 2.574445 -1.243483
H -3.911302 0.712894 1.908183
H -4.705303 2.266259 2.167441
H -5.399731 1.220670 -0.012959
H -4.590542 2.770800 -0.260947
H -3.323340 -0.008186 -0.560189
H -3.704000 1.106499 -1.882277
H -2.662357 3.470580 1.419450
C -0.651064 0.298787 -1.966139
H -1.469281 0.318338 -2.672064
C 0.620217 0.485690 -1.823874
C 1.835271 1.318408 -2.016781
Fe 0.073673 -1.038877 -0.717710
C 2.815242 -0.992928 0.522901
O 1.752328 -1.614983 0.213859
N 2.838031 -0.200767 1.594134
C 3.990611 0.596871 2.005647
H 3.695854 1.649767 2.060498
H 4.328119 0.272407 2.995533
H 4.811725 0.498143 1.299861
C 1.625977 -0.040422 2.399720
H 1.123182 -1.000983 2.518688
H 1.912454 0.346259 3.379096
H 0.939039 0.664120 1.919300
Br -1.687157 -2.622103 0.031829
C 4.056978 -1.189661 -0.307060
H 4.417137 -0.239764 -0.713231
H 4.863104 -1.627961 0.291170
H 3.816786 -1.860319 -1.132990
H 2.722698 0.678651 -2.086515
H 1.762399 1.865649 -2.968142
C 2.041317 2.326280 -0.868330
H 1.198527 3.028202 -0.854087
H 2.017396 1.786080 0.083681
C 3.360495 3.087267 -0.997342
H 3.482139 3.808430 -0.180481
H 4.215567 2.400203 -0.968435
H 3.410010 3.640767 -1.943499

TS4 - Non aromatic system
Opt Eel: -855.866167
SP Eel: -4597.97790480
Gcorr: 0.358878
C -1.930956 -0.778647 0.076743
C -3.270587 -0.294949 0.613028
C -4.434743 -1.013268 -0.096662
C -4.288898 -2.538180 -0.012993
C -2.932564 -3.001708 -0.560716
C -1.773593 -2.292946 0.163850
H -5.390303 -0.695582 0.341251
H -3.336001 -0.501900 1.691618
H -3.366593 0.790012 0.488567
H -1.859133 -0.502052 -0.988587
H -4.376726 -2.850640 1.038205
H -5.106680 -3.027695 -0.557426
H -2.828469 -4.089783 -0.455343
H -2.878575 -2.778907 -1.636240
H -1.774640 -2.611671 1.215917
H -0.811364 -2.600447 -0.261554
H -4.453201 -0.709207 -1.153280
C -0.603162 -0.367009 1.722201
H -1.360636 -0.704351 2.424399
C 0.671745 -0.116772 1.646167
C 1.855938 -0.193216 2.555335
Fe -0.258984 0.712878 0.067834
C 1.999727 0.069291 -1.676369
O 0.729785 0.140683 -1.600966
N 2.603622 -1.115524 -1.709811
C 4.052983 -1.295920 -1.741844
H 4.572949 -0.354843 -1.581612
H 4.336700 -1.993148 -0.947756
H 4.353229 -1.718793 -2.706678
C 1.827542 -2.353453 -1.660106
H 0.794693 -2.153304 -1.935635
H 2.266414 -3.069470 -2.360591
H 1.861924 -2.776021 -0.650011
Br -1.126925 3.025005 -0.151857
C 2.810906 1.336997 -1.734853
H 2.124667 2.180425 -1.820226
H 3.400507 1.454150 -0.818507
H 3.498354 1.342199 -2.585970
H 1.637013 -0.812236 3.440243
H 2.067814 0.819860 2.928664
C 3.118307 -0.725757 1.857598
H 2.908226 -1.724660 1.451911
H 3.344922 -0.082971 0.997641
C 4.325866 -0.790594 2.792298
H 4.571958 0.203087 3.188269
H 4.132179 -1.450316 3.647650
H 5.212038 -1.171733 2.270742

TS5 - Non aromatic system
Opt Eel: -1569.078745
SP Eel: -9053.23992325
