Supplementary Information (SI) for Organic & Biomolecular Chemistry.
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S2Supporting Information

Using machine learning methods to predict diabatic bond dissociation energy of non-heme iron complex

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1. Details of the dataset

1.1 The chemical scope of the database

The molecules collected in this dataset are non heme iron complexes containing transition metal Fe, including six ligands: Cl^-, Br^-, F^-, NCS^-, N_3^-, and OH^-, with their distribution in the database shown in Table S1. The collected non-heme iron complexes contain one or two of the aforementioned monodentate ligands, typically exhibiting an octahedral spatial structure. In the molecular data collection section, we describe the data collection process and record key properties such as molecular weight, oxidation state of Fe, number of monodentate ligands, and molecular charge. Each molecule is also labeled with its corresponding literature source. In terms of the details of diabatic BDE calculation, we introduce the calculation method of BDE and demonstrate the distribution of each one of the BDEs per bond type as well as the full database. All calculations of structure and energy are achieved through quantum chemistry calculations.

Table S1. Six monodentate ligands involved in the dataset.

Ligand	Ligand field strength	Average diabatic BDE (kcal mol^{-1})	Number of ligands
Cl^-	Weak-field ligand	96.0	116
Br^-	Weak-field ligand	85.5	113
F^-	Weak-field ligand	122.0	112
N_3^-	Strong-field ligand	76.0	112
NCS^-	Strong-field ligand	84.5	109
OH^-	Strong-field ligand	92.9	327

1.2 Molecular data collection

This study cleaned and organized the molecular data based on the following principles: (1) Replace the L group (L = OTf, $NCCH_3$, ...) in the original structure with either an OH or X group (X = F, Cl, Br, NCS, N_3); (2) Hydrogenate structures containing Fe=O double bonds in the collected data to convert them into intermediate structures with Fe–OH bonds; (3) Without altering the structure of the non-heme ligand, obtain a new structure by swapping the positions of the OH group and the X group (Figure S1).

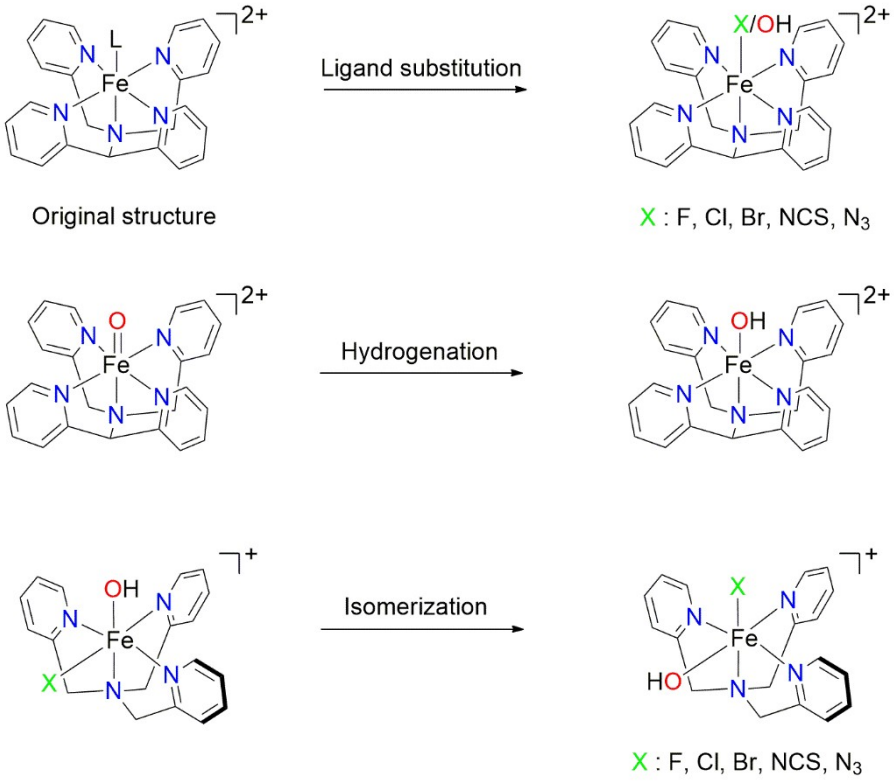

Figure S1. Principles of molecular processing for non-heme iron complexes

We calculated key information for each complex, with the spin multiplicity of each species labeled as a pre-superscript (e.g., ^{3}FeTMCBrOH refers to the non-heme iron complex FeTMCBrOH in a triplet state). Note that some complexes in the dataset contain molecules not directly coordinated to the Fe center (e.g., solvent molecules or counterions), as they were included in the original structural coordinates obtained from the literature. Additionally, we calculated important properties such as molecular weight, oxidation state of Fe, number of monodentate ligands, coordination number, atom count, and molecular charge. Corresponding literature sources can be found in the References (in the Supporting Information). These details are summarized in **Table S2**.

Table S2. Molecular properties of non-heme iron complexes used in this study.

Filename	Molecular weight (g mol^{-1})	Oxidation state of Fe	Monodentate ligand	Coordination number	Atom Count	Charge	Ref. (In SI)
^{3}FeTMCBrOH	409.2	4	2	6	54	2	1
^{3}FeTMCClOH	364.7	4	2	6	54	2	1
^{3}FeTMCFOH	348.3	4	2	6	54	2	1

^{3}FeTMCN3OH	371.3	4	2	6	56	2	1
^{3}FeTMCNCSOH	387.4	4	2	6	56	2	1
^{3}FeTMCOHBr	409.2	4	2	6	54	2	1
^{3}FeTMCOHCl	364.7	4	2	6	54	2	1
^{4}FeTMCOHF	348.3	3	2	6	54	1	1
^{3}FeTMCOHF	348.3	4	2	6	54	2	1
^{6}FeTMCOHN$_3$	371.3	3	2	6	56	1	1
^{3}FeTMCOHN$_3$	371.3	4	2	6	56	2	1
^{3}FeTMCOHNCS	387.4	4	2	6	56	2	1
^{4}FeTMCOHSR	374.4	3	1	6	56	1	1
^{6}FeTMCOHTF	442.3	3	2	6	60	1	1
^{5}FeNTBBrOH	602.3	2	2	6	65	0	2
^{5}FeNTBClOH	557.9	2	2	6	65	0	2
^{5}FeNTBFOH	541.4	2	2	6	65	0	2
^{5}FeNTBN3OH	564.4	2	2	6	67	0	2
^{5}FeNTBNCSOH	580.5	2	2	6	67	0	2
^{5}FeNTBOHBr	602.3	2	2	6	65	0	2
^{5}FeNTBOHCl	557.9	2	2	6	65	0	2
^{5}FeNTBOHF	541.4	2	2	6	65	0	2
^{4}FeNTBOHMeCN	563.5	1	2	6	70	0	2
^{5}FeNTBOHN$_3$	564.4	2	2	6	67	0	2
^{5}FeNTBOHNCS	580.5	2	2	6	67	0	2
^{6}Cisalpha	510.4	3	2	6	67	2	3
^{5}CisalphaBrOH	549.3	4	2	6	62	2	3
^{3}CisalphaClOH	504.8	4	2	6	62	2	3
^{5}CisalphaFOH	488.4	4	2	6	62	2	3
^{3}CisalphaN$_3$OH	511.4	4	2	6	64	2	3
^{3}CisalphaNCSOH	527.5	4	2	6	64	2	3
^{6}CisbetatranstoamineN	510.4	3	2	6	67	2	3
^{3}CisbetatranstoamineNBrOH	549.3	4	2	6	62	2	3
^{3}CisbetatranstoamineNClOH	504.8	4	2	6	62	2	3
^{3}CisbetatranstoamineNFOH	488.4	4	2	6	62	2	3
^{5}CisbetatranstoamineNN$_3$OH	511.4	4	2	6	64	2	3
^{3}CisbetatranstoamineNNCSOH	527.5	4	2	6	64	2	3
^{5}CisbetatranstoamineNOHBr	549.3	4	2	6	62	2	3
^{5}CisbetatranstoamineNOHCl	504.8	4	2	6	62	2	3
^{5}CisbetatranstoamineNOHF	488.4	4	2	6	62	2	3
^{3}CisbetatranstoamineNOHN$_3$	511.4	4	2	6	64	2	3
^{3}CisbetatranstoamineNOHNCS	527.5	4	2	6	64	2	3
^{6}CisbetatranstoquinolylN	510.4	3	2	6	67	2	3
^{5}CisbetatranstoquinolylNBrOH	549.3	4	2	6	62	2	3
^{5}CisbetatranstoquinolylNClOH	504.8	4	2	6	62	2	3
^{5}CisbetatranstoquinolylNFOH	488.4	4	2	6	62	2	3
^{3}CisbetatranstoquinolylNN$_3$OH	511.4	4	2	6	64	2	3

^{3}CisbetatranstoquinolylNNCSOH	527.5	4	2	6	64	2	3
^{3}CisbetatranstoquinolylNOHBr	549.3	4	2	6	62	2	3
^{5}CisbetatranstoquinolylNOHCl	504.8	4	2	6	62	2	3
^{3}CisbetatranstoquinolylNOHF	488.4	4	2	6	62	2	3
^{3}CisbetatranstoquinolylNOHN$_3$	511.4	4	2	6	64	2	3
^{3}CisbetatranstoquinolylNOHNCS	527.5	4	2	6	64	2	3
^{6}FeN4PyBr	503.2	3	1	6	51	2	4
^{6}FeN4PyCl	458.7	3	1	6	51	2	4
^{6}FeN4PyF	442.3	3	1	6	51	2	4
^{6}FeN4PyN$_3$	465.3	3	1	6	53	2	4
^{6}FeN4PyNCS	481.4	3	1	6	53	2	4
^{2}FeN4PyOH	440.3	3	1	6	52	2	4
^{6}FeTMCBr	392.2	3	1	5	52	2	4
^{6}FeTMCCl	347.7	3	1	5	52	2	4
^{6}FeTMCF	331.3	3	1	5	52	2	4
^{6}FeTMCN$_3$	354.3	3	1	5	54	2	4
^{6}FeTMCNCS	370.4	3	1	5	54	2	4
^{6}FeTMCOH	329.3	3	1	5	53	2	4
^{6}Fe13TMCBr	378.2	3	1	5	49	2	5
^{6}Fe13TMCCl	333.7	3	1	5	49	2	5
^{6}Fe13TMCF	317.2	3	1	5	49	2	5
^{6}Fe13TMCN$_3$	340.3	3	1	5	51	2	5
^{6}Fe13TMCNCS	356.3	3	1	5	51	2	5
^{6}Fe13TMCOH	315.3	3	1	5	50	2	5
^{2}Fe13TMCOOCCH33Br	467.3	3	2	6	64	1	6
^{2}Fe13TMCOOCCH33Cl	422.8	3	2	6	64	1	6
^{2}Fe13TMCOOCCH33F	406.4	3	2	6	64	1	6
^{2}Fe13TMCOOCCH33N$_3$	429.4	3	2	6	66	1	6
^{2}Fe13TMCOOCCH33NCS	445.4	3	2	6	66	1	6
^{2}Fe13TMCOOCCH33OH	404.4	3	2	6	65	1	6
^{6}FeBQENBrOH	495.2	5	2	6	52	3	7
^{4}FeBQENClOH	450.7	5	2	6	52	3	7
^{6}FeBQENFOH	434.3	5	2	6	52	3	7
^{4}FeBQENN$_3$OH	457.3	5	2	6	54	3	7
^{6}FeBQENNCSOH	473.4	5	2	6	54	3	7
^{6}FeBQENOHBr	495.2	5	2	6	52	3	7
^{4}FeBQENOHCl	450.7	5	2	6	52	3	7
^{4}FeBQENOHF	434.3	5	2	6	52	3	7
^{4}FeBQENOHN$_3$	457.3	5	2	6	54	3	7
^{6}FeBQENOHNCS	473.4	5	2	6	54	3	7
^{2}FeBnTPENOH	440.3	3	1	6	52	2	8
^{6}FeBnTPENBr	503.2	3	1	6	51	2	8
^{6}FeBnTPENCl	458.7	3	1	6	51	2	8
^{6}FeBnTPENF	442.3	3	1	6	51	2	8

^{6}FeBnTPENN$_3$	465.3	3	1	6	53	2	8
^{6}FeBnTPENNCS	481.4	3	1	6	53	2	8
^{1}FetpenaBr	526.2	4	1	6	55	2	9
^{5}FetpenaCl	481.8	4	1	6	55	2	9
^{5}FetpenaF	465.3	4	1	6	55	2	9
^{5}FetpenaN$_3$	488.3	4	1	6	57	2	9
^{1}FetpenaNCS	504.4	4	1	6	57	2	9
^{5}FetpenaOH	463.3	3	1	6	56	2	9
^{6}FeOPhIOTf3BrOH	785.9	5	1	6	41	0	10
^{6}FePhIOTf3FOH	759.1	5	2	6	41	0	10
^{6}FePhIOTf3OHNCS	896.1	5	2	6	43	0	10
^{5}FeiPrBIPO2BrOHC	666.5	2	2	6	85	0	11
^{5}FeiPrBIPO2Cl2C	640.5	2	2	6	84	0	11
^{5}FeiPrBIPO2ClOHC	622.0	2	2	6	85	0	11
^{5}FeiPrBIPO2FOHC	605.6	2	2	6	85	0	11
^{5}FeiPrBIPO2N3OHC	628.6	2	2	6	87	0	11
^{5}FeiPrBIPO2NCSOHC	644.6	2	2	6	87	0	11
^{5}FeiPrBIPO2OHBrC	666.5	2	2	6	85	0	11
^{5}FeiPrBIPO2OHClC	622.0	2	2	6	85	0	11
^{5}FeiPrBIPO2OHFC	605.6	2	2	6	85	0	11
^{5}FeiPrBIPO2OHN$_3$C	628.6	2	2	6	87	0	11
^{5}FeiPrBIPO2OHNCSC	644.6	2	2	6	87	0	11
^{3}FeiPrBIPSPhO2ClA	714.2	2	2	6	95	0	11
^{5}FeiPrBIPSPhO2ClB	714.2	2	2	6	95	0	11
^{4}FeN4Py2PhamideBrOtBu2	754.5	3	1	6	87	0	12
^{4}FeN4Py2PhamideClOtBu2	710.1	3	1	6	87	0	12
^{6}FeN4Py2PhamideFOtBu2	693.6	3	1	6	87	0	12
^{4}FeN4Py2PhamideN$_3$OtBu2	716.6	3	1	6	89	0	12
^{4}FeN4Py2PhamideNCSOtBu2	732.7	3	1	6	89	0	12
^{6}FeN4Py2PhamideOHOtBu2	691.6	3	1	6	88	0	12
^{6}FeN4Py2PhBr	655.4	3	1	6	71	2	12
^{6}FeN4Py2PhCl	610.9	3	1	6	71	2	12
^{6}FeN4Py2PhF	594.5	3	1	6	71	2	12
^{6}FeN4Py2PhN$_3$	617.5	3	1	6	73	2	12
^{6}FeN4Py2PhNCS	633.6	3	1	6	73	2	12
^{6}FeN4Py2PhOH	592.5	3	1	6	72	2	12
^{6}FeN3PyamideSRBr	686.5	3	1	6	76	2	13
^{6}FeN3PyamideSRCl	642.0	3	1	6	76	2	13
^{6}FeN3PyamideSRF	625.6	3	1	6	76	2	13
^{6}FeN3PyamideSRN$_3$	648.6	3	1	6	78	2	13
^{6}FeN3PyamideSRNCS	664.6	3	1	6	78	2	13
^{6}FeN3PyamideSROH	623.6	3	1	6	77	2	13
^{6}FeN4Py2PhF2Br	727.3	3	1	6	71	2	14
^{6}FeN4Py2PhF2Cl	682.9	3	1	6	71	2	14

^{6}FeN4Py2PhF2F	666.4	3	1	6	71	2	14
^{6}FeN4Py2PhF2N_3	689.5	3	1	6	73	2	14
^{6}FeN4Py2PhF2NCS	705.5	3	1	6	73	2	14
^{6}FeN4Py2PhF2OH	664.5	3	1	6	72	2	14
^{6}FeN3PyO2PhBr	669.4	3	1	6	72	1	15
^{6}FeN3PyO2PhCl	624.9	3	1	6	72	1	15
^{6}FeN3PyO2PhF	608.5	3	1	6	72	1	15
^{6}FeN3PyO2PhN_3	631.5	3	1	6	74	1	15
^{5}FeN3PyO2PhNCCH3	630.5	2	1	6	77	1	15
^{6}FeN3PyO2PhNCS	647.6	3	1	6	74	1	15
^{6}FeN3PyO2PhOH	606.5	3	1	6	73	1	15
^{4}FetsalenpyBr	513.3	3	1	6	47	0	16
^{4}FetsalenpyCl	468.8	3	1	6	47	0	16
^{4}FetsalenpyF	452.4	3	1	6	47	0	16
^{4}FetsalenpyN_3	475.4	3	1	6	49	0	16
^{4}FetsalenpyNCS	491.5	3	1	6	49	0	16
^{2}FetsalenpyOH	450.4	3	1	6	48	0	16
^{4}FeN2S2Br	444.2	3	1	5	38	-2	16
^{4}FeN2S2Cl	399.7	3	1	5	38	-2	16
^{4}FeN2S2F	383.3	3	1	5	38	-2	16
^{4}FeN2S2N_3	406.3	3	1	5	40	-2	16
^{4}FeN2S2NCS	422.3	3	1	5	40	-2	16
^{4}FeN2S2OH	381.3	3	1	5	39	-2	16
^{4}FeBNPAPh2OBrOTf	849.6	3	1	6	98	0	17
^{6}FeBNPAPh2OClOTf	805.2	3	1	6	98	0	17
^{6}FeBNPAPh2OFOTf	788.7	3	1	6	98	0	17
^{6}FeBNPAPh2ON_3OTf	811.7	3	1	6	100	0	17
^{6}FeBNPAPh2ONCSOTf	827.8	3	1	6	100	0	17
^{6}FeBNPAPh2OOHOTf	786.7	3	1	6	99	0	17
^{6}FeN3PyO2PhBr	669.4	3	1	6	72	1	18
^{6}FeN3PyO2PhCl	624.9	3	1	6	72	1	18
^{6}FeN3PyO2PhF	608.5	3	1	6	72	1	18
^{6}FeN3PyO2PhN_3	631.5	3	1	6	74	1	18
^{6}FeN3PyO2PhNCS	647.6	3	1	6	74	1	18
^{6}FeN3PyO2PhOH	606.5	3	1	6	73	1	18
^{6}FeMe3TACNBrS2SiMe2	429.3	3	1	6	46	0	19
^{6}FeMe3TACNClS2SiMe2	384.9	3	1	6	46	0	19
^{6}FeMe3TACNFS2SiMe2	368.4	3	1	6	46	0	19
^{6}FeMe3TACNN_3S2SiMe2	391.4	3	1	6	48	0	19
^{6}FeMe3TACNNCSS2SiMe2	407.5	3	1	6	48	0	19
^{6}FeMe3TACNOHS2SiMe2	366.4	3	1	6	47	0	19
^{6}FeBrMe3TACNOSiPh22O	719.6	3	1	6	84	0	20
^{6}FeClMe3TACNOSiPh22O	675.2	3	1	6	84	0	20
^{6}FeFMe3TACNOSiPh22O	658.7	3	1	6	84	0	20

$^{6}FeN_3Me3TACNOSiPh22O$	681.7	3	1	6	86	0	20
$^{6}FeNCSMe3TACNOSiPh22O$	697.8	3	1	6	86	0	20
$^{6}FeOHMe3TACNOSiPh22O$	656.7	3	1	6	85	0	20
$^{6}FeBNPAPh2OBrOH$	717.5	3	2	6	92	0	21
$^{6}FeBNPAPh2OClCl$	691.5	3	2	6	91	0	21
$^{6}FeBNPAPh2OClOH$	673.1	3	2	6	92	0	21
$^{6}FeBNPAPh2OFOH$	656.6	3	2	6	92	0	21
$^{6}FeBNPAPh2ON_3OH$	679.7	3	2	6	94	0	21
$^{6}FeBNPAPh2ONCSOH$	695.7	3	2	6	94	0	21
$^{6}FeBNPAPh2OOHBr$	717.5	3	2	6	92	0	21
$^{6}FeBNPAPh2OOHCl$	673.1	3	2	6	92	0	21
$^{6}FeBNPAPh2OOHF$	656.6	3	2	6	92	0	21
$^{6}FeBNPAPh2OOHN_3$	679.7	3	2	6	94	0	21
$^{6}FeBNPAPh2OOHNCS$	695.7	3	2	6	94	0	21
$^{5}FeMe2PyTACNBrOH$	401.1	2	2	6	46	0	22
$^{5}FeMe2PyTACNClOH$	356.7	2	2	6	46	0	22
$^{5}FeMe2PyTACNFOH$	340.2	2	2	6	46	0	22
$^{5}FeMe2PyTACNN_3OH$	363.2	2	2	6	48	0	22
$^{5}FeMe2PyTACNNCSOH$	379.3	2	2	6	48	0	22
$^{5}FeMe2PyTACNOHBr$	401.1	2	2	6	46	0	22
$^{5}FeMe2PyTACNOHCl$	356.7	2	2	6	46	0	22
$^{5}FeMe2PyTACNOHF$	340.2	2	2	6	46	0	22
$^{5}FeMe2PyTACNOHN_3$	363.2	2	2	6	48	0	22
$^{5}FeMe2PyTACNOHNCS$	379.3	2	2	6	48	0	22
$^{4}FeMe2PyTACNOOHOH2PA$	355.2	1	2	6	49	0	22
$^{6}FemepBrOH$	423.1	3	2	6	46	1	23
$^{6}FemepClOH$	378.7	3	2	6	46	1	23
$^{6}FemepFOH$	362.2	3	2	6	46	1	23
$^{6}FemepN_3OH$	385.2	3	2	6	48	1	23
$^{6}FemepNCSOH$	401.3	3	2	6	48	1	23
$^{6}FemepOHBr$	423.1	3	2	6	46	1	23
$^{6}FemepOHCl$	378.7	3	2	6	46	1	23
$^{6}FemepOHF$	362.2	3	2	6	46	1	23
$^{6}FemepOHN_3$	385.2	3	2	6	48	1	23
$^{6}FemepOHNCS$	401.3	3	2	6	48	1	23
$^{6}FeMePy2CHTACNBr$	461.2	3	1	6	53	2	23
$^{6}FeMePy2CHTACNCl$	416.7	3	1	6	53	2	23
$^{6}FeMePy2CHTACNF$	400.3	3	1	6	53	2	23
$^{6}FeMePy2CHTACNN_3$	423.3	3	1	6	55	2	23
$^{6}FeMePy2CHTACNNCS$	439.4	3	1	6	55	2	23
$^{6}FeMePy2CHTACNOH$	398.3	3	1	6	54	2	23
$^{3}FePyTACNBrOH$	401.1	4	2	6	46	2	23
$^{5}FePyTACNClOH$	356.7	4	2	6	46	2	23
$^{3}FePyTACNFOH$	340.2	4	2	6	46	2	23

^{3}FePyTACNN$_3$OH	363.2	4	2	6	48	2	23
^{3}FePyTACNNCSOH	379.3	4	2	6	48	2	23
^{3}FePyTACNOHBr	401.1	4	2	6	46	2	23
^{3}FePyTACNOHCl	356.7	4	2	6	46	2	23
^{3}FePyTACNOHF	340.2	4	2	6	46	2	23
^{3}FePyTACNOHN$_3$	363.2	4	2	6	48	2	23
^{3}FePyTACNOHNCS	379.3	4	2	6	48	2	23
^{5}FemepOOH	359.2	4	1	6	46	1	23
^{3}FeMePy2CHTACNOH	398.3	4	1	6	54	3	23
^{4}FePyTACNOOH	337.2	5	1	6	46	2	23
^{6}FeMeN4PyBr	503.2	3	1	6	51	2	24
^{6}FeMeN4PyCl	458.7	3	1	6	51	2	24
^{6}FeMeN4PyF	442.3	3	1	6	51	2	24
^{6}FeMeN4PyN$_3$	465.3	3	1	6	53	2	24
^{6}FeMeN4PyNCS	481.4	3	1	6	53	2	24
^{2}FeMeN4PyOH	440.3	3	1	6	52	2	24
^{5}FeMeOPyNMe3Br	414.1	4	1	5	48	3	25
^{6}FeMeOPyNMe3BrOH	431.1	5	2	6	50	3	25
^{5}FeMeOPyNMe3Cl	369.7	4	1	5	48	3	25
^{6}FeMeOPyNMe3ClOH	386.7	5	2	6	50	3	25
^{3}FeMeOPyNMe3F	353.2	4	1	5	48	3	25
^{6}FeMeOPyNMe3FOH	370.2	5	2	6	50	3	25
^{5}FeMeOPyNMe3N$_3$	376.3	4	1	5	50	3	25
^{6}FeMeOPyNMe3N$_3$OH	393.3	5	2	6	52	3	25
^{5}FeMeOPyNMe3NCS	392.3	4	1	5	50	3	25
^{6}FeMeOPyNMe3NCSOH	409.3	5	2	6	52	3	25
^{3}FeMeOPyNMe3OH	351.2	4	1	5	49	3	25
^{6}FeMeOPyNMe3OHBr	431.1	5	2	6	50	3	25
^{6}FeMeOPyNMe3OHCl	386.7	5	2	6	50	3	25
^{4}FeMeOPyNMe3OHF	370.2	5	2	6	50	3	25
^{3}FeMeOPyNMe3OHMeCN3cis	392.3	4	2	6	55	3	25
^{3}FeMeOPyNMe3OHMeCN3trans	392.3	4	2	6	55	3	25
^{2}FeMeOPyNMe3OHN$_3$	393.3	5	2	6	52	3	25
^{4}FeMeOPyNMe3OHNCS	409.3	5	2	6	52	3	25
^{5}FePyNMe3BrOCOcy22bCPCAcis	511.3	4	1	7	64	2	25
^{5}FePyNMe3BrOCOcy22bCPCAtrans	511.3	4	1	7	64	2	25
^{3}FePyNMe3BrOCOcy23bPAAtrans	473.2	4	1	7	55	2	25
^{5}FePyNMe3ClOCOcy22bCPCAcis	466.8	4	1	7	64	2	25
^{5}FePyNMe3ClOCOcy22bCPCAtrans	466.8	4	1	7	64	2	25
^{5}FePyNMe3ClOCOcy23bPAAtrans	428.7	4	1	7	55	2	25
^{5}FePyNMe3FOCOcy22bCPCAcis	450.4	4	1	7	64	2	25
^{3}FePyNMe3FOCOcy22bCPCAtrans	450.4	4	1	7	64	2	25
^{3}FePyNMe3FOCOcy23bPAAtrans	412.3	4	1	7	55	2	25
^{5}FePyNMe3N$_3$OCOcy22bCPCAcis	473.4	4	1	7	66	2	25