Gcorr: 0.599447
C 1.895060 2.667056 0.988526
C 1.290341 2.088217 2.280653
C 0.536304 3.137595 3.117960
C -0.545976 3.832146 2.282036
C 0.046275 4.452996 1.010279
C 0.813304 3.406623 0.180084
H 0.087160 2.668438 4.005455
H 0.578216 1.290319 2.022225
H 2.068329 1.615746 2.897523
H 2.681003 3.393668 1.265895
H -1.307277 3.090352 1.998594
H -1.060739 4.597731 2.878310
H -0.748944 4.914029 0.406968
H 0.736955 5.261757 1.293547
H 0.086315 2.673503 -0.204024
H 1.254396 3.887512 -0.703577
H 1.250601 3.890509 3.484056
C 0.942400 -0.404867 -0.721711
H 1.030852 -0.064955 -1.737686
C 0.589725 -1.041245 0.335654
Fe 2.689333 1.173157 -0.169543
Br 3.439919 1.760318 -2.555836
O 3.980227 -0.259832 0.566483
C 4.134811 -1.490111 0.316329
N 4.455667 -2.338875 1.299942
C 4.658341 -3.771317 1.106529
C 4.659122 -1.869510 2.667386
H 5.726844 -4.013822 1.146152
H 4.147564 -4.307064 1.912380
H 4.247846 -4.104607 0.156117
H 3.923143 -2.337581 3.329662
H 5.663671 -2.150800 3.002046
H 4.550871 -0.788213 2.705319
C 3.962974 -2.011320 -1.088055
H 4.842592 -2.577184 -1.411089
H 3.090726 -2.670236 -1.155025
H 3.818731 -1.163918 -1.759255

C 1.096874 -1.534541 1.651470
Fe -1.096579 -0.997067 -0.720820
C -3.433183 0.910884 -1.367870
O -2.190333 0.702353 -1.295466
N -3.933101 2.113139 -1.046845
C -5.347573 2.462180 -1.120059
H -5.454508 3.409381 -1.658837
H -5.919933 1.699087 -1.641832
H -5.753806 2.587555 -0.109362
C -3.058764 3.183292 -0.574897
H -2.076021 2.778526 -0.352382
H -2.969107 3.960968 -1.342555
H -3.490615 3.628018 0.326855
Br -1.408056 -2.705789 -2.617275
C -4.373758 -0.180848 -1.817737
H -5.153056 -0.367036 -1.072787
H -4.865405 0.098554 -2.756442
H -3.799389 -1.092539 -1.981217
O -2.602296 -1.617378 0.599378
C -3.318948 -0.897486 1.345925
N -4.564670 -1.287640 1.658693
C -2.805019 0.409667 1.902385
C -5.463780 -0.532036 2.524287
C -5.131527 -2.504640 1.084910
H -3.479519 1.236693 1.663913
H -2.710392 0.355522 2.992063
H -1.823650 0.614066 1.477836
H -6.207992 0.006818 1.925030
H -5.986868 -1.230748 3.184172
H -4.916587 0.178255 3.140678
H -6.119249 -2.279450 0.669807
H -4.478209 -2.876226 0.298540
H -5.243415 -3.270250 1.861610
H 1.929426 -0.898945 1.974281
H 1.521476 -2.535190 1.483695
C 0.056778 -1.619660 2.773112
H -0.776567 -2.252948 2.450173
H -0.358947 -0.622276 2.953978
C 0.669802 -2.162708 4.063911
H 1.482513 -1.515865 4.418301
H -0.078328 -2.226035 4.862986
H 1.084943 -3.167682 3.913893

TS6 - Non aromatic system
Opt Eel: -1569.085949
SP Eel: -9053.24005279
Gcorr: 0.604503
C 1.691433 -1.701778 -0.995549
C 1.180293 -1.183402 -2.336558
C 1.669201 -2.067852 -3.497739
C 1.300452 -3.540468 -3.280246
C 1.822294 -4.050880 -1.931426
C 1.317335 -3.168058 -0.778668
H 1.246038 -1.704057 -4.443733