^{5}FePyNMe3N$_3$OCOcy22bCPCAtrans	473.4	4	1	7	66	2	25
^{5}FePyNMe3N$_3$OCOcy23bPAAtrans	435.3	4	1	7	57	2	25
^{5}FePyNMe3NCSOCOcy22bCPCAcis	489.5	4	1	7	66	2	25
^{5}FePyNMe3NCSOCOcy22bCPCAtrans	489.5	4	1	7	66	2	25
^{3}FePyNMe3NCSOCOcy23bPAAtrans	451.4	4	1	7	57	2	25
^{3}FePyNMe3OHOCOcy22bCPCAcis	448.4	4	1	7	65	2	25
^{5}FePyNMe3OHOCOcy22bCPCAtrans	448.4	4	1	7	65	2	25
^{5}FePyNMe3BrOH	401.1	4	2	6	46	2	26
^{5}FePyNMe3ClOH	356.7	4	2	6	46	2	26
^{3}FePyNMe3FOH	340.2	4	2	6	46	2	26
^{5}FePyNMe3N3OH	363.2	4	2	6	48	2	26
^{3}FePyNMe3NCSOH	379.3	4	2	6	48	2	26
^{5}FePyNMe3OHBr	401.1	4	2	6	46	2	26
^{5}FePyNMe3OHCl	356.7	4	2	6	46	2	26
^{5}FePyNMe3OHF	340.2	4	2	6	46	2	26
^{6}FePyNMe3OHMeCN2cis	362.3	3	2	6	51	2	26
^{6}FePyNMe3OHMeCN2trans	362.3	3	2	6	51	2	26
^{5}FePyNMe3OHN3	363.2	4	2	6	48	2	26
^{3}FePyNMe3OHNCS	379.3	4	2	6	48	2	26
^{4}FeTpMePhBrSOCH2CHNH2CO2EtC	783.3	3	1	6	87	0	27
^{4}FeTpMePhBrSOCH2CHNH2CO2EtD	783.3	3	1	6	87	0	27
^{4}FeTpMePhClSOCH2CHNH2CO2EtC	738.9	3	1	6	87	0	27
^{6}FeTpMePhClSOCH2CHNH2CO2EtD	738.9	3	1	6	87	0	27
^{6}FeTpMePhFSOCH2CHNH2CO2EtC	722.4	3	1	6	87	0	27
^{6}FeTpMePhFSOCH2CHNH2CO2EtD	722.4	3	1	6	87	0	27
^{6}FeTpMePhN$_3$SOCH2CHNH2CO2EtC	745.5	3	1	6	89	0	27
^{6}FeTpMePhN$_3$SOCH2CHNH2CO2EtD	745.5	3	1	6	89	0	27
^{6}FeTpMePhNCSSOCH2CHNH2CO2EtC	761.5	3	1	6	89	0	27
^{6}FeTpMePhNCSSOCH2CHNH2CO2EtD	761.5	3	1	6	89	0	27
^{6}FeTpMePhOHSOCH2CHNH2CO2EtC	720.4	3	1	6	88	0	27
^{6}FeTpMePhOHSOCH2CHNH2CO2EtD	720.4	3	1	6	88	0	27
^{5}FeBPMENCNBrOH	473.1	2	2	6	48	0	28
^{5}FeBPMENCNClOH	428.7	2	2	6	48	0	28
^{5}FeBPMENCNFOH	412.2	2	2	6	48	0	28
^{5}FeBPMENCNN$_3$OH	435.3	2	2	6	50	0	28
^{5}FeBPMENCNNCSOH	451.3	2	2	6	50	0	28
^{5}FeBPMENFBrOH	459.1	2	2	6	46	0	28
^{5}FeBPMENFClOH	414.7	2	2	6	46	0	28
^{5}FeBPMENFFOH	398.2	2	2	6	46	0	28
^{5}FeBPMENFN$_3$OH	421.2	2	2	6	48	0	28
^{5}FeBPMENFNCSOH	437.3	2	2	6	48	0	28
^{5}FeBPMENHBrOH	423.1	2	2	6	46	0	28
^{5}FeBPMENHClOH	378.7	2	2	6	46	0	28
^{5}FeBPMENHFOH	362.2	2	2	6	46	0	28

^{5}FeBPMENHN$_3$OH	385.2	2	2	6	48	0	28
^{5}FeBPMENHNCSOH	401.3	2	2	6	48	0	28
^{5}FeBPMENMeBrOH	451.2	2	2	6	52	0	28
^{5}FeBPMENMeClOH	406.7	2	2	6	52	0	28
^{5}FeBPMENMeFOH	390.3	2	2	6	52	0	28
^{5}FeBPMENMeN$_3$OH	413.3	2	2	6	54	0	28
^{5}FeBPMENMeNCSOH	429.4	2	2	6	54	0	28
^{5}FeBPMENOHBrOH	455.1	2	2	6	48	0	28
^{5}FeBPMENOHClOH	410.7	2	2	6	48	0	28
^{3}FeBPMENOHFOH	394.2	2	2	6	48	0	28
^{5}FeBPMENOHN$_3$OH	417.2	2	2	6	50	0	28
^{5}FeBPMENOHNCSOH	433.3	2	2	6	50	0	28
^{5}FeBPMENSiH3BrOH	483.3	2	2	6	52	0	28
^{5}FeBPMENSiH3ClOH	438.9	2	2	6	52	0	28
^{5}FeBPMENSiH3N$_3$OH	445.4	2	2	6	54	0	28
^{5}FeBPMENSiH3NCSOH	461.5	2	2	6	54	0	28
^{5}FeBPMENtBuBrOH	535.3	2	2	6	70	0	28
^{5}FeBPMENtBuClOH	490.9	2	2	6	70	0	28
^{5}FeBPMENtBuFOH	474.4	2	2	6	70	0	28
^{5}FeBPMENtBuN$_3$OH	497.5	2	2	6	72	0	28
^{5}FeBPMENtBuNCSOH	513.5	2	2	6	72	0	28
^{6}FeH1CYPBrK	581.4	3	1	5	68	0	29
^{6}FeH1CYPClK	536.9	3	1	5	68	0	29
^{6}FeH1CYPFK	520.5	3	1	5	68	0	29
^{6}FeH1CYPN$_3$K	543.5	3	1	5	70	0	29
^{6}FeH1CYPNCSK	559.6	3	1	5	70	0	29
^{6}FeH1CYPOH	518.5	3	1	5	69	0	29
^{6}FeH1CYPOHK	518.5	3	1	5	69	0	29
^{6}FeH3BueaBrK	615.5	3	1	5	76	0	29
^{6}FeH3BueaClK	571.0	3	1	5	76	0	29
^{6}FeH3BueaFK	554.5	3	1	5	76	0	29
^{6}FeH3BueaN$_3$K	577.6	3	1	5	78	0	29
^{6}FeH3BueaNCSK	593.6	3	1	5	78	0	29
^{6}FeH3BueaOH	552.6	3	1	5	77	0	29
^{6}FeH3BueaOHK	552.6	3	1	5	77	0	29
^{6}FeH3BueaBr	363.0	3	1	5	33	-1	30
^{6}FeH3BueaCl	318.5	3	1	5	33	-1	30
^{6}FeH3BueaF	302.1	3	1	5	33	-1	30
^{6}FeH3BueaN$_3$	325.1	3	1	5	35	-1	30
^{6}FeH3BueaNCS	341.2	3	1	5	35	-1	30
^{6}FeH3BueaNMeBr	450.1	3	1	5	48	-1	30
^{6}FeH3BueaNMeCl	405.7	3	1	5	48	-1	30
^{6}FeH3BueaNMeF	389.2	3	1	5	48	-1	30
^{6}FeH3BueaNMeN$_3$	412.2	3	1	5	50	-1	30

^{6}FeH3BueaNMeNCS	428.3	3	1	5	50	-1	30
^{6}FeH3BueaNMeOH	387.2	3	1	5	49	-1	30
^{6}FeH3BueaOH	300.1	3	1	5	34	-1	30
^{6}FeMeBzImTPABrA	556.3	3	1	6	58	2	31
^{6}FeMeBzImTPAClA	511.8	3	1	6	58	2	31
^{6}FeMeBzImTPAFA	495.4	3	1	6	58	2	31
^{6}FeMeBzImTPAN$_3$A	518.4	3	1	6	60	2	31
^{6}FeMeBzImTPANCSA	534.4	3	1	6	60	2	31
^{6}FeMeBzImTPAOHA	493.4	3	1	6	59	2	31
^{6}FeMeBzImTPAOH	493.4	3	1	6	59	2	31
^{6}FebisMeBzImTPABr	609.3	3	1	6	65	2	32
^{6}FebisMeBzImTPACl	564.9	3	1	6	65	2	32
^{6}FebisMeBzImTPAF	548.4	3	1	6	65	2	32
^{6}FebisMeBzImTPAN$_3$	571.4	3	1	6	67	2	32
^{6}FebisMeBzImTPANCS	587.5	3	1	6	67	2	32
^{6}FebisMeBzImTPAOH2	546.4	3	1	6	66	2	32
^{3}FeMeHPyTACNBrOH	401.1	4	2	6	46	2	33
^{3}FeMeHPyTACNClOH	356.7	4	2	6	46	2	33
^{3}FeMeHPyTACNFOH	340.2	4	2	6	46	2	33
^{3}FeMeHPyTACNN$_3$OH	363.2	4	2	6	48	2	33
^{3}FeMeHPyTACNNCSOH	379.3	4	2	6	48	2	33
^{3}FeMeHPyTACNOHBr	401.1	4	2	6	46	2	33
^{3}FeMeHPyTACNOHCl	356.7	4	2	6	46	2	33
^{3}FeMeHPyTACNOHF	340.2	4	2	6	46	2	33
^{3}FeMeHPyTACNOHN$_3$	363.2	4	2	6	48	2	33
^{3}FeMeHPyTACNOHNCS	379.3	4	2	6	48	2	33
^{4}FeMeHPyTACNOHOH	338.2	4	2	6	47	2	33
^{4}FeL2Br	510.2	1	1	4	52	-2	34
^{4}FeL2Cl	465.7	1	1	4	52	-2	34
^{4}FeL2F	449.3	1	1	4	52	-2	34
^{4}FeL2N$_3$	472.3	1	1	4	54	-2	34
^{4}FeL2NCS	488.4	1	1	4	54	-2	34
^{4}FeL2OH	447.3	1	1	4	53	-2	34
^{6}FeLABrOH	432.1	5	2	6	42	1	35
^{6}FeLAClOH	387.6	5	2	6	42	1	35
^{6}FeLAFOH	371.2	5	2	6	42	1	35
^{6}FeLAN$_3$OH	394.2	5	2	6	44	1	35
^{6}FeLANCSOH	410.3	5	2	6	44	1	35
^{6}FeLAOHBr	432.1	5	2	6	42	1	35
^{6}FeLAOHCl	387.6	5	2	6	42	1	35
^{6}FeLAOHF	371.2	5	2	6	42	1	35
^{6}FeLAOHN$_3$	394.2	5	2	6	44	1	35
^{6}FeLAOHNCS	410.3	5	2	6	44	1	35
^{6}FeLBBrOH	449.1	3	2	6	46	1	35

^{6}FeLBClOH	404.7	3	2	6	46	1	35
^{6}FeLBFOH	388.2	3	2	6	46	1	35
^{6}FeLBN_3OH	411.2	3	2	6	48	1	35
^{6}FeLBNCSOH	427.3	3	2	6	48	1	35
^{6}FeLBOHBr	449.1	3	2	6	46	1	35
^{6}FeLBOHCl	404.7	3	2	6	46	1	35
^{6}FeLBOHF	388.2	3	2	6	46	1	35
^{6}FeLBOHN_3	411.2	3	2	6	48	1	35
^{6}FeLBOHNCS	427.3	3	2	6	48	1	35
^{3}FePh2TIPCysOEtBr	730.4	4	1	5	73	0	36
^{5}FePh2TIPCysOEtCl	685.9	4	1	5	73	0	36
^{5}FePh2TIPCysOEtN_3	692.5	4	1	5	75	0	36
^{5}FePh2TIPCysOEtNCS	708.6	4	1	5	75	0	36
^{5}FePh2TIPCysOEtOH	667.5	4	1	5	74	0	36
^{2}aCDOBr	501.2	3	1	6	50	0	36
^{4}aCDOCl	456.8	3	1	6	50	0	36
^{4}aCDOF	440.3	3	1	6	50	0	36
^{4}aCDON3	463.3	3	1	6	52	0	36
^{4}aCDONCS	479.4	3	1	6	52	0	36
^{6}aCDOOH	438.3	3	1	6	51	0	36
^{5}FePhTpBIHQBr	763.4	2	1	6	75	0	37
^{5}FePhTpBIHQCl	719.0	2	1	6	75	0	37
^{5}FePhTpBIHQF	702.5	2	1	6	75	0	37
^{5}FePhTpBIHQN_3	725.5	2	1	6	77	0	37
^{5}FePhTpBIHQNCS	741.6	2	1	6	77	0	37
^{3}FePhTpBIHQOH	700.5	2	1	6	76	0	37
^{3}FebBPMENBrOH	423.1	4	2	6	46	2	38
^{3}FebBPMENClOH	378.7	4	2	6	46	2	38
^{3}FebBPMENFOH	362.2	4	2	6	46	2	38
^{6}FebBPMENMeCNOH	384.3	3	2	6	51	2	38
^{3}FebBPMENN_3OH	385.2	4	2	6	48	2	38
^{3}FebBPMENNCSOH	401.3	4	2	6	48	2	38
^{3}FebBPMENOHBr	423.1	4	2	6	46	2	38
^{3}FebBPMENOHCl	378.7	4	2	6	46	2	38
^{3}FebBPMENOHF	362.2	4	2	6	46	2	38
^{6}FebBPMENOHMeCN	384.3	3	2	6	51	2	38
^{3}FebBPMENOHN_3	385.2	4	2	6	48	2	38
^{3}FebBPMENOHNCS	401.3	4	2	6	48	2	38
^{3}FebBPMENOHOOtBu	432.3	4	2	6	60	2	38
^{3}FebBPMENOOtBuOH	432.3	4	2	6	60	2	38
^{2}FeTMCOHNCOCH3	386.3	3	2	6	60	2	39
^{6}FeTPABrOH	443.1	3	2	6	44	1	40
^{6}FeTPAClOH	398.7	3	2	6	44	1	40
^{6}FeTPAFOH	382.2	3	2	6	44	1	40

^{6}FeTPAN$_3$OH	405.2	3	2	6	46	1	40
^{6}FeTPANCSOH	421.3	3	2	6	46	1	40
^{6}FeTPAOHBr	443.1	3	2	6	44	1	40
^{6}FeTPAOHCl	398.7	3	2	6	44	1	40
^{6}FeTPAOHF	382.2	3	2	6	44	1	40
^{2}FeTPAOHN$_3$	405.2	3	2	6	46	1	40
^{4}FeTPAOHNCS	421.3	3	2	6	46	1	40
^{5}FeTPAOCCPhBr	546.3	4	2	6	59	1	40
^{5}FeTPAOCCPhCl	501.8	4	2	6	59	1	40
^{5}FeTPAOCCPhF	485.4	4	2	6	59	1	40
^{4}FeTMCOHCN	355.3	3	1	6	55	1	41
^{6}FeTMCOHNCO	371.3	3	1	6	56	1	41
^{6}FeTMCOHO2CCF3	442.3	3	1	6	60	1	41
^{4}FeTMCOHOH	346.3	3	1	6	55	1	41
^{6}FeTMCSBr	437.3	3	1	6	55	1	41
^{6}FeTMCSCl	392.8	3	1	6	55	1	41
^{6}FeTMCSF	376.4	3	1	6	55	1	41
^{6}FeTMCSN$_3$	399.4	3	1	6	57	1	41
^{6}FeTMCSNCS	415.4	3	1	6	57	1	41
^{6}FeTMCSOH	374.4	3	1	6	56	1	41
^{4}FeBnTPENBr	559.3	1	1	6	63	0	42
^{4}FeBnTPENCl	514.9	1	1	6	63	0	42
^{4}FeBnTPENF	498.4	1	1	6	63	0	42
^{4}FeBnTPENN$_3$	521.4	1	1	6	65	0	42
^{4}FeBnTPENNCS	537.5	1	1	6	65	0	42
^{4}FeBnTPENOH	496.4	1	1	6	64	0	42
^{5}FeLBrCO2CH2CH3	511.1	2	1	6	51	0	43
^{5}FeLClCO2CH2CH3	466.6	2	1	6	51	0	43
^{5}FeLFCO2CH2CH3	450.2	2	1	6	51	0	43
^{5}FeLN$_3$CO2CH2CH3	473.2	2	1	6	53	0	43
^{5}FeLNCSCO2CH2CH3	489.3	2	1	6	53	0	43
^{6}FeTMCCH2CNMe2OBr	463.3	3	1	6	62	2	44
^{6}FeTMCCH2CNMe2OCl	418.8	3	1	6	62	2	44
^{6}FeTMCCH2CNMe2OF	402.4	3	1	6	62	2	44
^{6}FeTMCCH2CNMe2ON$_3$	425.4	3	1	6	64	2	44
^{6}FeTMCCH2CNMe2ONCS	441.4	3	1	6	64	2	44
^{6}FeTMCCH2CNMe2OOH	400.4	3	1	6	63	2	44
^{3}FeSSPDPBrOH	475.2	4	2	6	54	2	45
^{3}FeSSPDPClOH	430.8	4	2	6	54	2	45
^{3}FeSSPDPFOH	414.3	4	2	6	54	2	45
^{5}FeSSPDPN3OH	437.3	4	2	6	56	2	45
^{3}FeSSPDPNCSOH	453.4	4	2	6	56	2	45
^{5}FeTMCAcOH	372.3	2	1	6	55	0	46
^{5}FeTMCBrOPr	465.3	2	1	6	62	0	46

^{5}FeTMCClOPr	420.8	2	1	6	62	0	46
^{6}FeTMCdmaBr	463.3	3	1	6	62	2	46
^{6}FeTMCdmaCl	418.8	3	1	6	62	2	46
^{6}FeTMCdmaF	402.4	3	1	6	62	2	46
^{6}FeTMCdmaN_3	425.4	3	1	6	64	2	46
^{6}FeTMCdmaNCS	441.4	3	1	6	64	2	46
^{6}FeTMCdmaOH	400.4	3	1	6	63	2	46
^{5}FeTMCFOPr	404.3	2	1	6	62	0	46
^{5}FeTMCN_3OPr	427.4	2	1	6	64	0	46
^{5}FeTMCNCSOPr	443.4	2	1	6	64	0	46
^{5}FeTMCOHOPr	402.4	2	1	6	63	0	46
^{5}FeTMCPrBr	449.2	2	1	6	57	0	46
^{5}FeTMCPrCl	404.8	2	1	6	57	0	46
^{5}FeTMCPrF	388.3	2	1	6	57	0	46
^{5}FeTMCPrN_3	411.3	2	1	6	59	0	46
^{5}FeTMCPrNCS	427.4	2	1	6	59	0	46
^{5}FeTMCPrOH	386.3	2	1	6	58	0	46
^{1}FeTMCpyBr	429.2	2	1	6	56	2	46
^{1}FeTMCpyCl	384.8	2	1	6	56	2	46
^{1}FeTMCpyF	368.3	2	1	6	56	2	46
^{1}FeTMCpyN_3	391.3	2	1	6	58	2	46
^{1}FeTMCpyNCS	407.4	2	1	6	58	2	46
^{1}FeTMCpyOH	366.3	2	1	6	57	2	46
^{6}Fetmg3trenBr	576.4	3	1	5	81	2	47
^{6}Fetmg3trenCl	532.0	3	1	5	81	2	47
^{6}Fetmg3trenF	515.5	3	1	5	81	2	47
^{6}Fetmg3trenN_3	538.5	3	1	5	83	2	47
^{6}Fetmg3trenNCS	554.6	3	1	5	83	2	47
^{6}Fetmg3trenOH	513.5	3	1	5	82	2	47
^{6}FeTPOBzOH	863.6	1	1	6	103	0	47
^{6}FeTMG2dienANOH	427.4	3	2	5	66	2	48
^{5}FeTMG2dienBrOH	466.2	4	2	5	61	2	48
^{3}FeTMG2dienClOH	421.8	4	2	5	61	2	48
^{5}FeTMG2dienFOH	405.3	4	2	5	61	2	48
^{5}FeTMG2dienN_3OH	428.4	4	2	5	63	2	48
^{5}FeTMG2dienNCSOH	444.4	4	2	5	63	2	48
^{1}FeTMG2dienOHBr	466.2	6	2	5	61	2	48
^{3}FeTMG2dienOHCl	421.8	6	2	5	61	2	48
^{5}FeTMG2dienOHF	405.3	6	2	5	61	2	48
^{3}FeTMG2dienOHN_3	428.4	6	2	5	63	2	48
^{3}FeTMG2dienOHNCS	444.4	6	2	5	63	2	48
^{6}FeTPAbpyBr	583.3	3	1	6	63	3	48
^{6}FeTPAbpyCl	538.9	3	1	6	63	3	48
^{6}FeTPAbpyF	522.4	3	1	6	63	3	48

^{6}FeTPAbpyN$_3$	545.4	3	1	6	65	3	48
^{6}FeTPAbpyNCS	561.5	3	1	6	65	3	48
^{2}FeTPAbpyOH	520.4	3	1	6	64	3	48
^{4}FeBPMENBr	406.1	3	1	5	44	2	49
^{4}FeBPMENCl	361.7	3	1	5	44	2	49
^{4}FeBPMENF	345.2	3	1	5	44	2	49
^{4}FeBPMENN$_3$	368.2	3	1	5	46	2	49
^{6}FeBPMENNCS	384.3	3	1	5	46	2	49
^{4}FeBPMENOH	343.2	3	1	5	45	2	49
^{2}FePy5Me2Br	579.3	3	1	6	61	2	50
^{2}FePy5Me2Cl	534.8	3	1	6	61	2	50
^{2}FePy5Me2F	518.4	3	1	6	61	2	50
^{2}FePy5Me2N$_3$	541.4	3	1	6	63	2	50
^{6}FePy5Me2NCS	557.5	3	1	6	63	2	50
^{2}FePy5Me2OH	516.4	3	1	6	62	2	50
^{6}FeLBr2	583.3	5	1	6	63	3	51
^{6}FeLCl2	538.9	5	1	6	63	3	51
^{6}FeLF2	522.4	5	1	6	63	3	51
^{6}FeLN$_3$2	545.4	5	1	6	65	3	51
^{6}FeLNCS2	561.5	5	1	6	65	3	51
^{2}FeLOH2	520.4	5	1	6	64	3	51
^{5}FeTQABrOH	593.3	4	2	6	62	2	52
^{5}FeTQAClOH	548.8	4	2	6	62	2	52
^{3}FeTQAFOH	532.4	4	2	6	62	2	52
^{5}FeTQAN$_3$OH	555.4	4	2	6	64	2	52
^{5}FeTQANCSOH	571.5	4	2	6	64	2	52
^{6}FeTQAOH	513.4	3	2	6	61	2	52
^{3}FeTQAOHBr	593.3	4	2	6	62	2	52
^{5}FeTQAOHCl	548.8	4	2	6	62	2	52
^{3}FeTQAOHF	532.4	4	2	6	62	2	52
^{6}FeTQAOHMeCN	554.4	3	2	6	67	2	52
^{5}FeTQAOHN$_3$	555.4	4	2	6	64	2	52
^{1}FeTQAOHNCS	571.5	4	2	6	64	2	52
^{5}FeTQAOHOTF	662.5	4	2	6	69	2	52
^{6}FeTPPh2OBzBr	926.5	3	1	6	102	2	53
^{4}FeTPPh2OBzCl	882.0	3	1	6	102	2	53
^{6}FeTPPh2OBzF	865.6	3	1	6	102	2	53
^{6}FeTPPh2OBzN$_3$	888.6	3	1	6	104	2	53
^{6}FeTPPh2OBzNCS	904.6	3	1	6	104	2	53
^{6}FeTPPh2OBzOH	863.6	3	1	6	103	2	53
^{6}FeTMCpyBr	469.3	3	1	6	61	2	54
^{6}FeTMCpyCl	424.8	3	1	6	61	2	54
^{6}FeTMCpyF	408.4	3	1	6	61	2	54
^{6}FeTMCpyN$_3$	431.4	3	1	6	63	2	54

^{6}FeTMCpyNCS	447.4	3	1	6	63	2	54
^{6}FeTMCpyOH	406.4	3	1	6	62	2	54
^{6}FeMeTPENBrB	483.2	3	1	6	53	2	55
^{6}FeMeTPENBrC	483.2	3	1	6	53	2	55
^{6}FeMeTPENClB	438.8	3	1	6	53	2	55
^{6}FeMeTPENClC	438.8	3	1	6	53	2	55
^{6}FeMeTPENFB	422.3	3	1	6	53	2	55
^{2}FeMeTPENFC	422.3	3	1	6	53	2	55
^{6}FeMeTPENN$_3$B	445.3	3	1	6	55	2	55
^{2}FeMeTPENN$_3$C	445.3	3	1	6	55	2	55
^{6}FeMeTPENNCSB	461.4	3	1	6	55	2	55
^{6}FeMeTPENOHB	420.3	3	1	6	54	2	55
^{2}FeMeTPENOHC	420.3	3	1	6	54	2	55
^{5}FeMe3tacnClacacBr	440.6	4	1	6	49	2	56
^{5}FeMe3tacnClacacCl	396.1	4	1	6	49	2	56
^{5}FeMe3tacnClacacF	379.7	4	1	6	49	2	56
^{3}FeTp2Cl	517.4	2	1	6	54	1	56
^{3}FeTp2F	500.9	2	1	6	54	1	56
^{3}FeTp2NCS	540.0	2	1	6	56	1	56
^{6}FeCDOCABr*	748.5	3	1	6	79	0	57
^{6}FeCDOCACl*	704.0	3	1	6	79	0	57
^{6}FeCDOCAF*	687.6	3	1	6	79	0	57
^{6}FeCDOCAN$_3$*	710.6	3	1	6	81	0	57
^{4}FeCDOCAOH*	685.6	3	1	6	80	0	57
^{6}FeCDODMBr*	748.5	3	1	6	79	0	57
^{6}FeCDODMCl*	704.0	3	1	6	79	0	57
^{6}FeCDODMF*	687.6	3	1	6	79	0	57
^{6}FeCDODMN$_3$*	710.6	3	1	6	81	0	57
^{6}FeCDODMNCS*	726.7	3	1	6	81	0	57
^{6}FeCDODMOH*	685.6	3	1	6	80	0	57
^{6}FeTauDBr	390.0	3	1	6	34	0	58
^{6}FeTauDCl	345.5	3	1	6	34	0	58
^{6}FeTauDF	329.1	3	1	6	34	0	58
^{6}FeTauDN$_3$	352.1	3	1	6	36	0	58
^{6}FeTauDNCS	368.2	3	1	6	36	0	58
^{6}FeTauDOH	327.1	3	1	6	35	0	58
^{5}FeCDOBrC*	757.5	2	1	6	81	0	59
^{5}FeCDOBrC1*	757.5	2	1	6	81	0	59
^{3}FeCDOClC*	713.1	2	1	6	81	0	59
^{5}FeCDOClC1*	713.1	2	1	6	81	0	59
^{5}FeCDOFC*	696.6	2	1	6	81	0	59
^{5}FeCDOFC1*	696.6	2	1	6	81	0	59
^{5}FeCDON$_3$C*	719.6	2	1	6	83	0	59
^{5}FeCDON$_3$C1*	719.6	2	1	6	83	0	59

^{5}FeCDONCSC*	735.7	2	1	6	83	0	59
^{5}FeCDONCSC1*	735.7	2	1	6	83	0	59
^{5}FeCDOOHC*	694.6	2	1	6	82	0	59
^{5}FeCDOOHC1*	694.6	2	1	6	82	0	59
^{5}FeH3BueaBr	576.4	4	1	5	75	0	60
^{5}FeH3BueaCl	531.9	4	1	5	75	0	60
^{5}FeH3BueaF	515.4	4	1	5	75	0	60
^{5}FeH3BueaN_3	538.5	4	1	5	77	0	60
^{5}FeH3BueaNCS	554.5	4	1	5	77	0	60
^{5}FeH3BueaOH	513.5	4	1	5	76	0	60
^{5}FeAIkBBr*	599.3	2	1	6	66	2	61
^{5}FeAIkBCl*	554.8	2	1	6	66	2	61
^{3}FeAIkBF*	538.4	2	1	6	66	2	61
^{5}FeAIkBNCS*	577.4	2	1	6	68	2	61
^{4}FeAIkBBrOHR1*	600.3	3	1	6	67	2	61
^{4}FeAIkBBrR*	642.3	3	1	6	72	2	61
^{4}FeAIkBClR*	597.9	3	1	6	72	2	61
^{6}FeAIkBFR*	581.4	3	1	6	72	2	61
^{4}FeAIkBN_3R*	604.4	3	1	6	74	2	61
^{4}FeAIkBNCSR*	620.5	3	1	6	74	2	61
^{6}FeEgtBBrRe*	756.5	1	1	6	85	0	62
^{6}FeEgtBClRe*	712.0	1	1	6	85	0	62
^{6}FeEgtBFRe*	695.6	1	1	6	85	0	62
^{6}FeEgtBN_3Re*	718.6	1	1	6	87	0	62
^{6}FeEgtBNCSRe*	734.7	1	1	6	87	0	62
^{6}FeEgtBOHRe*	693.6	1	1	6	86	0	62
^{5}FeEgtBBrP*	771.5	2	1	6	85	0	62
^{3}FeEgtBClP*	727.0	2	1	6	85	0	62
^{5}FeEgtBFP*	710.6	2	1	6	85	0	62
^{5}FeEgtBN_3P*	733.6	2	1	6	87	0	62
^{5}FeEgtBNCSP*	749.6	2	1	6	87	0	62
^{5}FeEgtBOHP*	708.6	2	1	6	86	0	62

*** Complex contain molecules not directly coordinated to the Fe center**

1.3 Details of diabatic BDE calculation

The diabatic BDE is calculated using the single-point energy (E) of each structure. After optimizing the non-heme compounds at the B3LYP-D3/LANL2DZ-6-31G(d) level, single-point calculations for fragments A, B, and molecule AB were performed at the (U)B3LYP-D3/def2-TZVP level.

$$Fe(OH)(L) \rightarrow Fe(OH) + L\bullet$$

$$Fe(OH)(L) \rightarrow Fe(L) + OH\bullet$$

$$\text{diabatic BDEs}_{(Fe-L)} = E_{(L\bullet)} + E_{(Fe(OH))} - E_{(Fe(OH)(L))}$$

$$\text{diabatic BDEs}_{(Fe-OH)} = E_{(OH\bullet)} + E_{(Fe(L))} - E_{(Fe(OH)(L)}$$

We performed further calculations on Fe–X and Fe–OH bonds using other functionals including BP86, PBE0, MN15, wb97xd. The results indicate that the diabatic BDE values calculated with different functionals are comparable, with B3LYP-D3 yielding values closest to the average. The results are shown in Table S3.

Table S3. Calculated diabatic BDE of chemical bonds in different non-heme complexes

Bond	Diabatic BDE (kcal mol^{-1})					
	B3LYP-D3	BP86-D3	PBE0-D3	MN15	*ω*B97XD	Average[c]
Fe–Cl [a] (^{6}FeTPAClOH)	105.2	103.2	114.0	94.5	106.0	**104.6**
Fe–Cl [a] (^{5}FeNTBClOH)	145.1	129.6	152.1	142.2	152.2	**144.2**
Fe–F [a] (^{5}FeNTBFOH)	169.5	160.8	174.3	160.4	171.9	**167.4**
Fe–N_3 [a] (^{5}FeNTBN_3OH)	124.4	110.8	131.1	110.8	127.8	**121.0**
Fe–NCS [a] (^{5}FeNTBNCSOH)	135.6	119.3	142.1	132.0	142.2	**134.2**
Fe–OH [a] (^{5}FeNTBFOH)	144.1	134.9	149.7	139.1	147.8	**143.1**
Fe–OH [a] (^{5}FeNTBN_3OH)	131.8	121.9	138.3	125.9	135.5	**130.7**
Fe–OH [a] (^{5}FeNTBNCSOH)	129.1	120.4	135.6	122.4	132.3	**128.0**
Fe–F [a] (^{3}FeCDOF)	175.7	160.7	180.8	165.8	178.7	**172.4**
Fe–F [b] (^{3}FeCDOF)	175.2	160.7	179.9	165.5	177.4	**171.7**
Fe–F [a] (^{3}FeAIkBFR)	173.0	161.0	178.0	166.0	176.6	**170.9**
Fe–F [b] (^{3}FeAIkBFR)	174.9	162.2	179.9	169.9	178.2	**173.0**

[a] Diabatic BDE (kcal mol^{-1}) obtained at the DFT/def2TZVP//B3LYP-D3/6-31G(d)-LANL2DZ level.

[b] Diabatic BDE (kcal mol^{-1}) obtained at the DFT/def2TZVP//B3LYP-D3/6-31+G (d,p)-LANL2DZ level.

[c] Calculate the average BDE from the values obtained using five functionals: B3LYP-D3, BP86-D3, PBE0-D3, MN15, and ωB97XD.

There are some relatively small diabatic BDEs in the database, such as the Fe–N_3 bond of Fe(TMC)(OH)(N3)$^{+}$and the Fe–NCS bond of Fe(TQA)(OH)(NCS)$^{2+}$, as well as relatively large BDEs, such as the Fe-F bond of FeCDO(F) and FeAIkB(F)R^{2+}, which are mainly due to the influence of surrounding hydrogen bonds on the F atom. Considering the existence of hydrogen bonds, we conducted supplementary calculations. FeCDO(F) and FeAIkB(F)R^{2+} were calculated at the DFT/def2-TZVP//B3LYP-D3/6-31G(d)-LANL2DZ level ,as shown in Table S3. In addition, the structures of FeCDO(F) and FeAIkB(F)R^{2+} have been reoptimized at the DFT/def2TZVP//B3LYP-D3/6-31+G(d,p)-LANL2DZ level. We aligned the FeCDO(F)-a (B3LYP-D3/def2-TZVP//B3LYP-D3/6-31G(d)-LANL2DZ, in red) and FeCDO(F)-b (B3LYP-D3/def2TZVP//B3LYP-D3/6-31+G(d,p)-LANL2DZ, in blue), the structure of FeCDO(F)-a is almost identical to that of FeCDO(F)-b, RMSD = 0.087. A same trend is observed for FeAIkB(F)R^{2+}-a and FeAIkB(F)R^{2+}-b. Related results have been included in Figure S2.

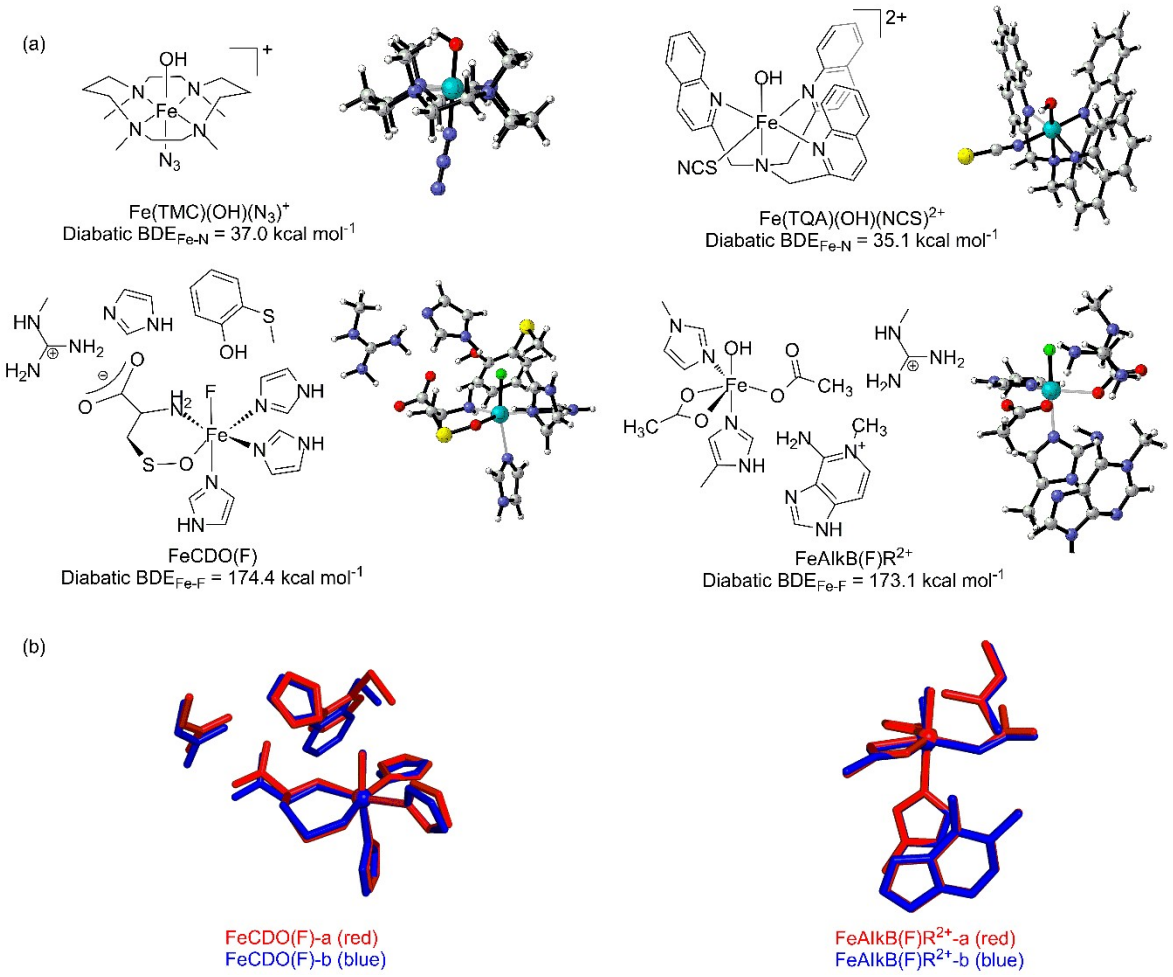

Figure S2. (a) Special diabatic BDE values and the corresponding non-heme iron complex structures, (b) Optimized geometries of FeCDO(F)-a, FeCDO(F)-b, FeAIkB(F)R^{2+}-a and FeAIkB(F)R^{2+}-b. The structures optimized at the B3LYP-D3/def2-TZVP//B3LYP-D3/6-31G(d)-LANL2DZ level are shown as red, and the structures optimized at the B3LYP-D3/def2-TZVP//B3LYP-D3/6-31+G(d,p)-LANL2DZ level are shown as blue.

The distribution of each one of the BDEs per bond type as well as the full database is shown in Figure S3.

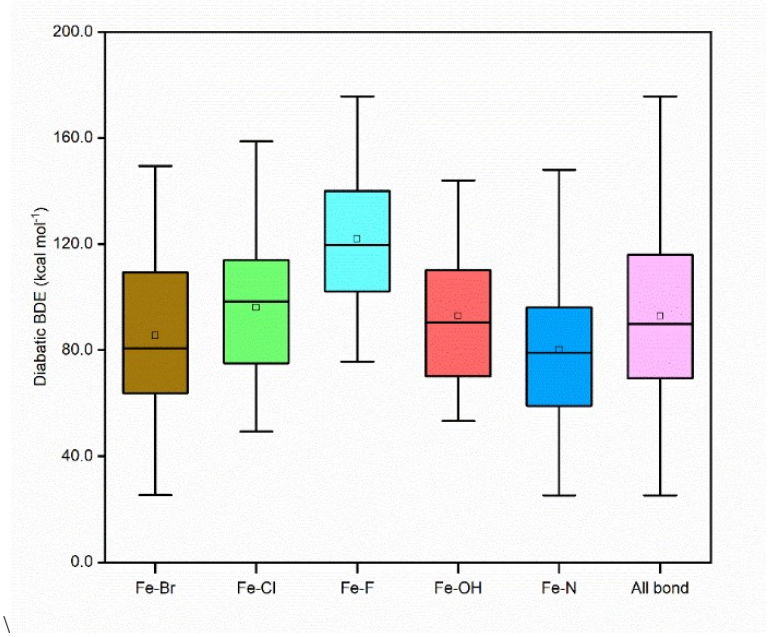

Figure S3. The distribution of each one of the BDEs per bond type as well as the full database.

Since non-heme iron complexes with a single monodentate ligand correspond to one diabatic BDE, while those with two monodentate ligands correspond to two diabatic BDEs, a total of 652 non-heme iron complex structures and 899 diabatic BDE values were ultimately collected. All diabatic BDE values are available on GitHub (https://github.com/rvsanshi/Nonheme.git).

2. Details of molecular descriptor

This study utilized four distinct molecular fingerprints: Morgan fingerprint, RDKit fingerprint, Topological Torsion (Topo) fingerprint, and Atom pair fingerprint, and three 3D descriptors: SOAP、MBTR、Coulomb Matrix. Feature selection was performed on these seven molecular descriptors, we first removed constant and duplicate features, then applied low-variance filtering (threshold = 0.01) to eliminate features with minimal variation. This is followed by feature ranking using a Random Forest model (n_estimators = 100, with Gini importance), retaining the top 150 fingerprint features and the top 200 3D descriptor features. For example, when using Morgan fingerprints, the initial molecular descriptor dimension is 6144, obtained by concatenating the Morgan fingerprints calculated separately for the molecule, fragment 1, and fragment 2. Removing constant and duplicate features reduces the descriptor dimension to 4005. Subsequently, low-variance filtering further reduces it to 3220. Finally, a Random Forest model is applied for feature ranking, retaining the top 150 fingerprint features. Detailed information can be obtained on GitHub (https://github.com/rvsanshi/Nonheme.git). A comprehensive list of the molecular descriptors employed is provided in **Table S4**.

Table S4. The molecular descriptors applied in this study.

Molecular descriptors	Original Feature Dimension	Selected Feature Dimension	Description
Morgan	6144	150	The Morgan fingerprint radius is 3, and the bit length is 2048. includeChirality = True
RDKit	6144	150	The bit length is 2048. includeChirality = True
Topological torsion (Topo)	6144	150	The bit length is 2048. includeChirality = True
Atom pair	6144	150	The bit length is 2048. includeChirality = True
SOAP	4000	170	species = ["H", "C", "N", "O", "F", "S", "Cl", "Br", "Fe"], r_cut = 6.0, n_max = 8, l_max = 6, length = 2000
MBTR	3000	200	k1{species= ["C", "H", "O", "N", "S", "P", "B", "Si", "I", "Fe", "K", "F", "Cl", "Br"], geometry = {"function": "atomic_number"}, grid = {"min": 0, "max": 10, "n": 100, "sigma": 0.1}, periodic=False, normalization="l2", sparse=False} k2{species= ["C", "H", "O", "N", "S", "P", "B", "Si", "I", "Fe", "K", "F", "Cl", "Br"], geometry= {"function": "inverse_distance"}, grid= {"min": 0, "max": 1, "n": 100, "sigma": 0.1}, weighting = {"function": "exp", "scale": 0.5, "threshold": 1e-3}, periodic=False, normalization="l2", sparse=False}, length = 2500
Coulomb Matrix	1000	187	Length = 1000

3. Details of model training

The 889 diabatic BDE values were randomly split into a 70% training dataset and a 30% testing dataset. During each machine learning iteration, the training dataset underwent a grid search using K-fold cross-validation to optimize hyperparameters. The SMARTS rule was applied to segment the two-dimensional molecular structures imported from SDF files, producing the molecular structure and the corresponding two radical structures after bond cleavage.

Fingerprints were generated for these three structures using RDKit (fpSize = 2048), Morgan (radius = 3, fpSize = 2048), Topological torsion (fpSize = 2048), and Atom pair (fpSize = 2048) fingerprints. The fingerprints of the three structures were then merged and optimized to create a new fingerprint. In addition, three 3D descriptors, SOAP, MBTR, and Coulomb Matrix, were introduced to combine with molecular fingerprints to create new molecular descriptors.

For each molecular descriptor, eight machine learning models—Linear Regression (LR), Random Forest (RF), Extra Trees (ET), K-Nearest Neighbor (KNN), Decision Tree (DT), Gradient Boosting Regression (GBR), AdaBoost Regressor (ABR), and Hist Gradient Boosting Regressor (HGBR)—were trained on the training dataset using optimized hyperparameters. The BDE prediction accuracy was assessed by comparing predictions to the test dataset. Mean absolute error (MAE) and the coefficient of determination (R^2) were used as metrics to evaluate prediction accuracy. The list of parameters used in different machine learning methods is shown in Table S5.

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|yi_{DFT} - yi_{ML}|$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(yi_{DFT} - yi_{ML})^2}{\sum_{i=1}^{n}(yi_{DFT} - yi_{average_DFT})^2}$$

The training and testing were performed 10 times (random state = 42), and the accuracy was evaluated a s the average of the results. The complete code for model training is available on GitHub (https://github. com/rvsanshi/Nonheme.git).

Table S5. The list of parameters used in different machine learning methods.

Method	Parameters
Linear Regression (LR)	n_jobs = -1
Random Forest (RF)	n_estimators: [100, 200, 300, 400, 500, 600], max_depth: [None, 5, 10, 15, 20], n_jobs = -1
Extra Trees (ET)	n_estimators: [100, 200, 300, 400, 500, 600], max_depth: [None, 5, 10, 15, 20], n_jobs = -1
K-Nearest Neighbor (KNN)	n_neighbors: [5, 10, 15], leaf_size: [25, 30, 35], n_jobs = -1
Decision Tree (DT)	max_depth: [None, 10, 20], min_samples_split: [2, 4, 6]

Gradient Boosting Regression (GBR)	n_estimators: [100, 200, 300, 400, 500, 600], max_depth: [5, 10, 15, 20]
AdaBoost Regressor (ABR)	n_estimators: [100, 200, 300, 400, 500, 600]
Hist Gradient Boosting Regressor (HGBR)	max_depth: [5, 10, 15, 20], min_samples_leaf: [5, 10, 15, 20]

4. Results

The final performance of seven algorithms (RF, ET, KNN, DT, GBR, ABR, HGBR) is shown in Figure S4-S10.

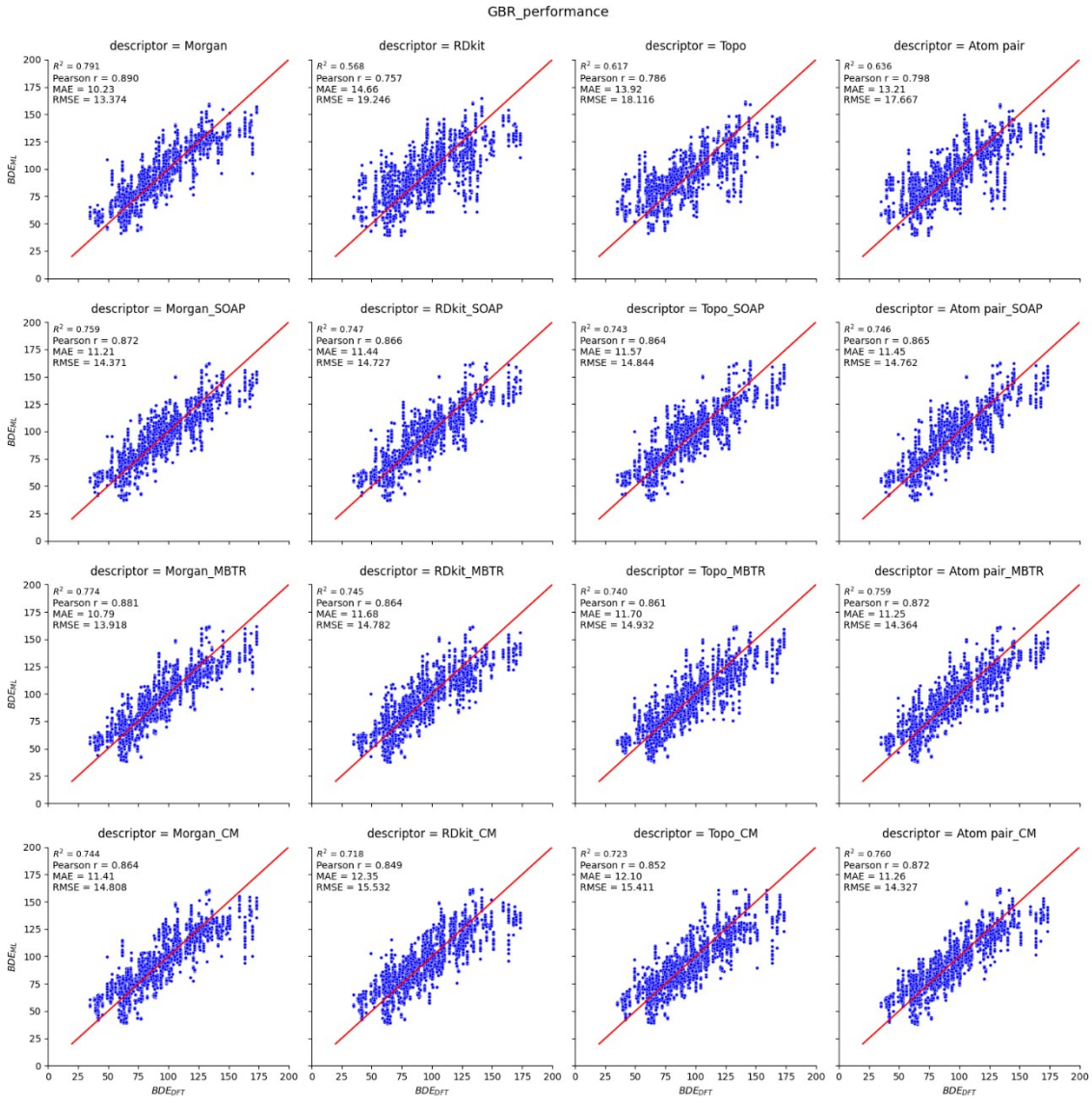

Figure S4. Performance of GBR algorithm combined with different molecular descriptors.

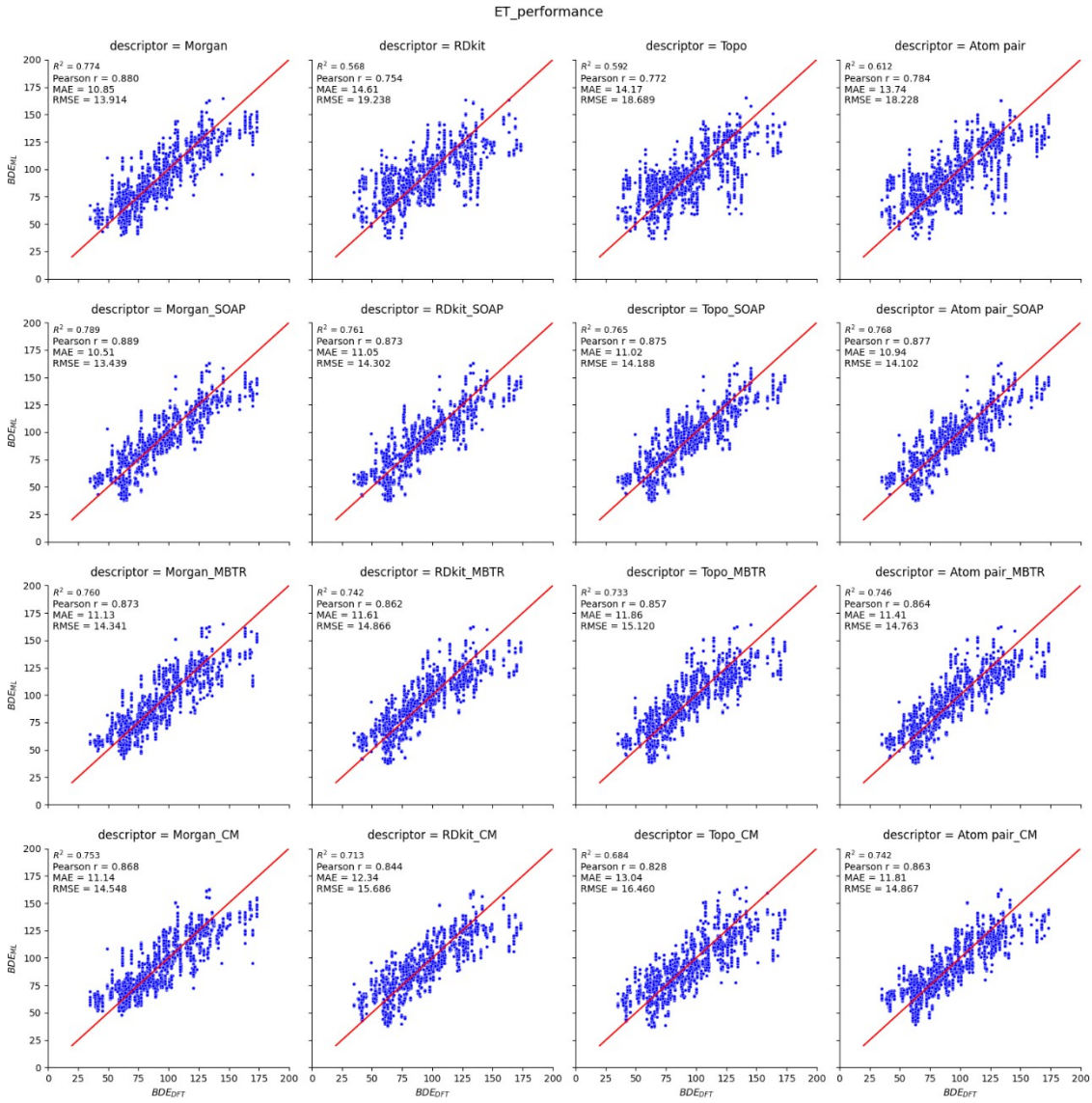

Figure S5. Performance of ET algorithm combined with different molecular descriptors.

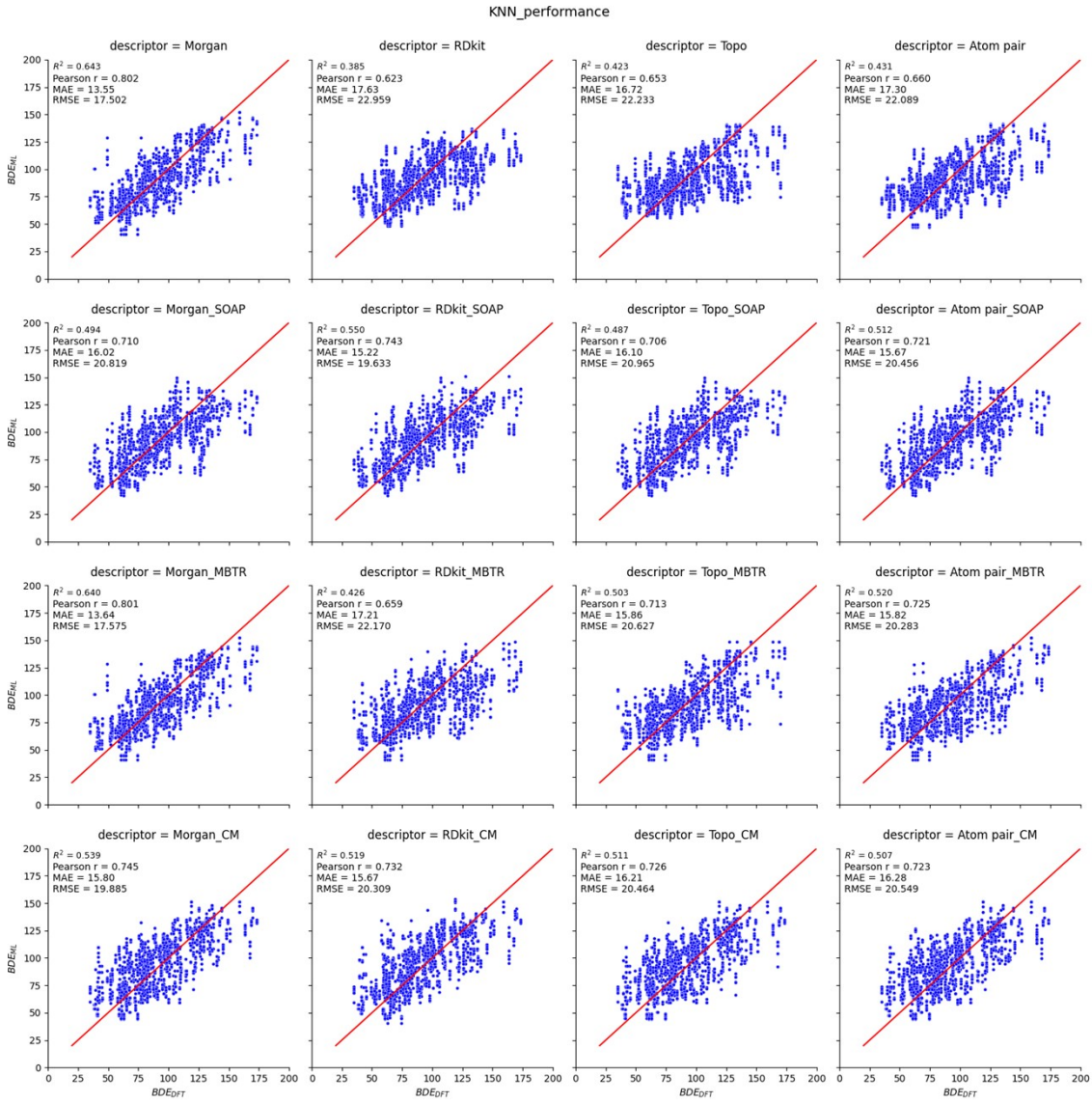

Figure S6. Performance of KNN algorithm combined with different molecular descriptors.