H 0.082203 -1.178161 -2.323358
H 1.502256 -0.151050 -2.502106
H 2.805166 -1.654955 -1.023681
H 0.205852 -3.641837 -3.301000
H 1.691743 -4.156990 -4.099814
H 1.509699 -5.091032 -1.768985
H 2.922167 -4.046338 -1.940173
H 0.225817 -3.256322 -0.725236
H 1.714992 -3.525587 0.179686
H 2.762061 -1.977399 -3.584478
C 0.494482 -0.840464 0.422613
H 0.131002 -1.726987 0.947014
C -0.349088 0.199556 0.159365
Fe 2.403344 -0.500167 0.649321
Br 3.742539 -1.368785 2.596118
O 3.482217 0.939722 -0.383504
C 3.690329 2.156384 -0.113506
N 3.863285 3.033159 -1.110590
C 4.242525 4.429553 -0.923096
C 3.773173 2.588600 -2.499707
H 5.193190 4.619490 -1.433977
H 3.475523 5.080850 -1.355130
H 4.358763 4.669286 0.130953
H 3.354398 3.400837 -3.099183
H 4.766890 2.336196 -2.889275
H 3.128436 1.713518 -2.567237
C 3.751826 2.630093 1.317004
H 4.770995 2.941884 1.572528
H 3.082527 3.476528 1.493840
H 3.469726 1.804494 1.972576
C 0.074107 1.437574 -0.608866
Fe -2.282992 0.048457 0.728709
C -3.419269 2.577781 -0.548259
O -3.441587 1.318549 -0.465177
N -3.228874 3.169763 -1.736408
C -3.319199 4.607806 -1.964454
H -2.393958 4.962135 -2.430543
H -4.154869 4.819519 -2.641728
H -3.476019 5.148171 -1.034091
C -3.025221 2.368188 -2.939837
H -2.775589 1.346482 -2.662175
H -3.934789 2.367398 -3.552888
H -2.208930 2.804944 -3.522706
Br -3.251594 0.109773 3.079700
C -3.620562 3.426652 0.683191
H -2.825103 4.167961 0.801877
H -4.575733 3.961349 0.627511
H -3.634797 2.769560 1.554222
O -3.020540 -1.606499 -0.359224
C -2.586710 -2.787621 -0.265672
N -2.399635 -3.509060 -1.380946
C -2.279929 -3.401014 1.078637
C -2.061613 -4.928516 -1.397223
C -2.704348 -2.905627 -2.677207
H -2.954410 -4.240744 1.280980
H -1.252419 -3.773278 1.127152
H -2.424631 -2.643392 1.850751
H -2.920124 -5.513329 -1.749075
H -1.222483 -5.092005 -2.079524
H -1.780466 -5.277152 -0.406233
H -3.778239 -2.962987 -2.893069
H -2.398565 -1.859385 -2.680652
H -2.157693 -3.449221 -3.449732
H -0.633613 1.622466 -1.430181
H 1.064304 1.330707 -1.069877
C 0.098923 2.689761 0.284733
H -0.855306 2.770655 0.821036
H 0.868082 2.553058 1.056521
C 0.362748 3.975753 -0.498569
H -0.435626 4.159478 -1.228423
H 0.417633 4.848231 0.164023
H 1.308434 3.913549 -1.049736

TS7e - Non aromatic system
Opt Eel: -1685.792727
SP Eel: -12182.7761763
Gcorr: 0.607695
C 0.121853 2.058391 2.015641
C 0.510934 2.839991 0.762037
C -0.054827 4.264648 0.785604
C 0.403533 5.022189 2.038406
C 0.062862 4.242748 3.315346
C 0.618215 2.812526 3.269553
H 0.251231 4.803858 -0.120234
H 1.606582 2.889963 0.691768
H 0.170285 2.322548 -0.137386
H -0.975684 2.046666 2.076331
H 1.492586 5.169909 1.987600
H -0.049666 6.021542 2.070317
H 0.449058 4.769959 4.197342
H -1.030458 4.195778 3.428247
H 1.718381 2.844071 3.257133