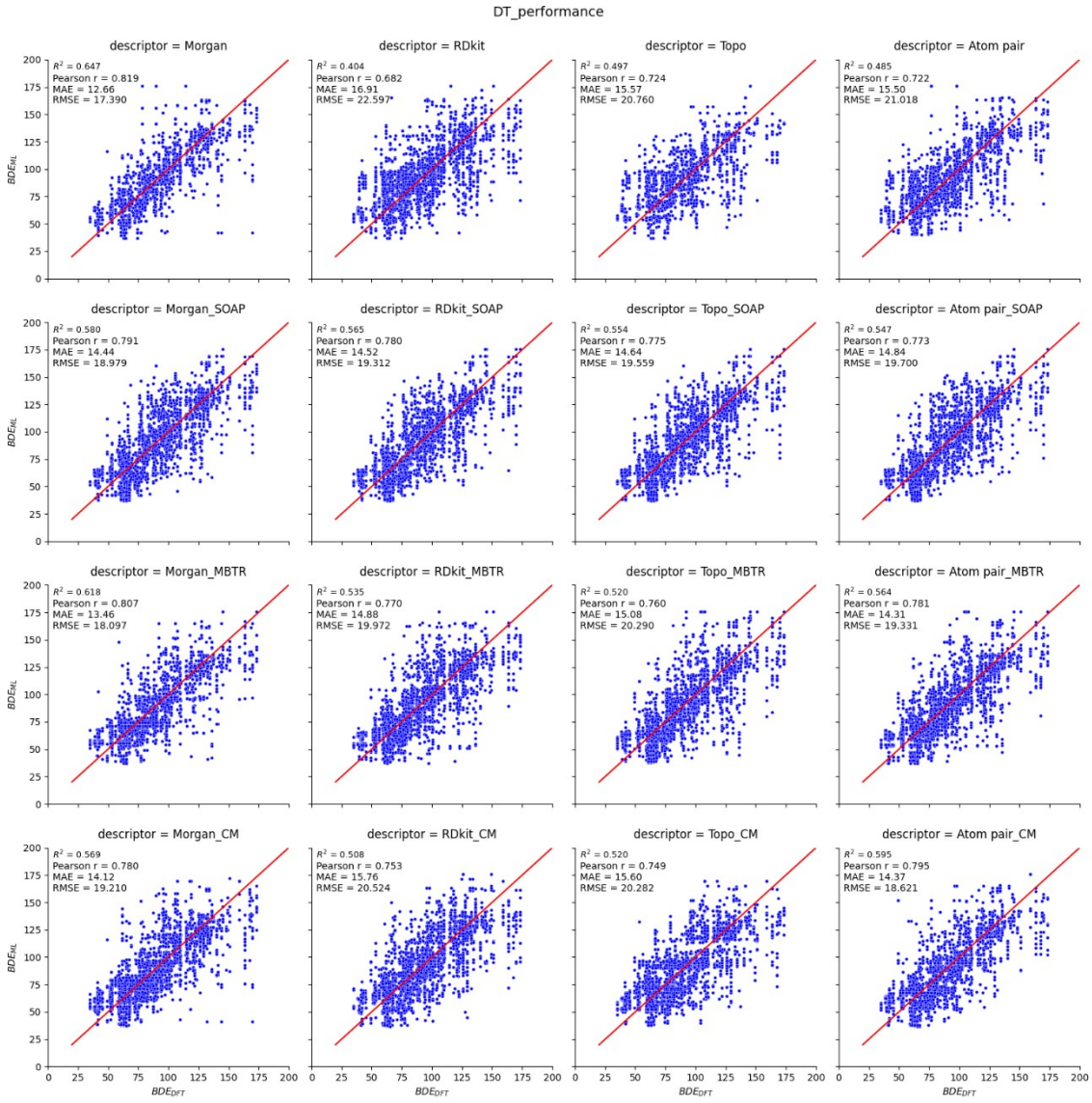

Figure S7. Performance of DT algorithm combined with different molecular descriptors.

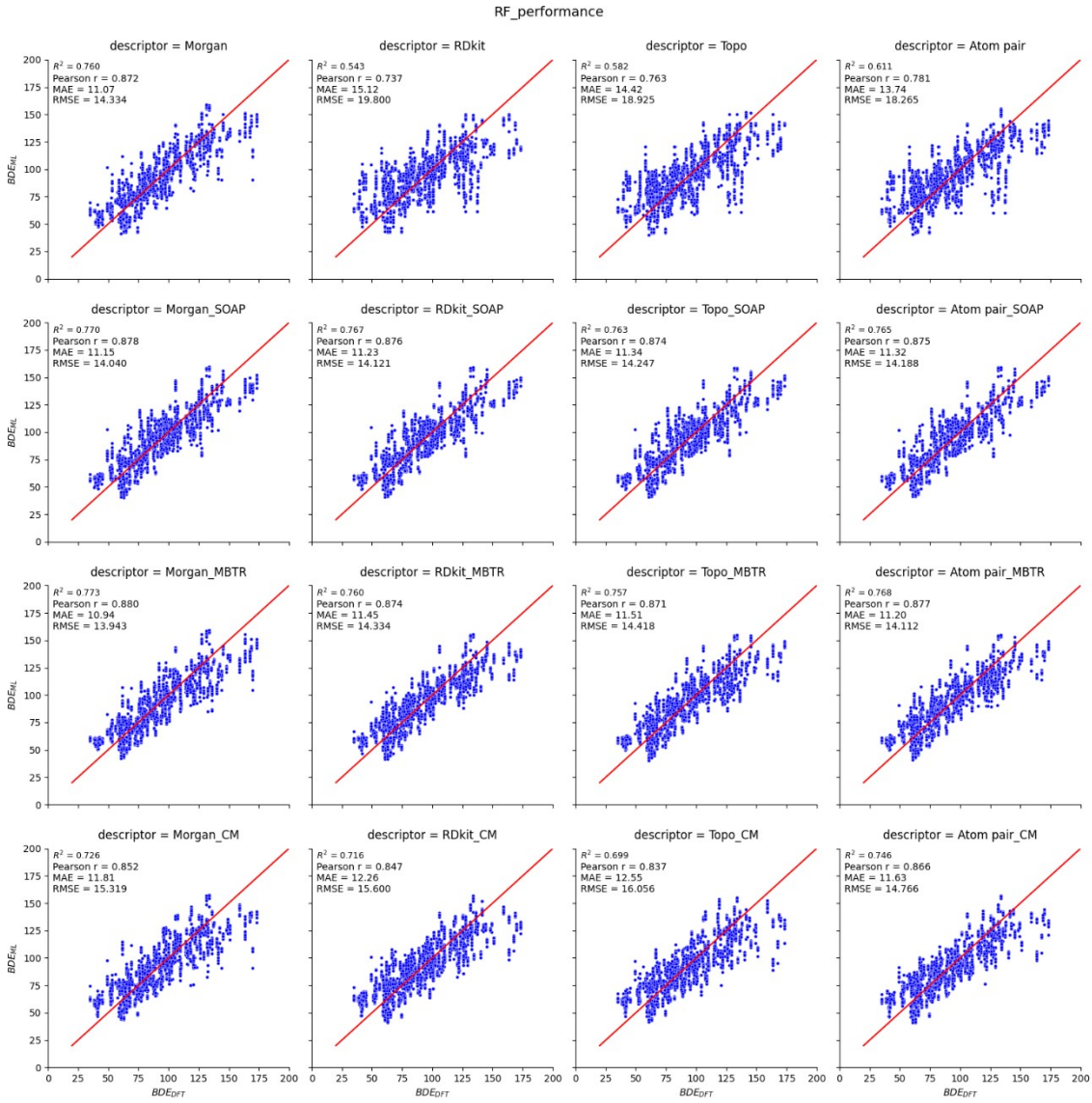

Figure S8. Performance of RF algorithm combined with different molecular descriptors.

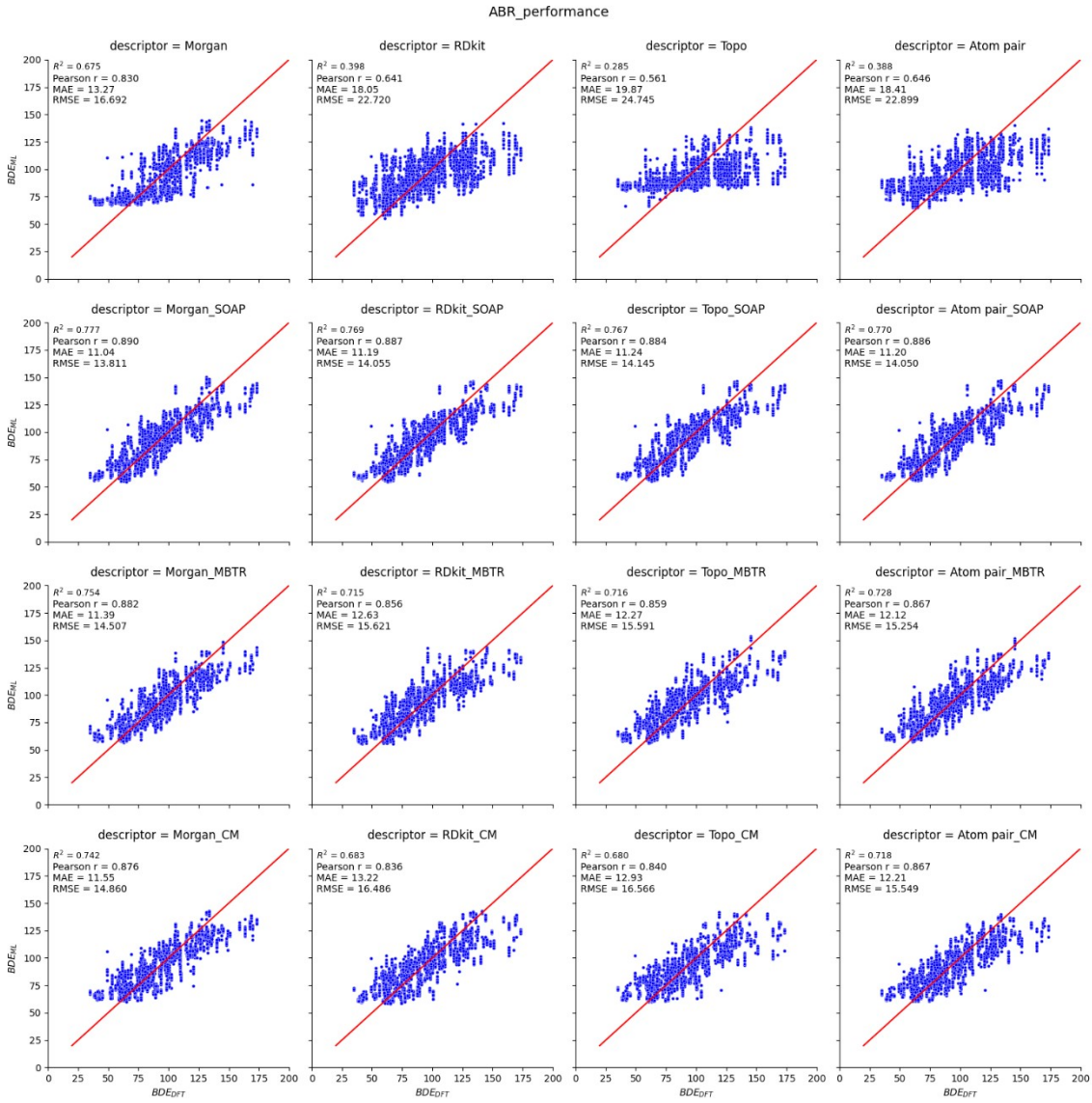

Figure S9. Performance of ABR algorithm combined with different molecular descriptors.

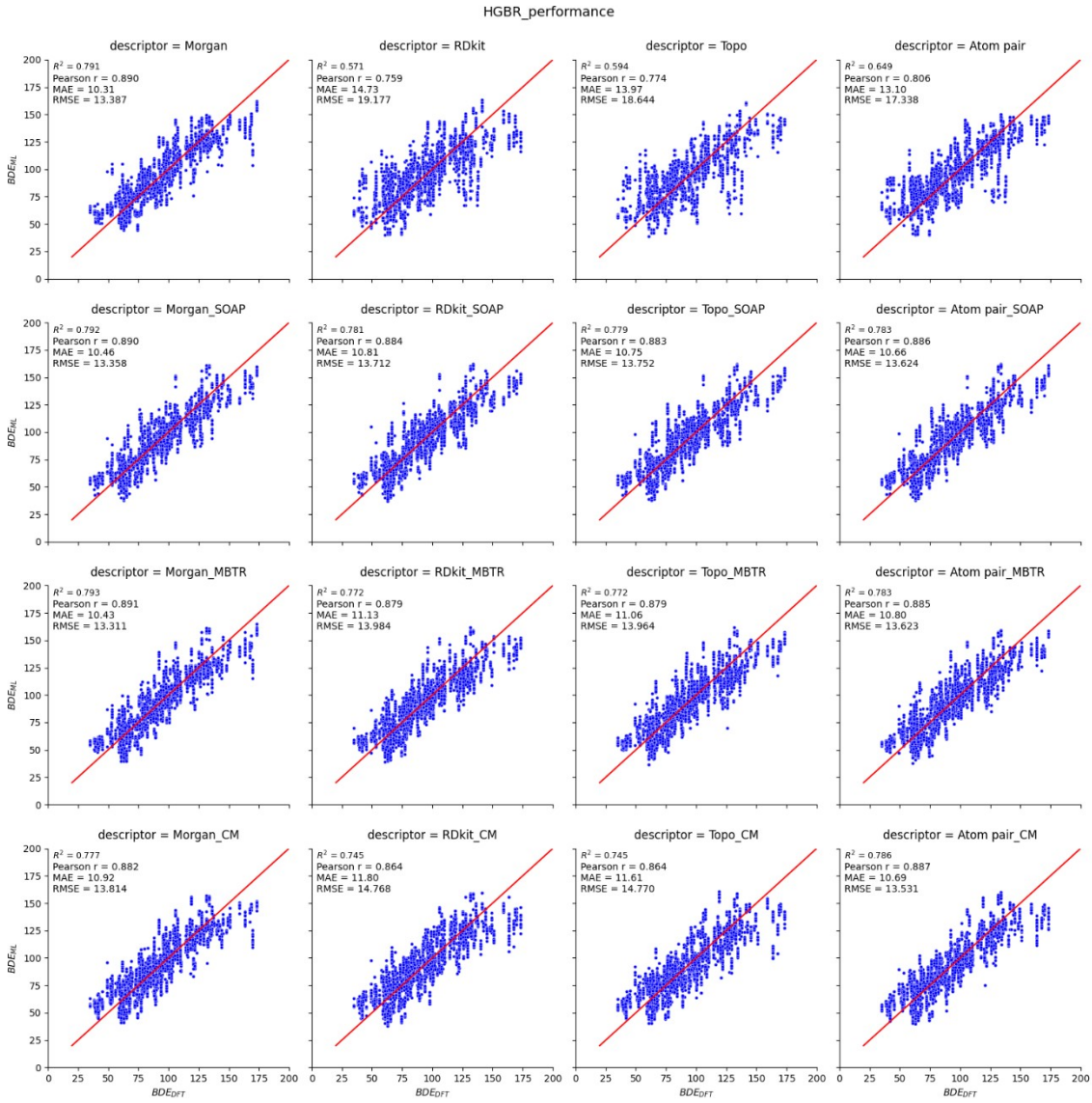

Figure S10. Performance of HGBR algorithm combined with different molecular descriptors.

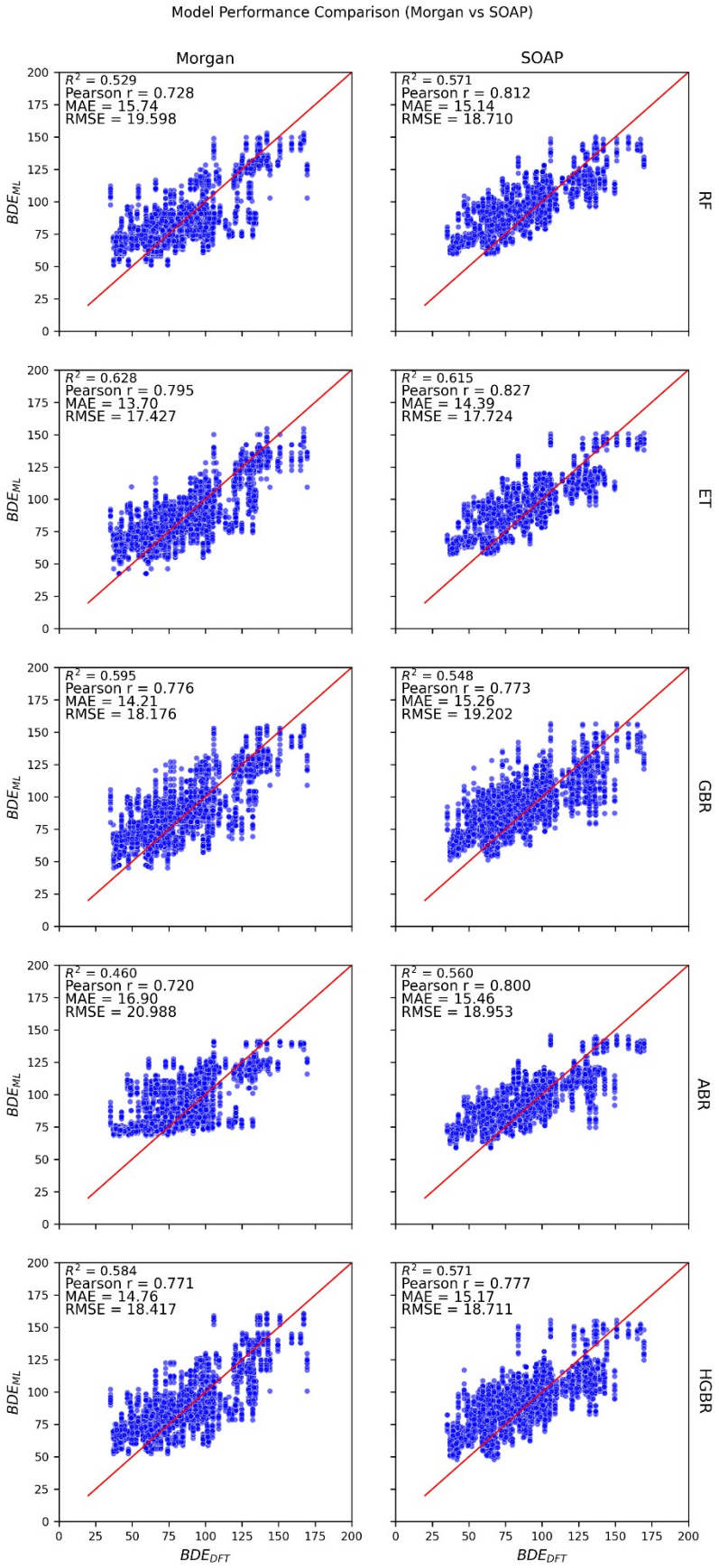

Figure S11. Predicting isomeric bonds using SOAP descriptors and Morgan fingerprints

5. Cartesian Coordinates

^{3}FeTMCBrOH
Charge: 2+
Energy: -2940147.9761543

Fe	0.01847	-0.00002	-0.36237
N	1.43964	-1.64487	-0.32591
N	-1.46907	-1.62752	-0.36702
N	-1.46944	1.62728	-0.36704
N	1.43928	1.64521	-0.32576
C	0.72054	-2.71955	0.43503
H	1.26133	-3.66635	0.30834
H	0.74954	-2.45755	1.48845
C	-0.72016	-2.91107	-0.03869
H	-1.27220	-3.45544	0.73295
H	-0.73624	-3.53065	-0.93581
C	-2.54506	-1.32928	0.65014
H	-3.28015	-2.14211	0.58119
H	-2.08631	-1.37985	1.63459
C	-3.29583	-0.00033	0.46709
H	-4.06745	-0.00040	1.24677
H	-3.85878	-0.00030	-0.47088
C	-2.54519	1.32867	0.65028
H	-2.08624	1.37913	1.63465
H	-3.28040	2.14141	0.58162
C	-0.72075	2.91097	-0.03865
H	-0.73682	3.53053	-0.93577
H	-1.27300	3.45527	0.73290
C	0.71991	2.71968	0.43522
H	0.74886	2.45756	1.48861
H	1.26052	3.66661	0.30869
C	2.72357	1.29149	0.37045
H	2.51593	1.22661	1.43826
H	3.41035	2.13331	0.21495
C	3.39315	0.00041	-0.10673
H	3.55042	0.00048	-1.18912
H	4.39867	0.00050	0.32947
C	2.72386	-1.29086	0.37032
H	2.51621	-1.22613	1.43814
H	3.41084	-2.13251	0.21473
C	1.73868	-2.10649	-1.71382
H	2.42767	-2.95717	-1.66135
H	0.82549	-2.40871	-2.21788
H	2.18867	-1.30154	-2.28891
C	-2.11255	-1.83396	-1.69926
H	-2.79847	-2.68717	-1.64426
H	-1.35522	-2.04106	-2.45405
H	-2.69175	-0.96142	-1.99135
C	-2.11324	1.83378	-1.69909
H	-2.69207	0.96104	-1.99135
H	-1.35616	2.04168	-2.45393
H	-2.79958	2.68663	-1.64383
C	1.73824	2.10690	-1.71366
H	0.82502	2.40915	-2.21766
H	2.18818	1.30198	-2.28882
H	2.42720	2.95761	-1.66123
O	0.09245	-0.00027	-2.11514
H	-0.74473	0.00223	-2.60923
Br	0.09649	-0.00010	2.11750

^{3}FeTMCClOH
Charge: 2+
Energy: -1613624.9241085

Fe	-0.02531	-0.00012	0.17106
N	-1.44972	-1.65355	0.09604
N	1.46917	-1.62106	0.18355
N	1.47060	1.62017	0.18363
N	-1.44856	1.65461	0.09552
C	-0.69009	-2.70697	-0.65981
H	-1.23587	-3.65715	-0.59575
H	-0.65778	-2.40815	-1.70357
C	0.71537	-2.90523	-0.10475
H	1.29344	-3.50648	-0.81353
H	0.67273	-3.46862	0.82787
C	2.50953	-1.33060	-0.86649
H	3.24813	-2.14154	-0.80922
H	2.02200	-1.39248	-1.83707
C	3.26692	-0.00120	-0.71666
H	4.00671	-0.00155	-1.52642
H	3.86353	-0.00144	0.19952
C	2.51061	1.32880	-0.86657
H	2.02297	1.39094	-1.83707
H	3.24985	2.13918	-0.80950
C	0.71739	2.90466	-0.10486
H	0.67456	3.46788	0.82786
H	1.29606	3.50579	-0.81325
C	-0.68791	2.70709	-0.66048
H	-0.65534	2.40776	-1.70409
H	-1.23305	3.65770	-0.59713
C	-2.70556	1.29538	-0.64702
H	-2.45429	1.22628	-1.70516
H	-3.40096	2.13560	-0.52303
C	-3.38911	0.00125	-0.19531
H	-3.58915	0.00153	0.88106
H	-4.37984	0.00150	-0.66433
C	-2.70660	-1.29360	-0.64649
H	-2.45541	-1.22522	-1.70469
H	-3.40261	-2.13322	-0.52196
C	-1.79881	-2.15388	1.45656
H	-2.38160	-3.07772	1.36717
H	-0.89931	-2.34775	2.03595
H	-2.41004	-1.41834	1.98059
C	2.12379	-1.78609	1.51469
H	2.78348	-2.66121	1.47816
H	1.36883	-1.91852	2.28545
H	2.71567	-0.91416	1.76697
C	2.12550	1.78542	1.51454
H	2.71841	0.91406	1.76641
H	1.37064	1.91700	2.28558
H	2.78440	2.66114	1.47801
C	-1.79736	2.15561	1.45590
H	-0.89773	2.34885	2.03526
H	-2.40911	1.42064	1.98012
H	-2.37951	3.07980	1.36614
O	0.01382	0.00044	1.92065
H	-0.83367	0.00027	2.39829
Cl	-0.07770	-0.00046	-2.07990

^{3}FeTMCFOH
Charge: 2+
Energy: -1387517.1631892

Fe	-0.03854	0.00011	0.17190
N	-1.45678	-1.64807	-0.01054
N	1.49138	-1.61050	0.10280
N	1.49067	1.61102	0.10293
N	-1.45735	1.64751	-0.01046
C	-0.63105	-2.65440	-0.75784
H	-1.18249	-3.60120	-0.82057
H	-0.49373	-2.26929	-1.76717
C	0.70676	-2.88237	-0.08360
H	1.30163	-3.58601	-0.67740
H	0.57129	-3.33141	0.90088
C	2.35360	-1.31836	-1.09069
H	3.07594	-2.14201	-1.17186
H	1.70794	-1.34380	-1.96812
C	3.13746	0.00067	-1.04997
H	3.75232	0.00081	-1.95794
H	3.85938	0.00091	-0.22898
C	2.35294	1.31927	-1.09068
H	1.70701	1.34434	-1.96792
H	3.07484	2.14328	-1.17200
C	0.70576	2.88273	-0.08363
H	0.57034	3.33211	0.90071
H	1.30034	3.58632	-0.67774
C	-0.63200	2.65416	-0.75776
H	-0.49448	2.26922	-1.76712
H	-1.18392	3.60068	-0.82053
C	-2.64443	1.27945	-0.84832
H	-2.29168	1.17667	-1.87555
H	-3.33798	2.12986	-0.81388
C	-3.37156	-0.00061	-0.43723
H	-3.64020	-0.00069	0.62386
H	-4.32789	-0.00077	-0.97248
C	-2.64396	-1.28041	-0.84833
H	-2.29126	-1.17754	-1.87556
H	-3.33728	-2.13103	-0.81388
C	-1.89038	-2.16896	1.31394
H	-2.43798	-3.10954	1.18170
H	-1.02912	-2.33397	1.95806
H	-2.55471	-1.44836	1.79203
C	2.28810	-1.75535	1.35053
H	2.86404	-2.68766	1.30221
H	1.61443	-1.77127	2.20589
H	2.98123	-0.93061	1.46977
C	2.28718	1.75592	1.35074
H	2.97856	0.92993	1.47132
H	1.61320	1.77393	2.20581
H	2.86483	2.68714	1.30158
C	-1.89129	2.16853	1.31388
H	-1.03010	2.33461	1.95783
H	-2.55528	1.44773	1.79215
H	-2.43954	3.10872	1.18137
O	0.00707	-0.00041	1.92440
H	-0.82736	-0.00025	2.42509

F	-0.07502	-0.00021	-1.57397

^{3}FeTMCN$_3$OH
Charge: 2+
Energy: -1427887.9747556

Fe	-0.01130	0.08468	-0.28179
N	1.47645	-1.41850	-0.49638
N	-1.40852	-1.51950	-0.48947
N	-1.56163	1.55464	-0.02523
N	1.33069	1.72266	-0.02371
C	0.79421	-2.63761	0.05240
H	1.39012	-3.52802	-0.18503
H	0.76424	-2.56362	1.13644
C	-0.59428	-2.79284	-0.53217
H	-1.13229	-3.58717	-0.00394
H	-0.52450	-3.09988	-1.57575
C	-2.33675	-1.51185	0.69703
H	-3.03512	-2.34860	0.56495
H	-1.74569	-1.73057	1.58496
C	-3.16906	-0.23534	0.88411
H	-3.76863	-0.40220	1.78714
H	-3.90448	-0.14735	0.07992
C	-2.45443	1.10564	1.10017
H	-1.84712	1.08224	2.00389
H	-3.22281	1.87862	1.23232
C	-0.85647	2.84450	0.32682
H	-0.81779	3.45232	-0.57760
H	-1.45809	3.39879	1.05512
C	0.53977	2.63312	0.87164
H	0.50737	2.17760	1.85890
H	1.05335	3.59897	0.95637
C	2.60320	1.35498	0.68541
H	2.34248	1.11484	1.71741
H	3.23391	2.25263	0.70797
C	3.38101	0.19277	0.07577
H	3.62325	0.36711	-0.97698
H	4.34991	0.16145	0.58755
C	2.73196	-1.17055	0.29422
H	2.49483	-1.29373	1.35191
H	3.44174	-1.96539	0.03287
C	1.85136	-1.66080	-1.92304
H	2.49291	-2.54664	-1.98732
H	0.96428	-1.80829	-2.53370
H	2.41046	-0.80881	-2.31067
C	-2.21378	-1.51519	-1.75108
H	-2.74910	-2.46821	-1.83037
H	-1.55349	-1.37950	-2.60415
H	-2.94219	-0.71468	-1.74819
C	-2.38392	1.86028	-1.23575
H	-3.06514	1.05021	-1.46455
H	-1.72857	2.01617	-2.08978
H	-2.97840	2.76035	-1.04161
C	1.66587	2.42570	-1.29631
H	0.76165	2.66943	-1.84942
H	2.30299	1.79243	-1.91536
H	2.21673	3.34715	-1.07665
O	-0.13013	0.33433	-2.01623
H	0.69787	0.50498	-2.49439
N	0.08689	-0.09041	1.55191
N	0.32104	-0.77947	2.52208
N	0.52765	-1.39311	3.47064

^{3}FeTMCNCSOH
Charge: 2+
Energy: -1633001.8451639

Fe	0.11990	0.00003	-0.49492
N	-1.29186	1.65724	-0.71866
N	1.59390	1.62240	-0.15097
N	1.59333	-1.62284	-0.15133
N	-1.29227	-1.65676	-0.71900
C	-0.69084	2.69247	0.18822
H	-1.22024	3.64462	0.05318
H	-0.84818	2.36645	1.21356
C	0.79000	2.90069	-0.09363
H	1.21294	3.55854	0.67357
H	0.92014	3.40774	-1.05021
C	2.27912	1.33221	1.15397
H	3.00386	2.14024	1.32349
H	1.52529	1.39584	1.93717
C	3.04268	-0.00061	1.23804
H	3.51192	-0.00081	2.22942
H	3.88300	-0.00073	0.53872
C	2.27863	-1.33313	1.15366
H	1.52477	-1.39668	1.93684
H	3.00310	-2.14145	1.32304
C	0.78920	-2.90096	-0.09420
H	0.91924	-3.40793	-1.05083
H	1.21194	-3.55901	0.67293
C	-0.69158	-2.69236	0.18769
H	-0.84878	-2.36644	1.21308
H	-1.22130	-3.64431	0.05252
C	-2.66716	-1.29387	-0.23894
H	-2.62836	-1.22151	0.84867
H	-3.32979	-2.13290	-0.48788
C	-3.24818	0.00050	-0.81598
H	-3.22782	0.00062	-1.91037
H	-4.31274	0.00060	-0.55465
C	-2.66683	1.29460	-0.23868
H	-2.62808	1.22205	0.84892
H	-3.32926	2.13384	-0.48746
C	-1.36058	2.16591	-2.11685
H	-1.93322	3.10039	-2.14259
H	-0.36059	2.33876	-2.50842
H	-1.86654	1.43801	-2.75203
C	2.58953	1.77574	-1.24865
H	3.18154	2.68209	-1.07287
H	2.07067	1.84128	-2.20269
H	3.26113	0.92556	-1.28474
C	2.58879	-1.77586	-1.24917
H	3.25930	-0.92486	-1.28617
H	2.06975	-1.84267	-2.20301
H	3.18187	-2.68144	-1.07296
C	-1.36110	-2.16518	-2.11730
H	-0.36108	-2.33785	-2.50894
H	-1.86714	-1.43714	-2.75227
H	-1.93369	-3.09967	-2.14321
O	0.55672	0.00021	-2.19466
H	-0.15963	0.00026	-2.85235
N	-0.32694	-0.00004	1.28409
C	-0.74825	-0.00015	2.41404
S	-1.29431	-0.00024	3.89635

^{3}FeTMCOHBr
Charge: 2+
Energy: -2940150.7976816

Fe	0.02318	-0.00018	-0.15943
N	1.44845	1.65589	-0.35003
N	-1.50235	1.59076	-0.18721
N	-1.49714	-1.59450	-0.18698
N	1.45357	-1.65164	-0.35140
C	0.60354	2.66532	-1.06805
H	1.14257	3.62020	-1.11214
H	0.46256	2.30886	-2.08647
C	-0.72441	2.87074	-0.37056
H	-1.33370	3.58522	-0.93641
H	-0.57115	3.29758	0.62046
C	-2.39615	1.33002	-1.36874
H	-3.14167	2.13510	-1.39628
H	-1.79886	1.45037	-2.27474
C	-3.16027	-0.00487	-1.35147
H	-3.77994	-0.00589	-2.25638
H	-3.87688	-0.00771	-0.52664
C	-2.38660	-1.33418	-1.37199
H	-1.78189	-1.44262	-2.27381
H	-3.12670	-2.14400	-1.40644
C	-0.71545	-2.87217	-0.36982
H	-0.56066	-3.29778	0.62149
H	-1.32324	-3.58859	-0.93484
C	0.61125	-2.66407	-1.06866
H	0.46818	-2.30832	-2.08689
H	1.15327	-3.61729	-1.11150
C	2.60369	-1.26900	-1.23682
H	2.21557	-1.15695	-2.24870
H	3.29755	-2.11898	-1.23490
C	3.34165	0.00502	-0.83329
H	3.61897	0.00488	0.22482
H	4.28918	0.00668	-1.38360
C	2.60017	1.27739	-1.23535
H	2.21255	1.16479	-2.24736
H	3.29173	2.12924	-1.23253
C	1.98197	2.22825	0.92283
H	2.61887	3.08785	0.68374
H	1.17335	2.54647	1.57456
H	2.56620	1.47786	1.45032
C	-2.36235	1.79198	1.02259
H	-3.03447	2.63877	0.83835
H	-1.74211	2.00201	1.88952
H	-2.95830	0.91049	1.23091
C	-2.35908	-1.79926	1.02040
H	-2.95764	-0.91957	1.22887
H	-1.74031	-2.00908	1.88849
H	-3.02896	-2.64729	0.83360
C	1.98939	-2.22172	0.92167
H	1.18206	-2.54341	1.57322
H	2.57074	-1.46918	1.44923
H	2.62965	-3.07871	0.68223
O	0.13894	-0.00573	-1.93376
H	-0.66337	0.03932	-2.47316
Br	0.10661	-0.00069	2.22574

^{3}FeTMCOHCl
Charge: 2+
Energy: -1613626.1202482

Fe	0.03638	-0.00046	0.04434

N	1.45636	1.65671	-0.11583
N	-1.48755	1.60063	0.00603
N	-1.48140	-1.60531	0.00710
N	1.46235	-1.65184	-0.11720
C	0.63244	2.66577	-0.85735
H	1.17655	3.61825	-0.89401
H	0.51420	2.30297	-1.87657
C	-0.71259	2.88084	-0.19387
H	-1.31209	3.57645	-0.79233
H	-0.58377	3.33645	0.78769
C	-2.39639	1.33025	-1.15952
H	-3.14373	2.13413	-1.18328
H	-1.81017	1.44531	-2.07432
C	-3.15782	-0.00614	-1.12631
H	-3.79402	-0.00758	-2.01967
H	-3.85947	-0.00982	-0.28865
C	-2.38355	-1.33499	-1.16382
H	-1.78595	-1.43304	-2.07211
H	-3.12356	-2.14522	-1.19822
C	-0.70188	-2.88275	-0.19178
H	-0.57088	-3.33650	0.79038
H	-1.29980	-3.58099	-0.78876
C	0.64145	-2.66477	-0.85735
H	0.52035	-2.30307	-1.87643
H	1.18921	-3.61519	-0.89209
C	2.63980	-1.27020	-0.96366
H	2.28391	-1.16083	-1.98802
H	3.33457	-2.11936	-0.93725
C	3.36431	0.00578	-0.53960
H	3.61233	0.00558	0.52565
H	4.32692	0.00769	-1.06306
C	2.63578	1.27995	-0.96198
H	2.28057	1.16999	-1.98650
H	3.32792	2.13120	-0.93446
C	1.93209	2.20756	1.18730
H	2.56861	3.07863	0.99267
H	1.09305	2.50036	1.81208
H	2.50124	1.45093	1.72236
C	-2.31489	1.79023	1.23781
H	-2.98486	2.64496	1.08454
H	-1.66938	1.97941	2.09145
H	-2.91177	0.90965	1.44715
C	-2.31191	-1.79922	1.23543
H	-2.91346	-0.92158	1.44383
H	-1.66865	-1.98663	2.09126
H	-2.97803	-2.65647	1.07918
C	1.94077	-2.19947	1.18651
H	1.10318	-2.49638	1.81119
H	2.50631	-1.44000	1.72128
H	2.58148	-3.06743	0.99180
O	0.16502	-0.00824	-1.72379
H	-0.63537	0.05555	-2.26503
Cl	0.08026	-0.00047	2.23083

^{4}FeTMCOHF
Charge: 1+
Energy: -1387745.1573906

Fe	0.02821	0.00058	0.09713
N	1.20586	1.80928	-0.01746
N	-1.71230	1.44788	0.10151
N	-1.22191	-1.79022	0.09798
N	1.70205	-1.47313	-0.01137
C	0.30256	2.71906	-0.77729
H	0.72273	3.73518	-0.80679
H	0.24565	2.33740	-1.79579
C	-1.10323	2.78314	-0.17355
H	-1.74473	3.36544	-0.84815
H	-1.06724	3.33397	0.76852
C	-2.60175	1.01054	-1.01279
H	-3.45089	1.70895	-1.08266
H	-2.01796	1.08722	-1.93029
C	-3.16900	-0.41698	-0.89378
H	-3.86479	-0.52355	-1.73557
H	-3.79852	-0.50732	-0.00309
C	-2.21958	-1.62492	-1.00581
H	-1.64928	-1.55100	-1.93125
H	-2.83609	-2.53585	-1.04675
C	-0.31184	-2.95173	-0.16736
H	-0.15694	-3.47387	0.77860
H	-0.80187	-3.66538	-0.84087
C	1.04594	-2.56981	-0.76571
H	0.90540	-2.22469	-1.78967
H	1.68249	-3.46763	-0.78815
C	2.88224	-0.95188	-0.74915
H	2.62839	-0.92607	-1.81493
H	3.71415	-1.66586	-0.65160
C	3.35648	0.44235	-0.31263
H	3.52745	0.47285	0.76740
H	4.34288	0.59436	-0.76694
C	2.48662	1.62644	-0.76028
H	2.24034	1.51247	-1.82104
H	3.07026	2.55517	-0.67931
C	1.48131	2.33779	1.33990
H	1.96409	3.32256	1.27611
H	0.55614	2.41189	1.90560
H	2.12602	1.64543	1.87839
C	-2.44694	1.53773	1.38372
H	-3.16217	2.37237	1.37060
H	-1.73260	1.66580	2.19744
H	-2.99904	0.62166	1.57473
C	-1.89548	-2.02583	1.39818
H	-2.59197	-1.22254	1.61528
H	-1.15057	-2.03381	2.19248
H	-2.44462	-2.97708	1.38070
C	2.10037	-1.90950	1.34444
H	1.22256	-2.20027	1.91716
H	2.55991	-1.07751	1.87670
H	2.80872	-2.74885	1.29245
F	0.06152	0.00806	1.83558
O	-0.02893	-0.00918	-1.70587
H	0.83449	0.04923	-2.13976

^{3}FeTMCOHF
Charge: 2+
Energy: -1387512.5248714

Fe	0.04802	-0.00011	0.07498
N	1.45464	1.64987	-0.00426
N	-1.47289	1.63354	0.09789
N	-1.47329	-1.63338	0.09832
N	1.45411	-1.65010	-0.00454
C	0.67088	2.67809	-0.76384
H	1.22991	3.62285	-0.77428
H	0.58540	2.31687	-1.78731
C	-0.70332	2.91054	-0.15478
H	-1.28681	3.56086	-0.81570
H	-0.61264	3.42991	0.79955
C	-2.45319	1.34055	-0.99653
H	-3.20506	2.14155	-0.98929
H	-1.91697	1.43277	-1.94448
C	-3.20879	0.00009	-0.90200
H	-3.90486	0.00008	-1.74967
H	-3.85459	-0.00045	-0.02040
C	-2.45155	-1.33937	-0.99766
H	-1.91246	-1.42847	-1.94408
H	-3.20275	-2.14103	-0.99322
C	-0.70385	-2.91045	-0.15408
H	-0.61299	-3.42944	0.80044
H	-1.28766	-3.56090	-0.81459
C	0.67009	-2.67850	-0.76374
H	0.58411	-2.31740	-1.78716
H	1.22914	-3.62324	-0.77382
C	2.68021	-1.28449	-0.78139
H	2.38126	-1.19125	-1.82627
H	3.37308	-2.13249	-0.69995
C	3.38636	-0.00043	-0.33959
H	3.60962	-0.00063	0.73101
H	4.36273	-0.00056	-0.83716
C	2.68078	1.28404	-0.78103
H	2.38190	1.19101	-1.82594
H	3.37399	2.13174	-0.69935
C	1.80250	2.10372	1.37003
H	2.42502	3.00398	1.30657
H	0.90219	2.31534	1.94042
H	2.34584	1.31748	1.88952
C	-2.15724	1.76982	1.41487
H	-2.75995	2.68595	1.41659
H	-1.41275	1.80721	2.20801
H	-2.81192	0.92589	1.60091
C	-2.15874	-1.76993	1.41453
H	-2.81442	-0.92662	1.59992
H	-1.41492	-1.80663	2.20839
H	-2.76075	-2.68653	1.41594
C	1.80194	-2.10333	1.37000
H	0.90162	-2.31509	1.94030
H	2.34496	-1.31677	1.88933
H	2.42474	-3.00341	1.30678
O	0.16298	-0.00238	-1.69655
H	-0.63380	0.01517	-2.24813
F	0.05812	0.00026	1.79773

^{6}FeTMCOHN$_{3}$
Charge: 1+
Energy: -1428128.8703069

Fe	0.06716	0.00004	-0.05338
N	-1.33646	-1.71917	-0.48557
N	1.58364	-1.63853	0.16354
N	1.58438	1.63792	0.16377
N	-1.33558	1.71975	-0.48549
C	-0.37452	-2.67673	-1.10309
H	-0.85903	-3.64931	-1.27648
H	-0.07183	-2.26087	-2.06189
C	0.86133	-2.89589	-0.22870
H	1.55011	-3.56966	-0.75458
H	0.57187	-3.40527	0.69218
C	2.68057	-1.32779	-0.80731

H	3.41712	-2.14446	-0.76460
H	2.22509	-1.31390	-1.79687
C	3.42683	-0.00069	-0.57784
H	4.24477	-0.00082	-1.30910
H	3.92583	-0.00084	0.39623
C	2.68106	1.32670	-0.80723
H	2.22534	1.31284	-1.79667
H	3.41792	2.14310	-0.76472
C	0.86260	2.89562	-0.22834
H	0.57333	3.40496	0.69262
H	1.55170	3.56918	-0.75408
C	-0.37337	2.67718	-1.10276
H	-0.07094	2.26186	-2.06188
H	-0.85755	3.65001	-1.27566
C	-2.38438	1.31028	-1.46264
H	-1.91050	1.21615	-2.44288
H	-3.11992	2.12332	-1.54741
C	-3.11964	0.00080	-1.12507
H	-3.44562	0.00082	-0.07972
H	-4.04282	0.00104	-1.71631
C	-2.38497	-1.30900	-1.46274
H	-1.91097	-1.21496	-2.44292
H	-3.12092	-2.12166	-1.54773
C	-1.97650	-2.31273	0.71076
H	-2.49710	-3.24501	0.45053
H	-1.22903	-2.51628	1.47600
H	-2.69726	-1.61416	1.13545
C	2.12139	-1.83563	1.53162
H	2.77739	-2.71628	1.56747
H	1.29135	-1.95646	2.22764
H	2.69041	-0.96555	1.84804
C	2.12230	1.83486	1.53179
H	2.69156	0.96484	1.84797
H	1.29234	1.95544	2.22796
H	2.77818	2.71560	1.56770
C	-1.97532	2.31330	0.71109
H	-1.22775	2.51615	1.47640
H	-2.69647	1.61495	1.13550
H	-2.49541	3.24593	0.45113
N	-0.37800	-0.00005	1.83672
N	-1.26096	-0.00011	2.66134
N	-2.10376	-0.00016	3.44866
O	0.40383	-0.00018	-1.91971
H	-0.22536	0.00048	-2.65183

^{3}FeTMCOHN$_{3}$
Charge: 2+
Energy: -1427890.6184718

Fe	0.05376	0.04701	-0.06155
N	1.55367	1.65678	0.06407
N	-1.39225	1.73622	0.11973
N	-1.53590	-1.45970	-0.39731
N	1.38663	-1.60606	-0.47526
C	0.80667	2.80753	-0.53510
H	1.39336	3.72741	-0.41175
H	0.71553	2.61264	-1.60239
C	-0.55685	2.99559	0.10629
H	-1.10235	3.78874	-0.41766
H	-0.44400	3.32249	1.14009
C	-2.33724	1.69225	-1.04381
H	-3.05542	2.51379	-0.91902
H	-1.77276	1.93752	-1.94901
C	-3.13810	0.39079	-1.21785
H	-3.78855	0.56016	-2.08453
H	-3.82737	0.26371	-0.37884
C	-2.40313	-0.92887	-1.50538
H	-1.77831	-0.85187	-2.39500
H	-3.16545	-1.69178	-1.71160
C	-0.82095	-2.71774	-0.83160
H	-0.75940	-3.37471	0.03650
H	-1.42758	-3.24061	-1.57950
C	0.56189	-2.45400	-1.39927
H	0.49623	-1.92426	-2.34682
H	1.07594	-3.40888	-1.56810
C	2.62109	-1.16041	-1.20217
H	2.31512	-0.86539	-2.20581
H	3.26999	-2.04101	-1.29207
C	3.39125	-0.01210	-0.55053
H	3.59563	-0.19935	0.50786
H	4.37421	0.01664	-1.03404
C	2.75361	1.35806	-0.78017
H	2.44383	1.43670	-1.82262
H	3.48970	2.14862	-0.58450
C	1.97002	1.94933	1.46271
H	2.62486	2.82884	1.47037
H	1.10196	2.13183	2.09096
H	2.50530	1.09471	1.87211
C	-2.16877	1.74243	1.39408
H	-2.77188	2.65680	1.44864
H	-1.48093	1.70565	2.23647
H	-2.83401	0.88676	1.44852
C	-2.38042	-1.81355	0.77864
H	-2.87017	-0.93648	1.18830
H	-1.77178	-2.26956	1.55614
H	-3.14768	-2.53586	0.47406
C	1.76685	-2.36037	0.75143
H	0.88291	-2.73669	1.26183
H	2.31295	-1.70878	1.43112
H	2.40140	-3.21091	0.47716
O	0.20301	0.28584	-1.82166
H	-0.48263	0.79359	-2.28024
N	0.08108	-0.14187	1.75254
N	-0.10848	-0.89396	2.69003
N	-0.26133	-1.55900	3.61092

^{3}FeTMCOHNCS
Charge: 2+
Energy: -1633002.1830275

Fe	0.02428	-0.29375	0.00732
N	-1.32785	-0.66480	1.67151
N	1.52964	-0.00847	1.62803
N	1.53110	-0.09188	-1.62442
N	-1.32618	-0.75000	-1.63644
C	-0.40015	-1.24544	2.69659
H	-0.93690	-1.36339	3.64684
H	-0.11071	-2.23215	2.34059
C	0.82160	-0.36968	2.91274
H	1.52158	-0.88021	3.58369
H	0.53999	0.56207	3.40383
C	2.67486	-0.93932	1.35944
H	3.41027	-0.79744	2.16276
H	2.30075	-1.95999	1.46944
C	3.40873	-0.74714	0.02050
H	4.24380	-1.45800	0.03909
H	3.88615	0.23583	-0.00481
C	2.67516	-1.00865	-1.30685
H	2.29960	-2.03308	-1.36295
H	3.41111	-0.90962	-2.11608
C	0.82400	-0.51839	-2.88942
H	0.54249	0.38705	-3.42756
H	1.52467	-1.06221	-3.53295
C	-0.39771	-1.38232	-2.62981
H	-0.10830	-2.34941	-2.22354
H	-0.93383	-1.54866	-3.57313
C	-2.36497	-1.75392	-1.23595
H	-1.85545	-2.70852	-1.10210
H	-3.05566	-1.85471	-2.08301
C	-3.14592	-1.41793	0.03495
H	-3.55921	-0.40514	0.00868
H	-4.01540	-2.08466	0.05167
C	-2.36624	-1.68802	1.32222
H	-1.85656	-2.64817	1.23806
H	-3.05777	-1.74516	2.17268
C	-1.98183	0.57521	2.17480
H	-2.57015	0.34085	3.06967
H	-1.23601	1.32798	2.41830
H	-2.63774	0.98241	1.40762
C	2.03295	1.38725	1.77733
H	2.72339	1.43713	2.62815
H	1.19620	2.06061	1.95058
H	2.55579	1.71120	0.88355
C	2.03538	1.29388	-1.84514
H	2.55958	1.66252	-0.96963
H	1.19907	1.95833	-2.05175
H	2.72512	1.29967	-2.69798
C	-1.97975	0.46261	-2.20311
H	-1.23366	1.20166	-2.48481
H	-2.63578	0.90898	-1.45819
H	-2.56780	0.18262	-3.08495
O	0.24239	-2.05932	0.05157
H	1.13868	-2.42457	0.07104
N	-0.33666	1.47188	-0.03795
C	-0.61964	2.64462	-0.06785
S	-0.98542	4.17905	-0.10647

^{4}FeTMCOHSR
Charge: 1+
Energy: -1599235.8633287

Fe	-0.01477	0.04753	-0.03422
N	1.54667	1.69355	-0.20816
N	-1.40139	1.70917	0.25874
N	-1.76037	-1.49662	-0.08236
N	1.20639	-1.65607	-0.43151
C	0.67428	2.76478	-0.76333
H	1.21777	3.72004	-0.80982
H	0.39132	2.46558	-1.77035
C	-0.58049	2.95476	0.08741
H	-1.19845	3.74400	-0.35934
H	-0.30103	3.29996	1.08398
C	-2.43455	1.62645	-0.82778
H	-3.08718	2.50706	-0.73029
H	-1.90042	1.68931	-1.77354
C	-3.32759	0.37480	-0.83423
H	-4.05312	0.54635	-1.63938
H	-3.93065	0.32728	0.07793

C	-2.68718	-0.99033	-1.13783
H	-2.11221	-0.91221	-2.05899
H	-3.49330	-1.72758	-1.27973
C	-1.07524	-2.75096	-0.50688
H	-0.93904	-3.36432	0.38555
H	-1.71957	-3.33043	-1.18291
C	0.27504	-2.54873	-1.19770
H	0.11531	-2.09102	-2.17242
H	0.74359	-3.53052	-1.35543
C	2.37765	-1.31769	-1.30710
H	1.99829	-1.17178	-2.32269
H	3.02930	-2.20069	-1.35302
C	3.21661	-0.09030	-0.92430
H	3.56954	-0.16313	0.10689
H	4.11941	-0.14476	-1.54498
C	2.57657	1.27982	-1.19878
H	2.10174	1.26496	-2.18239
H	3.36580	2.04521	-1.23604
C	2.20982	2.16240	1.02995
H	2.80844	3.06218	0.82681
H	1.47148	2.37373	1.80002
H	2.86406	1.38545	1.42214
C	-2.05969	1.78434	1.58730
H	-2.73779	2.64763	1.63280
H	-1.30222	1.87821	2.36564
H	-2.62571	0.87802	1.78132
C	-2.51565	-1.81352	1.15393
H	-3.09455	-0.95434	1.48363
H	-1.81606	-2.06724	1.94976
H	-3.21133	-2.64703	0.97849
C	1.66056	-2.32942	0.84007
H	2.58066	-2.89431	0.63806
H	0.89335	-3.04901	1.12456
S	0.34946	-0.30015	2.17688
C	1.84248	-1.35678	1.99619
O	-0.26810	0.30658	-1.86624
H	1.97440	-1.92304	2.92433
H	2.73418	-0.73803	1.87108
H	0.42659	-0.05946	-2.43039

[6]FeTMCOHTF
Charge: 1+
Energy: -1655404.3292033

Fe	-0.70112	0.15727	0.09067
N	0.03597	1.46636	1.75317
N	-0.79177	-1.39925	1.68800
N	-1.59165	-1.19705	-1.45769
N	-0.76531	1.68519	-1.52214
C	-0.67570	0.83799	2.90443
H	-0.33382	1.28006	3.85176
H	-1.73747	1.04844	2.78618
C	-0.45254	-0.67316	2.95939
H	-1.03711	-1.08914	3.78986
H	0.59591	-0.87943	3.17978
C	-2.20880	-1.88709	1.70947
H	-2.30342	-2.62059	2.52406
H	-2.83242	-1.02435	1.94092
C	-2.71808	-2.54845	0.41443
H	-3.72993	-2.89980	0.65169
H	-2.15037	-3.45928	0.20160
C	-2.87154	-1.69734	-0.86117
H	-3.48542	-0.82512	-0.64189
H	-3.38262	-2.31031	-1.61846
C	-1.84389	-0.29319	-2.63191
H	-1.02325	-0.44702	-3.33403
H	-2.76331	-0.60260	-3.14571
C	-1.94920	1.19352	-2.28967
H	-2.83037	1.36809	-1.67452
H	-2.05674	1.76202	-3.22489
C	-1.02617	3.04701	-0.97124
H	-2.06574	3.07897	-0.63457
H	-0.93960	3.77359	-1.79162
C	-0.10638	3.47906	0.18225
H	0.94462	3.32634	-0.08150
H	-0.22579	4.56414	0.28368
C	-0.41301	2.87529	1.56228
H	-1.49098	2.91041	1.74084
H	0.05454	3.49733	2.33887
C	1.50477	1.43276	1.95181
H	1.77967	1.99491	2.85502
H	1.85412	0.40765	2.03192
H	2.00516	1.86276	1.08711
C	0.16431	-2.52662	1.54791
H	0.11412	-3.18262	2.42751
H	1.17187	-2.12988	1.43452
H	-0.06739	-3.11568	0.66507
C	-0.77034	-2.33409	-1.95208
H	-0.57647	-3.04280	-1.15170
H	0.18479	-1.96157	-2.31821
H	-1.30365	-2.86042	-2.75575
C	0.45117	1.71273	-2.37097
H	0.68267	0.71691	-2.74077
H	1.30330	2.03878	-1.77429
H	0.31337	2.40321	-3.21424
O	1.14414	-0.32817	-0.29972
O	-2.42834	0.72043	0.55855
C	2.14890	-0.69445	-1.03046
O	2.14715	-1.02370	-2.20356
C	3.48595	-0.63032	-0.24828
F	4.47592	-1.24681	-0.88112
F	3.82669	0.66900	-0.06632
F	3.35213	-1.18735	0.98482
H	-2.76293	1.61707	0.68915

[5]FeNTBBrOH
Charge: 0
Energy: -3352756.6425020

Fe	0.67437	-0.05299	-1.22030
C	-3.30255	-1.19065	2.73049
C	-3.36133	-2.57146	2.55558
C	-2.64415	1.86308	2.67671
C	-2.16029	-0.55375	2.24347
C	-2.31982	-3.27991	1.92039
N	-1.78855	0.78747	2.21688
C	4.87967	2.91448	0.81686
C	-1.11408	-1.24881	1.59902
C	-1.18640	-2.63647	1.43258
C	-0.56933	0.83906	1.57404
C	0.21791	2.08846	1.27239
N	-0.14195	-0.34433	1.19120
C	1.95022	2.61614	-0.40353
N	4.16323	1.68509	0.53321
C	2.90588	1.51958	-0.00312
C	5.93630	-0.04097	1.15759
N	0.57679	2.15827	-0.15296
C	4.70320	0.40804	0.67991
N	2.60767	0.25125	-0.18857
C	6.13189	-1.42132	1.16289
C	3.70576	-0.48000	0.22417
C	-0.45153	2.77596	-1.00531
C	5.13932	-2.31494	0.70535
C	3.91229	-1.86306	0.22870
C	-1.65951	1.87599	-1.03357
N	-1.53158	0.58243	-1.24029
N	-2.96349	2.23397	-0.75681
C	-3.52776	3.55705	-0.57002
C	-2.79181	0.03195	-1.09573
C	-3.19712	-1.30496	-1.15965
C	-3.71292	1.05890	-0.79534
C	-4.54050	-1.56887	-0.91430
C	-5.06581	0.79998	-0.56130
C	-5.45845	-0.53651	-0.62329
H	-4.10963	-0.64258	3.20718
H	-4.23297	-3.11354	2.91181
H	-2.41311	-4.35523	1.79779
H	-0.40197	-3.16067	0.89931
H	-2.16409	2.82743	2.50849
H	-3.59162	1.83634	2.12686
H	-2.85096	1.75657	3.74719
H	-0.31134	2.99709	1.59667
H	1.14651	2.03752	1.84935
H	2.18187	3.56905	0.09874
H	2.04177	2.74226	-1.48710
H	4.19266	3.76157	0.79876
H	5.33322	2.85374	1.81134
H	5.67038	3.08478	0.07726
H	6.70704	0.64247	1.50164
H	7.07655	-1.81869	1.52378
H	5.34417	-3.38154	0.72219
H	3.13582	-2.52393	-0.14618
H	-0.03748	2.79148	-2.01878
H	-0.70619	3.79762	-0.67981
H	-2.73228	4.28228	-0.39487
H	-4.10095	3.86685	-1.45117
H	-4.19425	3.55365	0.29871
H	-5.77775	1.59097	-0.34358
H	-6.49936	-0.78929	-0.44149
H	-4.89369	-2.59535	-0.93915
H	-2.46512	-2.07874	-1.37047
O	1.11712	1.02523	-2.72613
H	1.15799	0.51701	-3.54926
Br	0.57299	-2.58212	-1.74934

[5]FeNTBClOH
Charge: 0
Energy: -2026226.2648479

Fe	-0.70038	-0.06774	-1.39620
C	3.20735	1.92961	2.30265
C	3.27437	3.22958	1.80596
C	2.55497	-1.05946	2.94214
C	2.09104	1.18088	1.92742
C	2.26694	3.75235	0.96812
N	1.71933	-0.13157	2.20649
C	-4.92470	-2.44010	1.31541
C	1.07963	1.68920	1.08401