H 0.327345 2.264295 4.175364
H -1.153848 4.216283 0.769660
C 0.593822 0.623573 2.060429
H 0.387553 0.170371 3.036065
C 1.276678 -0.094386 1.130570
Fe 1.980884 0.362011 -0.793167
C 4.712422 -0.675458 -0.245352
O 3.697986 -0.702385 -1.008280
N 5.457921 -1.770389 -0.099016
C 6.679112 -1.823841 0.701151
H 6.487690 -2.348455 1.644056
H 7.439624 -2.374142 0.139588
H 7.058082 -0.825967 0.911516
C 5.069098 -3.029793 -0.731512
H 4.027104 -2.979928 -1.040869
H 5.702393 -3.226023 -1.604046
H 5.201396 -3.839032 -0.007600
Br 2.081377 2.215569 -2.488492
Zn -0.982942 -0.678135 0.112575
Br 0.253230 -1.392289 -1.921779
Br -1.891896 -2.385949 1.556041
O -3.164310 -0.969395 -1.565225
C -3.825127 -1.981803 -1.279631
N -4.929924 -1.907708 -0.490721
C -5.591576 -3.078334 0.066371
C -5.245311 -0.638726 0.151149
H -5.157477 -3.351990 1.038483
H -6.652677 -2.853335 0.211105
H -5.513434 -3.931461 -0.606504
H -4.906534 0.179527 -0.481542
H -6.327615 -0.569545 0.296163
H -4.748819 -0.560468 1.126767
O -2.005603 0.992745 0.211337
C -2.511193 1.780542 -0.638638
N -3.494249 2.599925 -0.249211
C -4.097503 3.621403 -1.098343
C -3.993004 2.577009 1.123997
H -5.174587 3.438686 -1.177088
H -3.941274 4.607262 -0.646415
H -3.663758 3.618330 -2.094953
H -3.657324 3.473304 1.658191
H -5.087025 2.568062 1.103937
H -3.627069 1.690176 1.634551
C -3.430332 -3.339380 -1.824227
H -3.163631 -4.021154 -1.010232
H -4.239244 -3.799444 -2.402618
H -2.559325 -3.201542 -2.466398
C -2.002538 1.845588 -2.051872
H -2.811533 1.672660 -2.766549
H -1.563327 2.827648 -2.254703
H -1.239301 1.084349 -2.196389
C 5.076110 0.581230 0.503062
H 5.194264 0.387107 1.573307
H 6.016070 0.998771 0.125099
H 4.290444 1.325637 0.360921
C 1.809422 -1.479739 1.536065
H 1.401844 -2.239974 0.854741
H 2.890275 -1.490781 1.337781
C 1.614146 -1.963486 2.977899
H 2.058141 -1.239025 3.674967
H 0.544663 -2.016543 3.208680
C 2.253022 -3.336583 3.196662
H 3.329267 -3.313568 2.978979
H 2.130103 -3.678835 4.231743
H 1.799871 -4.090746 2.540016

TS7z - Non aromatic system
Opt Eel: -1685.805239
SP Eel: -12182.7819140
Gcorr: 0.607458
C -0.052807 3.725932 -0.384512
C 1.453096 4.062639 -0.359580
C 1.723598 5.505342 -0.803438
C 0.931124 6.509606 0.043104
C -0.568917 6.189330 0.022225
C -0.841288 4.746487 0.467005
H 2.798440 5.721202 -0.744492
H 1.829748 3.919379 0.664213
H 1.991226 3.353317 -0.999627
H -0.403725 3.812121 -1.420026
H 1.293462 6.470620 1.081077
H 1.106060 7.532391 -0.314992
H -1.117739 6.889564 0.665252
H -0.953348 6.329209 -0.998731
H -0.549770 4.627936 1.521338
H -1.914657 4.524414 0.407635
H 1.436443 5.618004 -1.859394
C -0.285829 2.328382 0.124180
H 0.182320 2.141133 1.091218
C -0.975653 1.314984 -0.461478
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