C	1.16044	2.99674	0.59179
C	0.53470	-0.35042	1.53482
C	-0.24828	-1.63938	1.52137
N	0.12887	0.70188	0.85924
C	-2.01083	-2.48837	0.01583
N	-4.19685	-1.32475	0.74016
C	-2.94591	-1.31265	0.16160
C	-5.93319	0.53487	0.96274
N	-0.62745	-2.01445	0.15203
C	-4.71641	-0.03967	0.58854
N	-2.63552	-0.12956	-0.32188
C	-6.10537	1.88138	0.64392
C	-3.71432	0.69701	-0.07777
C	0.38254	-2.81771	-0.55668
C	-5.10668	2.62251	-0.02484
C	-3.89608	2.04588	-0.39760
C	1.61020	-1.96964	-0.76417
N	1.51531	-0.76401	-1.28298
N	2.89292	-2.25423	-0.33518
C	3.42546	-3.49652	0.19080
C	2.77329	-0.19834	-1.19955
C	3.19738	1.08805	-1.54718
C	3.66162	-1.12496	-0.61141
C	4.52741	1.40455	-1.29186
C	5.00267	-0.81699	-0.36777
C	5.41470	0.46854	-0.71725
H	3.98923	1.52151	2.93606
H	4.12615	3.85215	2.06573
H	2.36648	4.76842	0.59675
H	0.40389	3.36356	-0.09209
H	2.06719	-2.03173	3.01678
H	3.51379	-1.17913	2.42487
H	2.74140	-0.68374	3.95402
H	0.29564	-2.45378	2.02368
H	-1.16733	-1.47288	2.09300
H	-2.25710	-3.30048	0.71888
H	-2.11291	-2.85205	-1.01162
H	-4.24674	-3.27448	1.50035
H	-5.37032	-2.13501	2.26763
H	-5.72264	-2.77530	0.64284
H	-6.70947	-0.03143	1.46897
H	-7.03679	2.37165	0.91350
H	-5.29405	3.66715	-0.25631
H	-3.11101	2.58064	-0.92531
H	-0.03720	-3.02476	-1.54654
H	0.61466	-3.75811	-0.03076
H	2.61028	-4.15424	0.49465
H	4.03452	-4.01216	-0.56043
H	4.05001	-3.28820	1.06566
H	5.69145	-1.53369	0.07039
H	6.44652	0.75823	-0.53866
H	4.89334	2.39870	-1.53002
H	2.48457	1.79184	-1.96613
O	-1.16771	-1.47047	-2.60386
H	-1.19788	-1.17822	-3.52629
Cl	-0.55694	2.14151	-2.30994

^{5}FeNTBFOH
Charge: 0
Energy: -1800100.8200717

Fe	1.14573	0.64589	1.57488
C	-3.01796	2.46276	-1.77360
C	-3.06291	3.69233	-1.11826
C	-2.37823	-0.42685	-2.82156
C	-1.99567	1.59403	-1.38931
C	-2.11878	4.04102	-0.12800
N	-1.66203	0.30539	-1.79452
C	4.66496	-2.87679	-1.09795
C	-1.05922	1.92906	-0.39147
C	-1.10041	3.17090	0.25085
C	-0.57861	-0.08053	-1.03609
C	0.10243	-1.42844	-1.10041
N	-0.19744	0.86041	-0.19897
C	1.85348	-2.41516	0.34126
N	4.10401	-1.61928	-0.64023
C	2.90304	-1.38865	-0.00031
C	6.01055	-0.01275	-1.20971
N	0.52794	-1.83141	0.22951
C	4.76906	-0.39520	-0.69597
N	2.75899	-0.12447	0.33025
C	6.34351	1.33601	-1.08419
C	3.90308	0.53209	-0.08269
C	-0.46465	-2.46139	1.11747
C	5.47760	2.26613	-0.46767
C	4.24211	1.88228	0.04521
C	-1.82771	-1.85556	0.96790
N	-2.19307	-0.73068	1.53790
N	-2.80854	-2.36476	0.11260
C	-2.82549	-3.59870	-0.64705
C	-3.45259	-0.44790	1.04095
C	-4.27795	0.66198	1.25929
C	-3.86375	-1.46853	0.15130
C	-5.49528	0.71073	0.58713
C	-5.09145	-1.43700	-0.51596
C	-5.89945	-0.32420	-0.28235
H	-3.75074	2.19289	-2.52781
H	-3.84467	4.40079	-1.37856
H	-2.19063	5.01588	0.34640
H	-0.34134	3.40043	0.99262
H	-1.92419	-1.40718	-2.96873
H	-3.42297	-0.55916	-2.52270
H	-2.34000	0.12009	-3.77022
H	-0.54469	-2.17250	-1.59188
H	0.99518	-1.33096	-1.72924
H	1.98208	-3.33508	-0.25971
H	1.98725	-2.68157	1.39591
H	3.88802	-3.64144	-1.13509
H	5.07797	-2.74892	-2.10367
H	5.46366	-3.21604	-0.42825
H	6.68752	-0.72190	-1.67693
H	7.30027	1.67907	-1.46829
H	5.78984	3.30371	-0.39066
H	3.54343	2.55299	0.53957
H	-0.11437	-2.23441	2.13234
H	-0.51076	-3.55398	0.96175
H	-1.89389	-4.14373	-0.49599
H	-3.65969	-4.23362	-0.32719
H	-2.93902	-3.38962	-1.71787
H	-5.40313	-2.23295	-1.18689
H	-6.86040	-0.25175	-0.78431
H	-6.14871	1.56699	0.72699
H	-3.95049	1.46408	1.91253
O	1.09597	-0.71489	2.89374
H	0.76433	-0.43809	3.76003
F	1.50401	2.45396	1.67225

^{5}FeNTBN$_3$OH
Charge: 0
Energy: -1840486.3758892

Fe	-0.76485	0.11961	-1.36024
C	3.12815	1.60630	2.51331
C	3.21364	2.94775	2.14550
C	2.43464	-1.42521	2.85731
C	2.01206	0.90820	2.05189
C	2.22073	3.56216	1.35446
N	1.62716	-0.42336	2.18954
C	-5.02070	-2.58639	0.97749
C	1.01644	1.50803	1.25111
C	1.11164	2.85770	0.89698
C	0.45476	-0.56460	1.48018
C	-0.33241	-1.83914	1.30620
N	0.06511	0.55566	0.91155
C	-2.09859	-2.47117	-0.30002
N	-4.28801	-1.40721	0.55552
C	-3.03311	-1.32326	-0.00851
C	-6.02114	0.41313	1.00914
N	-0.71457	-2.02329	-0.10094
C	-4.80388	-0.11209	0.56989
N	-2.71753	-0.08853	-0.33316
C	-6.18775	1.79053	0.86985
C	-3.79552	0.70190	0.01156
C	0.28448	-2.74155	-0.91146
C	-5.18234	2.61000	0.31193
C	-3.97149	2.08190	-0.12611
C	1.55815	-1.94060	-0.94302
N	1.57228	-0.68047	-1.32672
N	2.78503	-2.35784	-0.45695
C	3.20600	-3.67956	-0.03376
C	2.85767	-0.21704	-1.09107
C	3.40473	1.05909	-1.27205
C	3.63832	-1.26255	-0.54794
C	4.73013	1.24140	-0.89009
C	4.97407	-1.08805	-0.17670
C	5.50275	0.18979	-0.35373
H	3.89952	1.13010	3.11079
H	4.06943	3.53215	2.47164
H	2.33309	4.60729	1.08226
H	0.34982	3.31063	0.27492
H	1.95202	-2.40103	2.79677
H	3.41700	-1.48143	2.37547
H	2.56846	-1.16552	3.91307
H	0.21246	-2.71345	1.69327
H	-1.24910	-1.74916	1.89880
H	-2.34867	-3.36719	0.29105
H	-2.19729	-2.70074	-1.36578
H	-4.34422	-3.43829	1.05844
H	-5.47296	-2.40559	1.95782
H	-5.81367	-2.83132	0.26159
H	-6.80219	-0.21182	1.43209
H	-7.11936	2.24435	1.19626
H	-5.36436	3.67703	0.22123
H	-3.18095	2.68134	-0.56836
H	-0.11573	-2.75537	-1.93096
H	0.45430	-3.76737	-0.54652
H	2.33818	-4.32556	0.10128
H	3.87238	-4.13391	-0.77586

H	3.74042	-3.60926	0.91962
H	5.57322	-1.90040	0.22503
H	6.53536	0.37859	-0.07319
H	5.18121	2.22258	-1.00343
H	2.80642	1.86896	-1.68041
O	-1.20917	-1.11282	-2.75025
H	-1.22626	-0.71646	-3.63301
N	-0.68900	2.10729	-1.83170
N	0.27440	2.72668	-2.20812
N	1.18264	3.37013	-2.54895

^{5}FeNTBNCSOH
Charge: 0
Energy: -2045599.3199053

Fe	0.73743	0.06179	-1.27043
C	-3.26707	0.83446	2.69172
C	-3.40952	2.21482	2.56532
C	-2.40311	-2.16728	2.55473
C	-2.06415	0.29265	2.23723
C	-2.38807	3.01572	2.01367
N	-1.60893	-1.02075	2.16228
C	-3.25901	-3.77253	-0.68022
C	-1.03302	1.08119	1.68059
C	-1.18972	2.46678	1.56911
C	-0.35933	-0.96378	1.57892
C	0.50157	-2.14375	1.21386
N	0.01300	0.26089	1.28033
C	-0.23041	-2.81715	-1.05047
N	-2.76594	-2.41458	-0.80983
C	-1.48028	-1.97399	-1.03918
C	-4.95163	-1.11711	-0.60898
N	0.79866	-2.15883	-0.23089
C	-3.58072	-1.28281	-0.81924
N	-1.42141	-0.66742	-1.19323
C	-5.42608	0.19370	-0.63408
C	-2.71532	-0.19256	-1.05724
C	2.18357	-2.54107	-0.54432
C	-4.56705	1.28889	-0.86564
C	-3.20404	1.11818	-1.08391
C	3.09272	-1.39733	-0.16609
N	2.71363	-0.14668	-0.32278
N	4.37375	-1.49325	0.32788
C	5.16919	-2.68132	0.57698
C	3.77603	0.64354	0.07024
C	3.89530	2.03609	0.09900
C	4.83983	-0.18784	0.47974
C	5.10501	2.55784	0.54704
C	6.05652	0.33033	0.92840
C	6.16565	1.71999	0.95471
H	-4.05974	0.21617	3.10210
H	-4.33397	2.68321	2.89140
H	-2.54588	4.08495	1.91190
H	-0.41905	3.07823	1.11723
H	-1.88365	-3.09204	2.30164
H	-2.59402	-2.15470	3.63369
H	-3.36108	-2.14345	2.02402
H	1.45029	-2.03122	1.74642
H	0.06018	-3.09752	1.53948
H	-0.42986	-3.84931	-0.71977
H	0.14928	-2.81690	-2.07727
H	-2.42628	-4.46253	-0.53986
H	-3.92170	-3.84340	0.18861
H	-3.81842	-4.07117	-1.57385
H	-5.61653	-1.95877	-0.43764
H	-6.48465	0.37537	-0.47058
H	-4.97857	2.29349	-0.86608
H	-2.53729	1.95795	-1.24737
H	2.23897	-2.65247	-1.63175
H	2.48621	-3.48474	-0.06324
H	4.53419	-3.56793	0.55769
H	5.95280	-2.79106	-0.18120
H	5.63862	-2.60871	1.56320
H	6.87862	-0.30859	1.23709
H	7.09402	2.16974	1.29536
H	5.24122	3.63474	0.58291
H	3.06595	2.65627	-0.22679
O	1.18393	-0.95803	-2.81346
H	1.11724	-0.47818	-3.65137
N	0.42672	2.06998	-1.45542
C	-0.10259	3.12959	-1.51914
S	-0.86084	4.57519	-1.55825

^{5}FeNTBOHBr
Charge: 0
Energy: -3352762.4119684

Fe	-0.04004	-0.55189	-0.97287
C	0.27525	4.91413	0.76001
C	0.29474	5.39554	-0.54892
C	0.21766	3.16698	3.40167
C	0.18512	3.52874	0.90861
C	0.22898	4.52936	-1.66121
N	0.13693	2.70438	2.02976
C	-4.44790	-1.61814	2.41549
C	0.12090	2.65884	-0.19938
C	0.14114	3.14785	-1.50947
C	0.05985	1.40627	1.56334
C	-0.00426	0.20942	2.48614
N	0.04300	1.35016	0.25425
C	-1.31084	-1.80177	1.90055
N	-3.70750	-1.07079	1.29419
C	-2.35540	-1.15142	1.03229
C	-5.60987	-0.11307	-0.11904
N	-0.04568	-1.07458	1.79009
C	-4.29098	-0.45536	0.18808
N	-2.04841	-0.62925	-0.13250
C	-5.81621	0.52619	-1.34122
C	-3.22658	-0.17615	-0.69358
C	1.17398	-1.87711	1.89021
C	-4.75163	0.81102	-2.22421
C	-3.43912	0.46528	-1.91722
C	2.25027	-1.29167	1.01444
N	1.96847	-0.76247	-0.15342
N	3.60539	-1.27824	1.27391
C	4.31934	-1.85510	2.39753
C	3.16684	-0.37194	-0.71844
C	3.40909	0.25406	-1.94456
C	4.21732	-0.69969	0.16327
C	4.73670	0.53268	-2.25479
C	5.55121	-0.42525	-0.14733
C	5.78722	0.19794	-1.37244
H	0.33079	5.58516	1.61223
H	0.36448	6.46714	-0.71500
H	0.24888	4.95560	-2.66034
H	0.09081	2.44411	-2.33703
H	-0.04097	2.35810	4.08730
H	1.22742	3.52286	3.63913
H	-0.48927	3.98860	3.55653
H	0.86187	0.23821	3.16511
H	-0.89111	0.30827	3.13056
H	-1.65512	-1.89545	2.94425
H	-1.14810	-2.80660	1.49375
H	-3.77282	-1.81658	3.24938
H	-5.20061	-0.89415	2.74277
H	-4.95039	-2.55162	2.13719
H	-6.43629	-0.33531	0.54958
H	-6.82672	0.80892	-1.62304
H	-4.96809	1.30826	-3.16542
H	-2.58985	0.65848	-2.56848
H	0.94700	-2.86978	1.48435
H	1.51957	-1.99191	2.93139
H	3.63659	-2.01451	3.23352
H	4.77423	-2.81418	2.12439
H	5.10785	-1.16766	2.71933
H	6.36659	-0.68549	0.52113
H	6.81013	0.42872	-1.65687
H	4.97609	1.01571	-3.19783
H	2.56938	0.48915	-2.59438
O	-0.02288	0.24034	-2.68565
H	-0.04860	-0.42248	-3.39313
Br	-0.13006	-3.25730	-1.14125

^{5}FeNTBOHCl
Charge: 0
Energy: -2026231.1990867

Fe	-0.02809	-0.60955	-1.20732
C	0.15208	4.46313	1.50709
C	0.16349	5.17667	0.30866
C	0.12909	2.26136	3.78346
C	0.09780	3.07219	1.39866
C	0.12415	4.52740	-0.94378
N	0.06680	2.05573	2.34963
C	-4.41531	-2.24230	1.98514
C	0.06033	2.41818	0.14970
C	0.07205	3.13964	-1.04832
C	0.02443	0.86345	1.65258
C	-0.01255	-0.48440	2.33823
N	0.01475	1.04695	0.35518
C	-1.28604	-2.36650	1.37103
N	-3.68798	-1.51395	0.96286
C	-2.34284	-1.56577	0.65557
C	-5.60025	-0.27683	-0.19765
N	-0.03209	-1.61318	1.41229
C	-4.28267	-0.69340	0.00620
N	-2.05186	-0.84093	-0.39912
C	-5.81899	0.58609	-1.27131
C	-3.23168	-0.27148	-0.83435
C	1.19980	-2.40134	1.36062
C	-4.76756	1.01581	-2.11046
C	-3.45657	0.59534	-1.90768
C	2.27361	-1.63176	0.63626
N	1.99676	-0.90498	-0.42089
N	3.62072	-1.61078	0.93911
C	4.33376	-2.35273	1.96168
C	3.18824	-0.36513	-0.86182
C	3.42990	0.49356	-1.93805

C	4.23169	-0.80875	-0.02299
C	4.74969	0.88259	-2.14622
C	5.55808	-0.42407	-0.23251
C	5.79353	0.43033	-1.30942
H	0.18665	4.96765	2.46834
H	0.20561	6.26201	0.34214
H	0.13602	5.12991	-1.84781
H	0.04236	2.59751	-1.99070
H	-0.09639	1.33058	4.30699
H	1.12418	2.60652	4.08902
H	-0.60954	3.01247	4.08235
H	0.85632	-0.56585	3.00948
H	-0.89788	-0.52527	2.99127
H	-1.62569	-2.67760	2.37338
H	-1.10814	-3.26108	0.76456
H	-3.72420	-2.61689	2.74165
H	-5.13219	-1.57221	2.47019
H	-4.95916	-3.09006	1.55268
H	-6.41658	-0.60659	0.43825
H	-6.82892	0.93486	-1.46868
H	-4.99319	1.68804	-2.93339
H	-2.61668	0.89743	-2.52892
H	0.99145	-3.29066	0.75614
H	1.53862	-2.72149	2.36042
H	3.63748	-2.70156	2.72575
H	4.85008	-3.21897	1.53206
H	5.07292	-1.70003	2.43683
H	6.36855	-0.77101	0.40175
H	6.81074	0.75465	-1.51109
H	4.98827	1.54747	-2.97146
H	2.59521	0.81476	-2.55663
O	-0.01870	0.50689	-2.73428
H	-0.03157	0.00276	-3.56235
Cl	-0.06928	-3.05964	-1.72606

^{5}FeNTBOHF
Charge: 0
Energy: -1800097.0794125

Fe	-0.51248	-0.43035	-1.77920
C	2.15284	2.91140	2.19473
C	2.30149	3.95844	1.28588
C	1.49041	0.20939	3.69664
C	1.43021	1.80292	1.74931
C	1.75325	3.89620	-0.01271
N	1.08825	0.59950	2.36026
C	-4.61892	-1.85183	1.84495
C	0.88314	1.73210	0.45128
C	1.03801	2.78646	-0.45471
C	0.38438	-0.13373	1.42406
C	-0.18137	-1.51337	1.69550
N	0.24288	0.50906	0.28771
C	-1.91759	-2.58806	0.27398
N	-3.90334	-1.03790	0.88092
C	-2.77018	-1.34823	0.15012
C	-5.39288	1.03863	0.81892
N	-0.52296	-2.20813	0.47236
C	-4.32305	0.21897	0.45099
N	-2.45111	-0.38713	-0.68763
C	-5.47229	2.27776	0.18348
C	-3.38355	0.61517	-0.52416
C	0.51123	-3.05839	-0.12251
C	-4.52155	2.68611	-0.77806
C	-3.46109	1.86422	-1.14771
C	1.71275	-2.21498	-0.46248
N	1.67564	-1.33124	-1.43752
N	2.85829	-2.09371	0.30879
C	3.26571	-2.85838	1.46983
C	2.81625	-0.56066	-1.30688
C	3.20797	0.57732	-2.01843
C	3.58144	-1.02917	-0.21716
C	4.38964	1.19881	-1.62789
C	4.77499	-0.41771	0.17311
C	5.16456	0.70442	-0.55694
H	2.58291	2.95937	3.19106
H	2.85695	4.84289	1.58647
H	1.90018	4.73729	-0.68494
H	0.61315	2.68461	-1.45107
H	0.90145	-0.64530	4.03407
H	2.55499	-0.05514	3.72823
H	1.31712	1.03898	4.38958
H	0.53280	-2.09697	2.30030
H	-1.08192	-1.40698	2.31667
H	-2.30046	-3.26848	1.05288
H	-1.96014	-3.07822	-0.70194
H	-3.99274	-2.68365	2.16987
H	-4.87460	-1.24428	2.71926
H	-5.54289	-2.25319	1.41244
H	-6.12667	0.73495	1.55996
H	-6.28718	2.94939	0.43958
H	-4.62364	3.66696	-1.23392
H	-2.69386	2.14159	-1.86668
H	0.10669	-3.40025	-1.07733
H	0.77991	-3.91634	0.51726
H	2.61746	-3.72637	1.59192
H	4.29589	-3.20802	1.34429
H	3.21340	-2.24471	2.37823
H	5.36248	-0.77991	1.01207
H	6.07937	1.22217	-0.28212
H	4.71701	2.09724	-2.14291
H	2.56021	0.96994	-2.79586
O	-0.35173	1.23276	-2.68948
H	-0.49206	1.18091	-3.64650
F	-0.96512	-2.18529	-2.35323

^{4}FeNTBOHMeCN
Charge: 0
Energy: -1820728.8047223

Fe	0.34241	-0.29069	-1.07761
O	0.59714	-2.12618	-1.61638
C	-4.96246	0.58132	-1.64726
C	-5.18644	-0.67537	-2.22096
C	-3.78232	3.12042	-0.18325
C	-3.63541	0.97978	-1.48809
C	-4.12097	-1.50698	-2.60231
N	-3.06373	2.12752	-0.94614
C	-2.32227	1.40782	3.43364
C	-2.55785	0.15180	-1.87926
C	-2.79326	-1.10810	-2.43261
C	-1.68225	1.92376	-0.93866
C	-0.63845	2.90731	-0.54605
N	-1.35577	0.77369	-1.56155
C	0.17605	1.83606	1.52967
N	-1.74613	0.44218	2.52476
C	-0.74691	0.66177	1.58709
C	-3.30394	-1.55239	2.85589
N	0.45942	2.20677	0.13975
C	-2.25809	-0.83006	2.28011
N	-0.54205	-0.41946	0.83315
C	-3.54573	-2.83000	2.34156
C	-1.48603	-1.35713	1.22055
C	1.81460	2.69502	-0.08973
C	-2.77924	-3.35861	1.28636
C	-1.73989	-2.63143	0.70480
C	2.75311	1.53832	-0.30034
N	2.40184	0.44290	-0.95705
N	4.07728	1.52582	0.06513
C	4.73731	2.41010	1.01075
C	3.54096	-0.35552	-1.00902
C	3.72135	-1.63910	-1.53625
C	4.60138	0.31061	-0.36027
C	4.98327	-2.21294	-1.40496
C	5.86591	-0.26368	-0.21952
C	6.03957	-1.53600	-0.76184
H	-5.79175	1.20757	-1.33121
H	-6.20821	-1.01845	-2.35863
H	-4.33463	-2.48591	-3.02245
H	-1.95295	-1.75513	-2.66664
H	-3.88796	2.82805	0.87366
H	-3.26491	4.08250	-0.23027
H	-4.77945	3.25326	-0.61033
H	-0.19148	3.36965	-1.44386
H	-1.06309	3.72415	0.06225
H	-0.22287	2.68910	2.10482
H	1.13384	1.54406	1.98271
H	-1.55118	2.08772	3.80336
H	-3.11456	1.99825	2.95036
H	-2.75016	0.88320	4.29170
H	-3.91188	-1.14625	3.65915
H	-4.35278	-3.42323	2.76285
H	-3.01199	-4.35082	0.90959
H	-1.14256	-2.99042	-0.12938
H	2.17742	3.35667	0.71161
H	1.79889	3.29421	-1.01076
H	5.80609	2.43977	0.78538
H	4.34515	3.42448	0.91936
H	4.58716	2.04479	2.03265
H	6.67451	0.24365	0.29758
H	7.00825	-2.02040	-0.67510
H	5.15731	-3.21123	-1.79708
H	2.86834	-2.15789	-1.96103
N	2.74586	-0.24118	2.36953
C	2.35806	-1.24233	1.92531
C	1.88333	-2.51109	1.37967
H	2.65882	-3.27500	1.49760
H	0.97865	-2.82437	1.90959
H	1.63067	-2.41675	0.31526
H	0.59010	-2.31548	-2.56679

^{5}FeNTBOHN$_{3}$
Charge: 0
Energy: -1840491.9305591

Fe	-0.13685	-0.37013	-1.14843
C	0.90585	4.61789	1.44945
C	0.99523	5.30106	0.23705
C	0.58605	2.48763	3.77329

C	0.60540	3.25640	1.37291
C	0.79560	4.64990	-0.99877
N	0.43563	2.27586	2.34628
C	-4.62619	-2.02006	1.94025
C	0.40633	2.60019	0.14089
C	0.49862	3.29134	-1.07173
C	0.16451	1.09705	1.67896
C	-0.08902	-0.20005	2.41258
N	0.13111	1.25949	0.37829
C	-1.48490	-2.05105	1.58790
N	-3.85021	-1.26091	0.97666
C	-2.48662	-1.27340	0.77124
C	-5.71214	-0.10576	-0.33912
N	-0.18473	-1.38033	1.55690
C	-4.39970	-0.47003	-0.03092
N	-2.13942	-0.54528	-0.26595
C	-5.88094	0.73054	-1.44255
C	-3.30437	-0.02236	-0.79685
C	0.99369	-2.24729	1.57010
C	-4.78594	1.18250	-2.21062
C	-3.47932	0.81444	-1.90295
C	2.08509	-1.67224	0.70215
N	1.83227	-0.96036	-0.37255
N	3.43953	-1.84828	0.89644
C	4.11207	-2.66232	1.89229
C	3.05272	-0.63477	-0.93524
C	3.33155	0.12633	-2.07420
C	4.08280	-1.19817	-0.15527
C	4.67319	0.29106	-2.40592
C	5.42972	-1.03940	-0.48835
C	5.70208	-0.28328	-1.62829
H	1.06760	5.12232	2.39761
H	1.22787	6.36246	0.24617
H	0.87822	5.22691	-1.91563
H	0.34094	2.74943	-2.00136
H	0.10618	1.67914	4.32805
H	1.64345	2.53814	4.06049
H	0.10105	3.42760	4.05370
H	0.70543	-0.34396	3.16245
H	-1.02250	-0.09271	2.98497
H	-1.85351	-2.19523	2.61821
H	-1.37116	-3.04430	1.13492
H	-3.98339	-2.36453	2.75154
H	-5.40835	-1.38146	2.36240
H	-5.09407	-2.89091	1.46722
H	-6.56110	-0.45604	0.24044
H	-6.88507	1.03826	-1.72097
H	-4.97302	1.82882	-3.06344
H	-2.60833	1.13043	-2.47319
H	0.71049	-3.22001	1.14724
H	1.36499	-2.41978	2.59495
H	3.44591	-2.85088	2.73537
H	4.42490	-3.62320	1.46802
H	4.99564	-2.13102	2.25926
H	6.22758	-1.48125	0.10116
H	6.73621	-0.13432	-1.92637
H	4.93978	0.87252	-3.28388
H	2.50822	0.55200	-2.64366
O	-0.06719	0.72120	-2.69301
H	-0.14807	0.19199	-3.50170
N	-0.37834	-2.38856	-1.88640
N	-0.38365	-3.35854	-1.19485
N	-0.39481	-4.31217	-0.50203

[5]FeNTBOHNCS
Charge: 0
Energy: -2045606.8782443

Fe	-0.08945	-0.19571	-1.06648
C	0.81499	4.92811	1.29289
C	0.89056	5.56265	0.05339
C	0.55058	2.88766	3.70202
C	0.55751	3.55594	1.27186
C	0.71882	4.85489	-1.15522
N	0.41161	2.61200	2.28468
C	-4.57840	-1.89178	1.93769
C	0.38668	2.84338	0.06729
C	0.46469	3.48583	-1.17263
C	0.18021	1.39928	1.66594
C	-0.03499	0.12469	2.44859
N	0.15157	1.50642	0.35982
C	-1.44809	-1.74748	1.70459
N	-3.81830	-1.10159	0.98567
C	-2.45063	-1.04306	0.82717
C	-5.69329	-0.10857	-0.43999
N	-0.14447	-1.08526	1.63376
C	-4.37466	-0.38173	-0.07032
N	-2.10629	-0.33298	-0.22333
C	-5.86889	0.67209	-1.58234
C	-3.27916	0.10086	-0.81467
C	1.02340	-1.96607	1.68637
C	-4.77414	1.15624	-2.33068
C	-3.46104	0.87873	-1.96171
C	2.11811	-1.46855	0.77727
N	1.88452	-0.74270	-0.29216
N	3.45926	-1.75097	0.92650
C	4.09004	-2.62990	1.89493
C	3.10582	-0.52379	-0.90302
C	3.40161	0.19074	-2.06738
C	4.11462	-1.16281	-0.15396
C	4.73836	0.23905	-2.45202
C	5.45606	-1.12054	-0.53991
C	5.74576	-0.40511	-1.70157
H	0.95452	5.47636	2.21997
H	1.08983	6.63027	0.01925
H	0.78899	5.39567	-2.09488
H	0.32989	2.90181	-2.07980
H	0.11925	2.07466	4.28894
H	1.60393	3.00887	3.98240
H	0.01338	3.80876	3.94824
H	0.78608	0.01328	3.17415
H	-0.94941	0.24076	3.04944
H	-1.82187	-1.80935	2.74106
H	-1.34166	-2.77723	1.34332
H	-3.96181	-2.12741	2.80658
H	-5.44663	-1.31725	2.27384
H	-4.92179	-2.82840	1.48429
H	-6.54192	-0.48742	0.12169
H	-6.87805	0.90759	-1.90871
H	-4.96617	1.75362	-3.21738
H	-2.58996	1.21657	-2.51856
H	0.72736	-2.96549	1.34527
H	1.40345	-2.07774	2.71641
H	3.45699	-2.73176	2.77784
H	4.26338	-3.62428	1.46829
H	5.04812	-2.20084	2.20296
H	6.23671	-1.62140	0.02481
H	6.77632	-0.34728	-2.04067
H	5.01726	0.77948	-3.35208
H	2.59320	0.66271	-2.62111
O	-0.01348	0.79780	-2.67270
H	-0.08387	0.24214	-3.46399
N	-0.31460	-2.29880	-1.50913
C	-0.39222	-3.37867	-1.03374
S	-0.49680	-4.84036	-0.27794

[6]Cisalpha
Charge: 2+
Energy: -1693783.3419928

H	2.16621	-5.00549	-2.21011
H	2.52197	-5.26986	-0.48195
C	2.54754	-4.53784	-1.29624
H	3.58227	-4.22026	-1.46219
H	-3.40333	-3.49506	-2.64982
H	0.73694	-0.77415	-2.59245
H	0.83617	0.89651	-3.18893
H	-1.12613	-2.66938	-2.02099
H	5.33074	1.25180	-2.30756
H	2.92387	1.26636	-2.81583
C	1.72720	-3.38693	-0.94622
C	0.42510	0.25431	-2.40708
C	-3.29714	-2.71536	-1.90383
H	-0.66242	0.30333	-2.45059
C	-2.01475	-2.24463	-1.56707
C	4.63138	0.94186	-1.53792
C	3.24427	0.94536	-1.83131
N	1.07386	-2.47209	-0.66731
H	-5.39409	-2.55565	-1.46298
H	0.02661	2.84175	-2.54982
C	-4.39337	-2.19061	-1.24914
H	6.15088	0.60431	-0.06028
C	5.09013	0.58012	-0.29113
H	1.63806	3.15867	-1.90092
C	2.31991	0.56658	-0.87768
N	0.87376	0.63297	-1.04318
N	-1.81085	-1.28162	-0.67230
C	0.57687	3.10316	-1.63817
H	0.22383	5.21232	-1.93596
C	4.17156	0.15957	0.70625
C	2.78230	0.12920	0.39237
Fe	-0.01485	-0.86294	0.44506
H	-1.69578	1.59404	-0.97825
C	0.37611	2.00020	-0.58235
C	-4.21803	-1.16842	-0.28256
H	-2.00804	4.11842	-1.65810
C	-2.88942	-0.70897	-0.04560
C	0.06955	4.46692	-1.14942
N	1.86138	-0.34617	1.28709
C	4.55492	-0.25405	2.00787
H	5.60483	-0.22717	2.28667
H	0.99141	2.24088	0.29046
C	-1.09104	1.92987	-0.13048
C	-1.41119	4.37246	-0.77136
H	0.65590	4.79743	-0.28109
H	-6.29791	-0.95023	0.28933
C	-5.28514	-0.59837	0.46067
O	-0.47714	-1.82921	1.91485

C	2.25523	-0.75079	2.49317
N	-1.28743	0.85584	0.93506
C	3.60010	-0.69401	2.90338
C	-2.65270	0.34750	0.87532
H	-1.78260	5.33522	-0.40640
C	-1.60772	3.30934	0.31788
H	1.47524	-1.15414	3.12994
H	3.86832	-1.01817	3.90277
H	-2.66467	3.22492	0.59111
C	-5.02739	0.37974	1.39429
H	-1.06194	3.63236	1.21201
C	-3.71040	0.86387	1.59605
H	0.18084	1.56608	2.27419
C	-0.86400	1.25610	2.30608
H	-5.83798	0.80742	1.97505
H	-0.95412	0.38066	2.94877
H	-3.55314	1.65661	2.31820
H	-1.46256	2.07563	2.70779
H	-1.24062	-2.41456	2.04761

[5]CisalphaBrOH
Charge: 2+
Energy: -3225738.6598523

H	3.79731	-1.07848	3.91969
H	-0.83536	0.41365	2.95887
H	-1.25403	2.13842	2.76838
H	1.40172	-1.04233	3.15443
H	-5.66212	0.98426	2.33173
H	-3.32035	1.67312	2.61729
C	-0.71533	1.29581	2.33036
C	3.55125	-0.74528	2.91755
H	0.34044	1.55374	2.26289
C	2.20672	-0.70838	2.50853
C	-4.91039	0.58645	1.65816
C	-3.56589	0.97585	1.82539
H	5.58716	-0.45590	2.28585
H	-0.87313	3.68107	1.28466
C	4.53742	-0.39617	2.01246
H	-6.31867	-0.55183	0.50035
C	-5.27891	-0.26875	0.63478
H	-2.48633	3.35883	0.63839
C	-2.58528	0.51162	0.95752
N	-1.21440	0.94953	0.97566
N	1.83933	-0.29749	1.29443
C	-1.42372	3.40616	0.37813
H	-1.48816	5.45144	-0.29699
C	-4.29486	-0.80606	-0.23816
C	-2.93525	-0.43322	-0.05203
Fe	-0.03556	-0.85472	0.36715
H	1.12724	2.19748	0.33910
C	-0.96581	2.01052	-0.09716
C	4.17785	0.01786	0.70534
H	0.92086	4.78589	-0.15384
C	2.79209	0.09046	0.40109
C	-1.15937	4.48177	-0.68459
N	-1.92480	-1.00529	-0.76864
C	-4.58432	-1.73466	-1.26849
H	-5.61275	-2.03640	-1.44605
H	-1.58742	1.71041	-0.94440
C	0.49735	2.02020	-0.53608
C	0.32934	4.51098	-1.03747
H	-1.75580	4.28180	-1.58488
H	6.17879	0.24706	-0.10293
C	5.11681	0.30314	-0.32253
C	-2.22936	-1.89121	-1.71852
N	0.93432	0.64792	-1.06665
C	-3.55193	-2.26078	-2.02172
C	2.35724	0.48128	-0.89795
H	0.53471	5.26673	-1.80248
C	0.76863	3.13782	-1.56563
H	-1.39146	-2.34328	-2.23707
H	-3.73721	-2.97749	-2.81409
H	1.83376	3.13442	-1.81936
C	4.67877	0.61538	-1.59699
H	0.20843	2.93335	-2.48459
C	3.30110	0.69804	-1.89231
H	-0.63404	0.41917	-2.45351
C	0.45162	0.33752	-2.43638
H	5.39790	0.81561	-2.38429
H	0.73954	-0.68687	-2.67067
H	2.99812	0.96525	-2.89768
H	0.86731	1.01313	-3.18655
O	-0.69620	-1.65029	1.84403
H	-0.63569	-2.62236	1.89317
Br	1.00907	-2.77959	-0.70849

[3]CisalphaClOH
Charge: 2+
Energy: -1899210.6412448

H	3.58274	-2.07322	3.58674
H	-0.61494	-0.14795	2.94888
H	-1.04236	1.57895	2.98209
H	1.22507	-1.83794	2.77467
H	-5.51784	0.82737	2.28910
H	-3.15349	1.37235	2.71073
C	-0.49540	0.80710	2.43932
C	3.38814	-1.58467	2.63855
H	0.55765	1.08044	2.40346
C	2.05699	-1.44002	2.20613
C	-4.76382	0.44973	1.60660
C	-3.40207	0.75500	1.85556
H	5.45294	-1.28696	2.12323
H	-0.49640	3.32389	1.73185
C	4.41700	-1.14505	1.82876
H	-6.18101	-0.50539	0.30902
C	-5.13491	-0.29237	0.50655
H	-2.17031	3.18022	1.17904
C	-2.42435	0.28591	1.00211
N	-1.00809	0.64793	1.05156
N	1.75189	-0.83658	1.06086
C	-1.12804	3.20024	0.84502
H	-1.10811	5.31758	0.43601
C	-4.14565	-0.80623	-0.37454
C	-2.78050	-0.53233	-0.09046
Fe	-0.02315	-0.96241	0.14115
H	1.32672	1.90547	0.45291
C	-0.79036	1.86947	0.14975
C	4.12061	-0.52197	0.59069
H	1.25612	4.51951	0.27925
C	2.75033	-0.35839	0.25581
C	-0.87597	4.38939	-0.09527
N	-1.76462	-1.07640	-0.83684
C	-4.42763	-1.60134	-1.51320
H	-5.45940	-1.82813	-1.76683
H	-1.48259	1.72707	-0.68477
C	0.63266	1.86189	-0.39067
C	0.57869	4.38736	-0.57513
H	-1.55555	4.33978	-0.95668
H	6.14776	-0.21494	-0.11572
C	5.09498	-0.08873	-0.34878
C	-2.06155	-1.83063	-1.89674
N	0.92513	0.51089	-1.06498
C	-3.38880	-2.08959	-2.28164
C	2.36652	0.25915	-0.95155
H	0.76349	5.22403	-1.25583
C	0.89736	3.07160	-1.30312
H	-1.22799	-2.26428	-2.43376
H	-3.57067	-2.70143	-3.15813
H	1.93982	3.05370	-1.63608
C	4.70202	0.46024	-1.54942
H	0.26219	3.01065	-2.19388
C	3.32919	0.64691	-1.85803
H	-0.63605	0.63137	-2.48878
C	0.43138	0.41853	-2.46956
H	5.44625	0.77088	-2.27509
H	0.61433	-0.59482	-2.82364
H	3.06460	1.10323	-2.80460
H	0.94397	1.12756	-3.12022
O	-0.66363	-1.97239	1.42979
H	-0.62360	-2.92050	1.19245
Cl	0.89156	-2.65086	-1.03695

[5]CisalphaFOH
Charge: 2+
Energy: -1673086.4072606

H	-3.84548	-2.54947	-3.29371
H	0.70334	-0.48895	-2.85237
H	0.98608	1.25993	-3.08395
H	-1.44749	-2.14350	-2.64697
H	5.49054	0.57744	-2.45720
H	3.10662	1.02572	-2.85401
C	0.52044	0.50565	-2.44583
C	-3.61172	-1.97048	-2.40715
H	-0.55247	0.69041	-2.41143
C	-2.26733	-1.73226	-2.06744
C	4.76691	0.27952	-1.70568
C	3.39977	0.53324	-1.93449
H	-5.65368	-1.69634	-1.79012
H	0.49683	3.08823	-1.96977
C	-4.60807	-1.49440	-1.57522
H	6.25238	-0.50037	-0.36056
C	5.19532	-0.31963	-0.53189
H	2.13707	3.03463	-1.31277
C	2.45291	0.20459	-0.97055
N	1.05547	0.52594	-1.06161
N	-1.91651	-1.01885	-0.99840
C	1.07687	3.06364	-1.04031
H	0.99820	5.20766	-0.83545
C	4.25100	-0.72975	0.44678
C	2.87226	-0.47998	0.21019
Fe	-0.00923	-1.18136	0.00212
H	-1.37779	1.72270	-0.67055
C	0.72879	1.78353	-0.25184
C	-4.26342	-0.75457	-0.41584
H	-1.35675	4.36840	-0.75687

C	-2.88280	-0.50678	-0.18608
C	0.74669	4.32806	-0.23399
N	1.90437	-0.95571	1.03726
C	4.59192	-1.42895	1.63223
H	5.63623	-1.62933	1.85492
H	1.37583	1.73037	0.62744
C	-0.72926	1.78825	0.20713
C	-0.73511	4.33397	0.14789
H	1.36865	4.37417	0.67006
H	-6.26300	-0.48632	0.38273
C	-5.20594	-0.29670	0.54364
C	2.24887	-1.64586	2.12458
N	-1.05483	0.54637	1.03303
C	3.59134	-1.87540	2.47702
C	-2.46124	0.22805	0.95892
H	-0.98299	5.22414	0.73514
C	-1.07102	3.08408	0.97396
H	1.42646	-2.04912	2.70611
H	3.82140	-2.42685	3.38197
H	-2.13145	3.06442	1.24558
C	-4.77545	0.35648	1.68405
H	-0.49164	3.12043	1.90350
C	-3.40472	0.61543	1.90016
H	0.54829	0.73726	2.38823
C	-0.52334	0.54671	2.41934
H	-5.49624	0.69295	2.42188
H	-0.70259	-0.44444	2.83481
H	-3.11051	1.15252	2.79404
H	-0.99686	1.30528	3.04621
O	0.68247	-2.26156	-1.27357
H	0.71081	-3.21002	-1.04696
F	-0.57900	-2.23630	1.29488

^{3}CisalphaN$_{3}$OH
Charge: 2+
Energy: -1713478.6231436

H	3.62474	-2.02981	3.47099
H	-0.57205	-0.19327	2.89025
H	-1.08593	1.51038	3.01497
H	1.25968	-1.87352	2.64040
H	-5.54301	0.68446	2.33590
H	-3.19329	1.29533	2.74266
C	-0.51284	0.79136	2.42823
C	3.41126	-1.50222	2.54815
H	0.52509	1.11725	2.38978
C	2.07805	-1.39992	2.11141
C	-4.78646	0.34273	1.63732
C	-3.43049	0.68636	1.87830
H	5.46204	-1.07157	2.07123
H	-0.63736	3.33894	1.81570
C	4.42261	-0.96817	1.77255
H	-6.19329	-0.62347	0.33689
C	-5.15090	-0.38711	0.52728
H	-2.30798	3.14678	1.27023
C	-2.44808	0.26266	1.00815
N	-1.04045	0.66615	1.04060
N	1.75304	-0.74755	0.99580
C	-1.27048	3.21977	0.92899
H	-1.34510	5.35018	0.59456
C	-4.15759	-0.85398	-0.37514
C	-2.79782	-0.54670	-0.09496
Fe	0.02153	-0.87875	0.05539
H	1.23049	2.05281	0.47896
C	-0.88391	1.92905	0.18656
C	4.10739	-0.29626	0.56394
H	1.04911	4.66225	0.39128
C	2.73277	-0.17815	0.22296
C	-1.07822	4.45136	0.03016
N	-1.77176	-1.03861	-0.86089
C	-4.42316	-1.62708	-1.53375
H	-5.44926	-1.87799	-1.78731
H	-1.57448	1.78703	-0.64989
C	0.53561	2.00202	-0.36437
C	0.37032	4.52925	-0.46204
H	-1.76293	4.40170	-0.82731
H	6.12644	0.14203	-0.09468
C	5.07165	0.23036	-0.33613
C	-2.05319	-1.76764	-1.93895
N	0.88493	0.68915	-1.07895
C	-3.37574	-2.06093	-2.32236
C	2.33078	0.48849	-0.95520
H	0.51158	5.39615	-1.11478
C	0.73949	3.25325	-1.23479
H	-1.20431	-2.14884	-2.49473
H	-3.54684	-2.65307	-3.21447
H	1.77910	3.29365	-1.57521
C	4.66604	0.82585	-1.51105
H	0.10188	3.19372	-2.12416
C	3.29001	0.96820	-1.82343
H	-0.67259	0.78442	-2.50124
C	0.40441	0.62085	-2.48615
H	5.40290	1.20981	-2.20869
H	0.62856	-0.37401	-2.86923
H	3.01300	1.46686	-2.74501
H	0.88284	1.36762	-3.12109
O	-0.50418	-2.06407	1.28572
H	-1.39234	-2.43073	1.12560
N	0.77463	-2.08209	-1.12031
N	1.08288	-3.19871	-0.68691
N	1.40356	-4.23767	-0.34671

^{3}CisalphaNCSOH
Charge: 2+
Energy: -1918583.1265612

H	3.46924	-0.35246	4.09185
H	-0.97996	0.46626	2.96063
H	-1.72820	2.04817	2.63199
H	1.15883	-0.74126	3.18793
H	-5.91866	0.34204	1.90594
H	-3.73561	1.40685	2.30440
C	-1.00358	1.31424	2.27843
C	3.25210	-0.12532	3.05404
H	-0.02161	1.78236	2.23418
C	1.94508	-0.32709	2.56767
C	-5.05697	-0.00936	1.34819
C	-3.79670	0.60041	1.58325
H	5.25845	0.44524	2.53735
H	-1.38770	3.61200	1.09509
C	4.23581	0.31869	2.19340
H	-6.16971	-1.46289	0.22890
C	-5.19925	-1.01451	0.41796
H	-2.97087	3.04814	0.54733
C	-2.68427	0.17196	0.89216
N	-1.35491	0.79376	0.92798
N	1.61041	-0.05273	1.31133
C	-1.93298	3.20430	0.23643
H	-2.28704	5.17213	-0.57614
C	-4.06456	-1.48964	-0.29320
C	-2.80158	-0.89765	-0.02061
Fe	-0.05114	-0.70369	0.37676
H	0.73382	2.36519	0.15637
C	-1.31581	1.85871	-0.17898
C	3.91220	0.60022	0.84139
H	0.18929	4.83525	-0.52682
C	2.55801	0.42737	0.44838
C	-1.85514	4.22391	-0.91069
N	-1.64810	-1.35981	-0.59909
C	-4.09811	-2.53838	-1.24519
H	-5.04524	-3.01254	-1.48676
H	-1.91768	1.43894	-0.99033
C	0.11347	2.02923	-0.67926
C	-0.40094	4.41654	-1.35319
H	-2.46248	3.88228	-1.75990
H	5.89009	1.14250	0.13544
C	4.84878	1.01423	-0.14374
C	-1.70968	-2.36006	-1.47714
N	0.68839	0.65981	-1.06499
C	-2.92681	-2.95813	-1.84705
C	2.14107	0.71286	-0.87062
H	-0.33832	5.13177	-2.17907
C	0.20030	3.07544	-1.80240
H	-0.76690	-2.70911	-1.87905
H	-2.92182	-3.76049	-2.57629
H	1.24551	3.19929	-2.10411
C	4.43667	1.23267	-1.43989
H	-0.35858	2.72692	-2.67850
C	3.07281	1.09611	-1.81105
H	-0.77702	0.20600	-2.52032
C	0.30811	0.21173	-2.43305
H	5.15514	1.53288	-2.19546
H	0.68690	-0.79985	-2.57616
H	2.78704	1.30984	-2.83443
H	0.71985	0.86136	-3.20630
O	-0.58339	-1.54924	1.84498
H	-0.32432	-2.48838	1.83588
N	1.02472	-2.08188	-0.29795
C	1.97561	-2.75472	-0.55952
S	3.22805	-3.67846	-0.93966

^{6}CisbetatranstoamineN
Charge: 2+
Energy: -1693777.6947840

H	2.61044	1.09008	4.80406
H	4.54516	1.35955	3.19204
H	3.32812	2.61034	2.96527
C	2.53064	0.76332	3.76242
C	3.51165	1.53107	2.87487
H	2.76974	-0.30908	3.74684
H	0.89085	2.06905	3.32609
H	0.37864	0.50929	3.92985
C	1.09820	0.99433	3.26665
H	4.04137	1.65177	0.77530
C	3.35413	1.08804	1.41463
H	3.63707	0.03243	1.34042
H	1.66097	2.32648	0.92915

H	-0.69922	-1.04145	3.46178
C	1.91189	1.26062	0.90048
C	0.90073	0.52002	1.80651
H	-1.33145	2.04481	2.75396
H	1.09168	-0.55620	1.73688
H	4.37059	0.38545	-1.23787
H	-0.40155	2.84278	1.45387
H	5.37682	-1.79193	-1.75412
H	3.27518	2.25728	-1.26903
C	-1.09515	2.03492	1.68687
H	-2.56847	-2.56414	3.90263
C	-1.49781	-1.09535	2.73410
C	3.73186	-0.48915	-1.24130
C	4.31542	-1.74365	-1.53441
N	-0.49879	0.72101	1.27859
N	1.75187	0.89357	-0.57531
H	1.62099	2.89462	-1.23260
C	-2.58236	-1.97339	2.99249
C	2.22457	2.01284	-1.44614
C	2.38650	-0.37535	-0.94191
H	-2.01010	2.19329	1.11709
C	-1.47314	-0.31568	1.59560
H	3.99936	-3.85705	-1.73589
C	3.55317	-2.88942	-1.52715
H	-0.97204	5.93336	-1.79944
C	1.57134	-1.53614	-0.99838
H	2.07699	1.72644	-2.48733
C	2.16116	-2.80991	-1.27055
C	-3.65529	-2.05213	2.13461
N	-0.87248	2.83750	-1.18393
Fe	-0.39986	0.67230	-1.01607
C	-1.22853	3.86074	-1.59268
N	0.21645	-1.40312	-0.83742
C	-1.66995	5.14813	-2.10902
H	-4.50203	-2.69425	2.35713
C	-2.52791	-0.46561	0.65009
C	1.30609	-3.93962	-1.30270
H	1.72913	-4.92187	-1.49390
H	-2.66726	5.38358	-1.72278
C	-3.64652	-1.30198	0.92908
C	-0.55550	-2.48297	-0.90412
H	-1.70627	5.11166	-3.20311
C	-0.04943	-3.77913	-1.11154
N	-2.39545	0.15518	-0.56454
H	-1.62167	-2.32240	-0.80264
H	-0.73157	-4.62138	-1.14156
O	-0.38470	0.60190	-2.82254
C	-4.67138	-1.36710	-0.05032
C	-3.35850	0.04913	-1.47733
H	-5.55077	-1.97597	0.14128
H	-3.16351	0.53190	-2.42960
C	-4.53960	-0.67895	-1.24114
H	-5.30710	-0.72002	-2.00603
H	-0.14519	-0.10836	-3.43978

[3]CisbetatranstoamineNBrOH
Charge: 2+
Energy: -3225734.4192123

H	2.32400	5.24141	0.35669
H	4.37322	3.79844	-0.01766
H	3.35220	3.87007	-1.44900
C	2.26878	4.14940	0.40525
C	3.39328	3.51206	-0.41180
H	2.36796	3.87342	1.46392
H	0.82149	4.02301	-1.17596
H	0.09926	4.18727	0.41279
C	0.90530	3.69545	-0.13402
H	4.06216	1.52701	-0.97623
C	3.26942	1.98209	-0.37512
H	3.40879	1.64139	0.65639
H	1.77949	1.82764	-1.92503
H	-1.35163	3.46534	1.41825
C	1.89329	1.51434	-0.88377
C	0.75416	2.15544	-0.06830
H	-1.30199	3.34871	-1.62905
H	0.81136	1.81970	0.97136
H	4.37353	-0.86785	-0.44585
H	-0.20733	2.30648	-2.59369
H	5.18487	-1.87135	1.64544
H	3.45376	-0.13222	-2.28515
C	-1.01077	2.32237	-1.86100
H	-3.51417	3.44433	2.58211
C	-2.03672	2.65294	1.21862
C	3.66539	-1.04197	0.35462
C	4.13384	-1.61648	1.55988
N	-0.57108	1.63669	-0.59213
N	1.77257	-0.02597	-0.96117
H	1.85908	-0.10571	-3.06860
C	-3.29257	2.64815	1.87912
C	2.42644	-0.49779	-2.22710
C	2.33502	-0.69562	0.21607
H	-1.86179	1.78331	-2.27128
C	-1.72243	1.65786	0.31717
H	3.63451	-2.28172	3.53856
C	3.27497	-1.84541	2.61173
C	1.43019	-0.98067	1.25527
H	2.41515	-1.58590	-2.24444
C	1.89421	-1.54750	2.47773
C	-4.23775	1.68524	1.60436
Fe	-0.26983	-0.39815	-0.96584
N	0.09213	-0.77341	1.01637
H	-5.21432	1.71376	2.07798
C	-2.64409	0.60244	0.10567
C	0.93237	-1.83307	3.47587
H	1.25192	-2.25963	4.42247
C	-3.93246	0.62696	0.70709
C	-0.78516	-1.08615	1.97110
C	-0.40293	-1.59309	3.22305
N	-2.22959	-0.47695	-0.63825
H	-1.83184	-0.95244	1.74231
H	-1.16871	-1.81681	3.95712
C	-4.81925	-0.43570	0.39273
C	-3.07880	-1.46285	-0.91665
H	-5.81982	-0.43874	0.81609
H	-2.69240	-2.28906	-1.50041
C	-4.40344	-1.45666	-0.43781
H	-5.06126	-2.27733	-0.70145
O	-0.41187	-0.15781	-2.68326
H	-0.46062	-0.99383	-3.18872
Br	0.01468	-2.84508	-1.27266

[3]CisbetatranstoamineNClOH
Charge: 2+
Energy: -1899205.7016722

H	2.30562	4.85147	1.38326
H	4.35903	3.53197	0.70474
H	3.34357	3.91920	-0.67915
C	2.25226	3.77624	1.18612
C	3.38150	3.33889	0.25223
H	2.34796	3.27069	2.15671
H	0.80818	4.00698	-0.38701
H	0.08420	3.80986	1.19798
C	0.89027	3.45368	0.55480
H	4.05446	1.52943	-0.74016
C	3.26068	1.83940	-0.05383
H	3.39801	1.27621	0.87549
H	1.77586	2.03516	-1.60294
H	-1.41864	2.93364	1.95650
C	1.88687	1.49669	-0.65796
C	0.74226	1.93823	0.27520
H	-1.30645	3.44274	-0.99199
H	0.79469	1.38037	1.21441
H	4.36822	-0.93849	-0.79441
H	-0.20815	2.64307	-2.16164
H	5.19241	-2.38770	1.01015
H	3.44096	0.17725	-2.40442
C	-1.01447	2.49454	-1.44733
H	-3.59041	2.65082	3.06596
C	-2.08583	2.16394	1.59404
C	3.66702	-1.28062	-0.04359
C	4.14323	-2.11204	0.99780
N	-0.58076	1.54272	-0.36024
N	1.76822	0.01448	-1.07611
H	1.84520	0.41721	-3.14672
C	-3.34764	2.00993	2.22482
C	2.40553	-0.16930	-2.42161
C	2.33876	-0.90297	-0.08391
H	-1.86439	2.06119	-1.96965
C	-1.74385	1.36743	0.52175
H	3.66040	-3.19581	2.78641
C	3.29453	-2.56194	1.98456
C	1.44379	-1.40203	0.88029
H	2.36633	-1.22486	-2.68451
C	1.91600	-2.22901	1.94050
C	-4.27161	1.10135	1.75871
Fe	-0.26485	-0.35484	-1.15162
N	0.10706	-1.12797	0.71717
H	-5.25159	1.01953	2.21885
C	-2.64720	0.36320	0.09415
C	0.96335	-2.71543	2.86735
H	1.28892	-3.34341	3.69181
C	-3.93897	0.24367	0.67634
C	-0.76205	-1.63160	1.59377
C	-0.37100	-2.40801	2.69647
N	-2.20964	-0.53862	-0.84508
H	-1.80929	-1.43344	1.42088
H	-1.13018	-2.77707	3.37675
C	-4.79851	-0.75833	0.15430
C	-3.02840	-1.47652	-1.31260
H	-5.80103	-0.86464	0.55934
H	-2.61413	-2.16466	-2.03937
C	-4.35407	-1.59385	-0.85079
H	-4.99070	-2.36492	-1.27013
O	-0.42408	0.26694	-2.76933
H	-0.45347	-0.45614	-3.42815
Cl	0.02084	-2.47193	-1.91541

^{3}CisbetatranstoamineNFOH
Charge: 2+
Energy: -1673081.3828927

H	-2.09512	4.56874	-2.03423
H	-4.19511	3.40817	-1.23262
H	-3.21300	3.97453	0.11306
C	-2.07038	3.53546	-1.67451
C	-3.23715	3.26378	-0.72370
H	-2.15047	2.89038	-2.56015
H	-0.64080	3.99068	-0.13082
H	0.08902	3.50532	-1.65684
C	-0.72806	3.28870	-0.96727
H	-3.97813	1.62959	0.50475
C	-3.15988	1.82499	-0.19591
H	-3.28019	1.12934	-1.03385
H	-1.72817	2.23934	1.35118
H	1.86706	2.89785	-1.84130
C	-1.81460	1.55984	0.49944
C	-0.62279	1.83814	-0.44691
H	1.35462	3.47548	0.75417
H	-0.65350	1.14705	-1.29209
H	-4.36347	-0.80427	1.15982
H	0.21576	2.79309	1.95581
H	-5.29020	-2.48233	-0.37575
H	-3.35901	0.52771	2.50278
C	1.05126	2.57680	1.29400
H	4.05583	2.40177	-2.82935
C	2.40668	2.03145	-1.48479
C	-3.70633	-1.25103	0.42408
C	-4.24332	-2.21253	-0.46636
N	0.67068	1.50747	0.30049
N	-1.74231	0.16023	1.14502
H	-1.73379	0.89459	3.12369
C	3.68245	1.75652	-2.04104
C	-2.31805	0.19749	2.52662
C	-2.37900	-0.88331	0.33306
H	1.88241	2.21149	1.89305
C	1.88952	1.23155	-0.48632
H	-3.87659	-3.51523	-2.13215
C	-3.46002	-2.78856	-1.44148
C	-1.54731	-1.50792	-0.61515
H	-2.24773	-0.80537	2.94796
C	-2.08452	-2.45237	-1.53646
C	4.45760	0.71832	-1.57334
Fe	0.24344	-0.29586	1.22108
N	-0.20983	-1.20134	-0.58794
H	5.44607	0.53425	-1.98301
C	2.66302	0.13534	-0.02668
C	-1.19643	-3.02184	-2.48044
H	-1.57060	-3.74120	-3.20336
C	3.96075	-0.12788	-0.54756
C	0.59640	-1.76598	-1.48568
C	0.13657	-2.66466	-2.46340
N	2.10307	-0.71180	0.89191
H	1.64638	-1.51444	-1.43594
H	0.84449	-3.08216	-3.17051
C	4.66070	-1.24510	-0.01872
C	2.75704	-1.76871	1.35788
H	5.66130	-1.46370	-0.38127
H	2.21008	-2.39878	2.05058
C	4.06991	-2.05215	0.93489
H	4.58555	-2.91260	1.34640
O	0.51556	0.44621	2.77121
H	0.47436	-0.25706	3.45166
F	-0.08296	-1.85551	1.97876

^{5}CisbetatranstoamineNN$_{3}$OH
Charge: 2+
Energy: -1713468.3620335

H	2.67990	4.96760	-0.13590
H	4.66758	3.41586	-0.38864
H	3.62623	3.37708	-1.80662
C	2.58276	3.88841	0.01967
C	3.67136	3.12747	-0.73819
H	2.67959	3.71276	1.09996
H	1.14707	3.65056	-1.54716
H	0.40884	4.01553	-0.00088
C	1.20426	3.43555	-0.47487
H	4.25463	1.06878	-1.09082
C	3.48756	1.61831	-0.53594
H	3.63090	1.39502	0.52678
H	1.97968	1.28106	-2.04659
H	-0.70815	3.21346	1.45281
C	2.09163	1.12428	-0.96923
C	0.97791	1.91833	-0.24939
H	-1.01934	3.13296	-1.86987
H	1.02165	1.68630	0.81973
H	4.38662	-0.99197	0.21570
H	-0.01317	1.94045	-2.75507
H	4.89730	-1.81549	2.47653
H	3.67092	-0.90154	-1.92711
C	-0.80231	2.07319	-2.01879
H	-2.76307	3.50954	2.75431
C	-1.54912	2.56807	1.23665
C	3.56832	-1.15487	0.90665
C	3.86348	-1.63026	2.20453
N	-0.38762	1.45361	-0.71091
N	1.91286	-0.37662	-0.79905
H	2.14401	-0.85632	-2.84268
C	-2.73988	2.74260	1.98707
C	2.60179	-1.12720	-1.89182
C	2.26636	-0.88891	0.51943
H	-1.69972	1.57260	-2.37477
C	-1.48531	1.62261	0.23248
H	3.07291	-2.21237	4.11326
C	2.85308	-1.85302	3.11254
C	1.20965	-1.16596	1.41989
H	2.47009	-2.19494	-1.71352
C	1.50224	-1.64427	2.73578
C	-3.86263	1.98836	1.72957
Fe	-0.29543	-0.74937	-1.07281
N	-0.08891	-1.02425	0.99613
H	-4.78246	2.15304	2.28242
C	-2.60242	0.76188	0.02763
C	0.41417	-1.92911	3.59557
H	0.61004	-2.28616	4.60277
C	-3.81262	0.96177	0.74911
C	-1.08503	-1.34944	1.81802
C	-0.87826	-1.78046	3.13808
N	-2.43676	-0.31161	-0.80535
H	-2.08763	-1.28252	1.41970
H	-1.73405	-2.01256	3.76184
C	-4.88738	0.07670	0.47341
C	-3.45286	-1.14375	-1.01720
H	-5.83553	0.21417	0.98593
H	-3.25279	-1.99904	-1.65522
C	-4.71640	-0.96109	-0.42205
H	-5.51982	-1.65406	-0.64621
O	-0.16262	-0.51119	-2.82445
H	-0.95573	-0.68982	-3.36429
N	-0.35079	-2.61725	-1.17435
N	-0.16302	-3.21651	-2.23913
N	0.01190	-3.83767	-3.18010

^{3}CisbetatranstoamineNNCSOH
Charge: 2+
Energy: -1918577.5973242

H	1.21199	5.63920	0.27660
H	3.50721	4.61987	-0.04633
H	2.51976	4.47955	-1.49631
C	1.36619	4.55718	0.33412
C	2.61006	4.14422	-0.45451
H	1.49579	4.31124	1.39710
H	0.00414	4.14231	-1.27229
H	-0.76846	4.18217	0.29933
C	0.12655	3.84448	-0.22529
H	3.65801	2.32039	-0.98872
C	2.78261	2.61977	-0.40392
H	2.96960	2.32095	0.63331
H	1.37695	2.16802	-1.97328
H	-2.08056	3.22310	1.25978
C	1.53112	1.89306	-0.92613
C	0.27357	2.30666	-0.14303
H	-1.94307	3.07492	-1.71932
H	0.37483	1.99901	0.90207
H	4.39834	0.04168	-0.46193
H	-0.66912	2.25752	-2.68252
H	5.39844	-0.78402	1.62431
H	3.36514	0.53946	-2.31190
C	-1.46422	2.12246	-1.95352
H	-4.20421	2.79630	2.41086
C	-2.58155	2.28229	1.07969
C	3.74002	-0.26676	0.34068
C	4.31745	-0.73642	1.54459
N	-0.90771	1.51728	-0.68780
N	1.69059	0.36210	-0.97952
H	1.78363	0.25036	-3.08180
C	-3.81798	2.04021	1.73522
C	2.42010	-0.00284	-2.23690
C	2.36782	-0.18212	0.20487
H	-2.19389	1.43433	-2.37298
C	-2.05766	1.34669	0.21394
H	3.96740	-1.46038	3.53443
C	3.52501	-1.11365	2.60550
C	1.53740	-0.62497	1.25813
H	2.61463	-1.07486	-2.23096
C	2.11241	-1.07750	2.48280
C	-4.54433	0.89617	1.49277
Fe	-0.22440	-0.39143	-0.99410
N	0.18350	-0.65500	1.03808
H	-5.51020	0.73969	1.96317
C	-2.74836	0.12307	0.03351
C	1.22835	-1.50402	3.50475
H	1.63134	-1.84328	4.45479

C	-4.01953	-0.10329	0.63048
C	-0.60895	-1.08738	2.01364
C	-0.12943	-1.49947	3.27187
N	-2.11409	-0.85894	-0.68306
H	-1.66943	-1.12341	1.80445
H	-0.83603	-1.82689	4.02627
C	-4.66055	-1.33618	0.34585
C	-2.73344	-2.00877	-0.92876
H	-5.64264	-1.53675	0.76481
H	-2.18037	-2.74491	-1.50008
C	-4.03098	-2.27280	-0.45070
H	-4.50139	-3.22020	-0.68908
O	-0.40109	-0.16718	-2.74148
H	-0.38316	-1.02969	-3.19618
N	0.35709	-2.17518	-1.21467
C	0.81207	-3.27405	-1.19467
S	1.42252	-4.76432	-1.18190

[5]CisbetatranstoamineNOHBr
Charge: 2+
Energy: -3225726.6593173

H	-3.55783	-1.04635	4.36070
H	-5.14939	-1.26068	2.40756
H	-3.87100	-2.46610	2.31350
C	-3.29325	-0.66287	3.36969
C	-4.07114	-1.38711	2.27102
H	-3.53968	0.40745	3.36563
H	-1.59030	-1.94409	3.24207
H	-1.19716	-0.36632	3.91377
C	-1.79529	-0.87331	3.14748
H	-4.25483	-1.30051	0.11466
C	-3.67298	-0.81663	0.90433
H	-3.93223	0.24637	0.90231
H	-1.93995	-2.03788	0.48979
H	0.07115	1.45327	3.21180
C	-2.17130	-0.97347	0.58828
C	-1.31524	-0.38202	1.75194
H	0.66410	-2.21441	2.94464
H	-1.39338	0.70740	1.69229
H	-4.16972	0.91886	-1.17077
H	-0.24530	-2.81049	1.52402
H	-4.53055	3.33071	-1.38430
H	-3.52160	-1.00489	-1.90337
C	0.52398	-2.12278	1.86213
H	2.05628	2.76625	3.83105
C	1.00367	1.28218	2.68666
C	-3.30817	1.57143	-1.11133
C	-3.51871	2.96236	-1.25140
N	0.12049	-0.71832	1.57384
N	-1.77489	-0.38924	-0.77418
H	-2.21776	-2.20983	-1.77621
C	2.14185	2.01273	3.05494
C	-2.44038	-1.15005	-1.89093
C	-2.04028	1.04764	-0.91872
H	1.45105	-2.36449	1.35096
C	1.11290	0.23105	1.75971
H	-2.60989	4.90399	-1.35419
C	-2.45525	3.83565	-1.23674
C	-0.92733	1.92958	-0.95118
H	-2.02123	-0.79505	-2.83368
C	-1.13464	3.33597	-1.11446
C	3.38490	1.73580	2.49440
Fe	0.40041	-0.72520	-1.24766
N	0.33424	1.40262	-0.90034
H	4.26620	2.27867	2.82396
C	2.35149	0.07272	1.03246
C	0.00827	4.16764	-1.20267
H	-0.12132	5.23965	-1.32254
C	3.50923	0.77547	1.44972
C	1.38007	2.21187	-1.04657
C	1.26743	3.60581	-1.17778
N	2.32627	-0.64506	-0.12248
H	2.35447	1.73917	-1.08046
H	2.16146	4.21005	-1.28386
C	4.70995	0.54626	0.72835
C	3.46425	-0.83666	-0.79286
H	5.62494	1.04638	1.03342
H	3.38354	-1.41434	-1.70814
C	4.69328	-0.29142	-0.37182
H	5.59283	-0.49252	-0.94331
O	0.72961	-0.39681	-2.98271
H	0.80029	-1.12372	-3.62810
Br	0.39151	-3.16811	-1.29938

[5]CisbetatranstoamineNOHCl
Charge: 2+
Energy: -1899199.5406901

H	-3.57012	-3.02318	3.23185
H	-5.17971	-2.19788	1.46513
H	-3.96372	-3.25813	0.76260
C	-3.29151	-2.21880	2.54300
C	-4.10984	-2.28674	1.25361
H	-3.48426	-1.27144	3.06419
H	-1.65412	-3.34792	1.76663
H	-1.18060	-2.30650	3.10331
C	-1.80693	-2.35691	2.20481
H	-4.30057	-1.15569	-0.58378
C	-3.68990	-1.14214	0.32354
H	-3.89285	-0.20188	0.84508
H	-2.02538	-2.08383	-0.68192
H	0.17702	-0.41591	3.31851
C	-2.20027	-1.19137	-0.07509
C	-1.30937	-1.27396	1.20511
H	0.58797	-3.53906	1.29802
H	-1.33132	-0.28882	1.68000
H	-4.10316	1.40253	-0.62497
H	-0.37562	-3.33268	-0.19594
H	-4.32364	3.63586	0.35667
H	-3.56183	0.03567	-2.23462
C	0.43617	-2.92906	0.40100
H	2.23017	0.35567	4.43014
C	1.09694	-0.35618	2.74854
C	-3.20443	1.90714	-0.29422
C	-3.33381	3.20309	0.25616
N	0.10625	-1.54624	0.84758
N	-1.78234	-0.03976	-0.99764
H	-2.31306	-1.12908	-2.74247
C	2.27293	0.05994	3.38699
C	-2.48843	-0.13897	-2.32413
C	-1.96719	1.29854	-0.42621
H	1.33886	-2.92885	-0.20204
C	1.14718	-0.84404	1.43023
H	-2.31270	4.91302	1.05600
C	-2.22017	3.91323	0.64258
C	-0.80431	2.03687	-0.08038
H	-2.05939	0.61264	-2.98887
C	-0.92974	3.35711	0.45668
C	3.49760	0.02944	2.72677
Fe	0.36931	-0.22098	-1.64938
N	0.42413	1.49315	-0.34097
H	4.40734	0.31069	3.24955
C	2.37329	-0.68962	0.67971
C	0.25945	4.07662	0.72838
H	0.19260	5.07956	1.14072
C	3.56735	-0.32129	1.34778
C	1.51422	2.22543	-0.12670
C	1.48294	3.51522	0.42870
N	2.30579	-0.76600	-0.67615
H	2.45794	1.78283	-0.42252
H	2.40973	4.05543	0.58638
C	4.75134	-0.22995	0.57019
C	3.42840	-0.66115	-1.38974
H	5.69226	0.02405	1.05034
H	3.31263	-0.72158	-2.46714
C	4.68641	-0.43844	-0.79531
H	5.57164	-0.38011	-1.41917
O	0.74265	0.86144	-3.03617
H	0.75213	0.51055	-3.94565
Cl	0.15480	-2.20789	-2.67557

[5]CisbetatranstoamineNOHF
Charge: 2+
Energy: -1673078.8006724

H	3.41461	-3.92447	-2.22878
H	5.10135	-2.59477	-0.88892
H	3.94943	-3.40735	0.16455
C	3.16017	-2.94878	-1.80147
C	4.04662	-2.62410	-0.59905
H	3.31065	-2.20409	-2.59467
H	1.57869	-3.77947	-0.62621
H	1.02612	-3.20418	-2.19492
C	1.69689	-2.97463	-1.35877
H	4.30279	-1.00347	0.81385
C	3.64821	-1.25959	-0.02447
H	3.80516	-0.50816	-0.80511
H	2.04555	-1.89218	1.28288
H	-0.28567	-1.46426	-2.95131
C	2.18145	-1.19833	0.45055
C	1.23749	-1.63439	-0.71552
H	-0.64216	-3.79926	-0.03498
H	1.24838	-0.83391	-1.46110
H	4.14657	1.41633	0.35130
H	0.32428	-3.11394	1.31282
H	4.40488	3.35133	-1.13692
H	3.56399	0.39291	2.28526
C	-0.48862	-2.93398	0.61840
H	-2.34729	-1.02480	-4.21498
C	-1.19176	-1.21303	-2.41265
C	3.25820	1.84547	-0.09512
C	3.40866	2.96923	-0.94010
N	-0.16850	-1.76907	-0.25585
N	1.79852	0.15593	1.04689
H	2.18604	-0.46742	3.02916
C	-2.37300	-0.98416	-3.13097
C	2.47615	0.35413	2.37426

C	2.01101	1.30688	0.17199
H	-1.38875	-2.73907	1.19247
C	-1.21969	-1.27008	-1.00750
H	2.41568	4.44642	-2.13911
C	2.30654	3.57926	-1.49475
C	0.85879	1.95704	-0.34600
H	2.11863	1.29547	2.79541
C	1.00655	3.10309	-1.18940
C	-3.58103	-0.77315	-2.47476
Fe	-0.34737	0.15137	1.72840
N	-0.37987	1.51146	0.03456
H	-4.49636	-0.63814	-3.04392
C	-2.42631	-0.86592	-0.32089
C	-0.17054	3.74733	-1.64244
H	-0.08694	4.61694	-2.28833
C	-3.62508	-0.68001	-1.05406
C	-1.45802	2.17834	-0.37126
C	-1.40405	3.28915	-1.22969
N	-2.33256	-0.52950	0.99386
H	-2.41114	1.83268	0.01092
H	-2.32226	3.78168	-1.52959
C	-4.78775	-0.31204	-0.32793
C	-3.43292	-0.15609	1.65029
H	-5.73169	-0.18814	-0.85144
H	-3.29010	0.13360	2.68611
C	-4.69694	-0.08302	1.03245
H	-5.56428	0.20336	1.61716
O	-0.76003	1.45600	2.89689
H	-0.69438	1.31449	3.85840
F	0.04008	-1.29723	2.68595

^{3}CisbetatranstoamineNOHN$_{3}$
Charge: 2+
Energy: -1713470.5014141

H	2.58896	-4.05431	-2.74467
H	4.53209	-3.17023	-1.38267
H	3.32791	-3.95301	-0.36601
C	2.51249	-3.11468	-2.18878
C	3.50159	-3.09043	-1.02297
H	2.74355	-2.30718	-2.89686
H	0.87343	-3.80667	-0.99301
H	0.36506	-3.03519	-2.48353
C	1.07881	-2.96338	-1.66115
H	4.04401	-1.76914	0.61087
C	3.34913	-1.78257	-0.23419
H	3.61791	-0.94642	-0.88820
H	1.66693	-2.39692	0.96771
H	-1.02672	-1.86780	-3.07182
C	1.90773	-1.58796	0.27228
C	0.89428	-1.63590	-0.88801
H	-1.25365	-3.41898	-0.49310
H	1.06391	-0.78929	-1.55916
H	4.35473	0.56677	1.39567
H	-0.36543	-3.09287	1.02854
H	5.36852	2.49947	0.27356
H	3.27352	-0.93675	2.49534
C	-1.05929	-2.68864	0.29445
H	-3.05322	-1.13280	-4.24833
C	-1.74474	-1.26420	-2.53380
C	3.73296	1.17169	0.74772
C	4.32008	2.28296	0.09790
N	-0.50033	-1.42769	-0.31409
N	1.74023	-0.31628	1.13054
H	1.60909	-1.32463	2.98523
C	-2.92238	-0.84811	-3.20952
C	2.24353	-0.57585	2.51715
C	2.40324	0.85679	0.54165
H	-2.00177	-2.45221	0.78506
C	-1.54726	-0.92306	-1.21332
H	4.02813	3.92498	-1.25293
C	3.57811	3.07517	-0.74892
C	1.61280	1.68855	-0.27799
H	2.19446	0.35640	3.07948
C	2.19994	2.80400	-0.94563
C	-3.90510	-0.13342	-2.56128
Fe	-0.27681	0.11926	1.12488
N	0.26901	1.42765	-0.35754
H	-4.81927	0.14670	-3.07562
C	-2.50953	-0.11212	-0.56229
C	1.35286	3.61192	-1.74230
H	1.76868	4.46500	-2.27095
C	-3.71658	0.26600	-1.21097
C	-0.49990	2.23190	-1.08743
C	0.00681	3.32117	-1.81683
N	-2.19700	0.36247	0.68636
H	-1.56043	2.02476	-1.09780
H	-0.67361	3.92826	-2.40324
C	-4.63103	1.06210	-0.47239
C	-3.05473	1.13586	1.34485
H	-5.57446	1.35153	-0.92673
H	-2.72362	1.51757	2.30329
C	-4.30869	1.47974	0.80363
H	-4.98404	2.09647	1.38599
O	-0.12513	1.53240	2.16682
H	-0.13685	1.28539	3.11071
N	-0.57703	-1.05117	2.54092
N	-1.70620	-1.17258	3.02686
N	-2.71730	-1.34723	3.52989

^{3}CisbetatranstoamineNOHNCS
Charge: 2+
Energy: -1918576.0087213

H	2.63073	0.83845	4.85339
H	4.45629	1.53617	3.24563
H	3.07567	2.62461	3.17194
C	2.56217	0.61215	3.78480
C	3.39986	1.59563	2.96615
H	2.94412	-0.40929	3.65172
H	0.73564	1.70695	3.53839
H	0.48232	0.02689	3.96908
C	1.09160	0.68791	3.35053
H	3.84321	1.99822	0.87985
C	3.26003	1.28433	1.46980
H	3.67692	0.28984	1.27964
H	1.40398	2.32804	1.16741
H	-0.73399	-1.36945	3.52479
C	1.78889	1.31487	1.01799
C	0.92088	0.35016	1.85089
H	-1.41411	1.53285	2.93798
H	1.23877	-0.67994	1.66440
H	4.25745	1.04889	-1.34687
H	-0.64275	2.54330	1.68169
H	5.53423	-0.92075	-2.06338
H	2.92137	2.68572	-1.05071
C	-1.22948	1.64484	1.86780
H	-2.54503	-3.00179	3.81282
C	-1.46360	-1.47347	2.73353
C	3.75605	0.08947	-1.36945
C	4.49506	-1.04576	-1.77797
N	-0.50635	0.43550	1.33588
N	1.60788	1.07833	-0.49354
H	1.20562	3.10807	-0.92785
C	-2.51870	-2.40903	2.90437
C	1.90492	2.33771	-1.24460
C	2.43298	-0.03207	-0.99036
H	-2.18390	1.73107	1.35144
C	-1.39804	-0.70353	1.59253
H	4.47815	-3.16554	-2.11418
C	3.91071	-2.29223	-1.80752
C	1.80170	-1.28909	-1.06967
H	1.78060	2.13541	-2.30803
C	2.54222	-2.44112	-1.46620
C	-3.51713	-2.54218	1.96541
Fe	-0.34204	0.48851	-0.77043
N	0.45489	-1.34562	-0.81468
H	-4.34102	-3.23119	2.12420
C	-2.36936	-0.89854	0.57825
C	1.84961	-3.67348	-1.53932
H	2.38443	-4.57333	-1.82954
C	-3.46171	-1.78885	0.76212
C	-0.16687	-2.51623	-0.93365
C	0.49849	-3.70877	-1.26676
N	-2.16981	-0.25472	-0.61513
H	-1.23494	-2.52596	-0.77507
H	-0.06928	-4.63016	-1.33024
C	-4.39822	-1.89556	-0.29950
C	-3.04562	-0.38956	-1.60338
H	-5.25743	-2.55122	-0.18946
H	-2.80076	0.10894	-2.53350
C	-4.20152	-1.18446	-1.46664
H	-4.89729	-1.25412	-2.29532
O	-0.19509	0.34795	-2.53808
H	-0.48853	1.15813	-2.99240
N	-1.03982	2.22895	-0.90501
C	-1.65075	3.21938	-1.15153
S	-2.44872	4.58214	-1.46627

^{6}CisbetatranstoquinolylN
Charge: 2+
Energy: -1693778.9568750

H	-3.75729	-4.42746	-0.05280
H	-5.34775	-2.49612	-0.43320
H	-4.27120	-2.72409	-1.80695
C	-3.42880	-3.39094	0.07295
C	-4.30064	-2.43845	-0.74682
H	-3.51835	-3.15652	1.14279
H	-1.92835	-3.54324	-1.44100
H	-1.33452	-3.98067	0.14699
C	-1.97043	-3.26641	-0.38222
H	-4.42204	-0.31099	-1.15493
C	-3.80305	-0.99811	-0.56870
H	-3.92148	-0.72982	0.48635
H	-2.22629	-1.03214	-2.04058
H	-0.00273	-3.40632	1.53528
C	-2.32473	-0.82992	-0.96907

C	-1.42221	-1.82995	-0.21388
H	0.30899	-3.51143	-1.76679
H	-1.41576	-1.55425	0.84657
H	-4.12900	1.60675	0.23743
H	-0.45054	-2.18220	-2.70553
H	-4.44495	2.58365	2.46591
H	-3.42280	1.58736	-1.86754
C	0.29762	-2.43623	-1.95695
H	1.94663	-3.96804	2.91423
C	0.93669	-2.91316	1.32191
C	-3.27108	1.67864	0.89409
C	-3.45484	2.24839	2.17515
N	0.00902	-1.68113	-0.68446
N	-1.80692	0.60100	-0.82779
H	-2.06372	1.02582	-2.87770
C	2.06657	-3.24425	2.11470
C	-2.33759	1.47085	-1.92213
C	-2.03411	1.21478	0.48133
H	1.26746	-2.12169	-2.33729
C	1.04545	-2.00602	0.28832
H	-2.52898	2.80223	4.03034
C	-2.39396	2.37292	3.04211
C	-0.91430	1.39485	1.33639
H	-1.86935	2.45310	-1.83432
C	-1.09820	1.96629	2.63563
C	3.30404	-2.69982	1.85688
O	0.23680	0.28636	-3.00755
Fe	0.37494	0.42904	-1.21754
N	0.33306	1.06099	0.87752
H	4.17305	-2.99076	2.43909
C	2.29629	-1.36129	0.07549
C	0.04663	2.13328	3.45273
H	-0.06684	2.55093	4.44930
C	3.44658	-1.73429	0.82542
C	1.38521	1.26976	1.66350
C	1.28897	1.78553	2.96801
N	2.33939	-0.34001	-0.83510
H	2.35480	1.02715	1.24660
H	2.18739	1.91426	3.56132
N	0.99015	2.61857	-1.49294
C	4.66733	-1.08518	0.50609
C	3.49600	0.25301	-1.10988
C	1.24613	3.73204	-1.68523
H	5.57176	-1.35922	1.04228
H	3.46134	1.05765	-1.83763
C	4.69930	-0.11266	-0.47450
H	0.64618	5.70219	-2.08616
C	1.56812	5.13213	-1.92944
H	5.62257	0.38837	-0.74352
H	2.10375	5.54827	-1.06995
H	2.19640	5.21994	-2.82209
H	0.36401	0.93069	-3.72195

[5]CisbetatranstoquinolylNBrOH
Charge: 2+
Energy: -3225726.6578113

H	-3.55733	-1.04727	4.36096
H	-5.14918	-1.26100	2.40795
H	-3.87096	-2.46658	2.31358
C	-3.29287	-0.66360	3.36999
C	-4.07096	-1.38756	2.27129
H	-3.53922	0.40675	3.36620
H	-1.59002	-1.94491	3.24181
H	-1.19670	-0.36735	3.91389
C	-1.79494	-0.87410	3.14753
H	-4.25481	-1.30071	0.11496
C	-3.67289	-0.81693	0.90463
H	-3.93207	0.24608	0.90274
H	-1.93986	-2.03815	0.48983
H	0.07118	1.45273	3.21222
C	-2.17122	-0.97376	0.58847
C	-1.31510	-0.38245	1.75205
H	0.66462	-2.21469	2.94426
H	-1.39336	0.70698	1.69267
H	-4.17004	0.91810	-1.17091
H	-0.24473	-2.81075	1.52358
H	-4.53132	3.32981	-1.38478
H	-3.52155	-1.00540	-1.90325
C	0.52445	-2.12295	1.86177
H	2.05615	2.76583	3.83164
C	1.00368	1.28187	2.68698
C	-3.30861	1.57082	-1.11151
C	-3.51942	2.96170	-1.25173
N	0.12068	-0.71849	1.57367
N	-1.77494	-0.38947	-0.77405
H	-2.21763	-2.21026	-1.77581
C	2.14179	2.01251	3.05534
C	-2.44033	-1.15052	-1.89072
C	-2.04063	1.04730	-0.91870
H	1.45154	-2.36441	1.35052
C	1.11299	0.23101	1.75976
H	-2.61104	4.90352	-1.35457
C	-2.45617	3.83523	-1.23700
C	-0.92787	1.92953	-0.95109
H	-2.02115	-0.79565	-2.83352
C	-1.13546	3.33585	-1.11447
C	3.38482	1.73594	2.49462
Fe	0.40050	-0.72494	-1.24754
N	0.33380	1.40285	-0.90007
H	4.26607	2.27886	2.82422
C	2.35152	0.07306	1.03236
C	0.00728	4.16778	-1.20245
H	-0.12254	5.23975	-1.32239
C	3.50919	0.77590	1.44966
C	1.37949	2.21232	-1.04607
C	1.26656	3.60625	-1.17725
N	2.32631	-0.64447	-0.12275
H	2.35400	1.73985	-1.07982
H	2.16047	4.21071	-1.28305
C	4.70987	0.54707	0.72810
C	3.46423	-0.83571	-0.79329
H	5.62481	1.04727	1.03321
H	3.38355	-1.41319	-1.70869
C	4.69322	-0.29033	-0.37227
H	5.59272	-0.49112	-0.94394
O	0.72972	-0.39677	-2.98261
H	0.80089	-1.12377	-3.62785
Br	0.39228	-3.16796	-1.29978

[5]CisbetatranstoquinolylNClOH
Charge: 2+
Energy: -1899199.5383181

H	-3.56604	-3.03078	3.22904
H	-5.17735	-2.20223	1.46521
H	-3.96198	-3.26138	0.75992
C	-3.28820	-2.22504	2.54145
C	-4.10765	-2.29078	1.25264
H	-3.48073	-1.27870	3.06458
H	-1.65126	-3.35229	1.76133
H	-1.17677	-2.31348	3.09971
C	-1.80391	-2.36222	2.20169
H	-4.29996	-1.15698	-0.58275
C	-3.68851	-1.14472	0.32406
H	-3.89108	-0.20520	0.84713
H	-2.02445	-2.08475	-0.68389
H	0.17914	-0.42213	3.31839
C	-2.19911	-1.19305	-0.07585
C	-1.30747	-1.27709	1.20372
H	0.59075	-3.54108	1.29205
H	-1.33001	-0.29282	1.68039
H	-4.10476	1.39952	-0.62456
H	-0.37260	-3.33247	-0.20176
H	-4.32784	3.63172	0.35910
H	-3.56257	0.03282	-2.23376
C	0.43883	-2.92951	0.39612
H	2.23214	0.34875	4.43070
C	1.09878	-0.36065	2.74816
C	-3.20666	1.90466	-0.29288
C	-3.33755	3.19993	0.25879
N	0.10817	-1.54766	0.84515
N	-1.78248	-0.04023	-0.99748
H	-2.31116	-1.12801	-2.74388
C	2.27471	0.05510	3.38695
C	-2.48876	-0.13899	-2.32389
C	-1.96881	1.29732	-0.42475
H	1.34170	-2.92775	-0.20667
C	1.14886	-0.84591	1.42886
H	-2.31849	4.90986	1.06127
C	-2.22480	3.91062	0.64677
C	-0.80679	2.03633	-0.07737
H	-2.06173	0.61476	-2.98748
C	-0.93375	3.35581	0.46112
C	3.49916	0.02684	2.72616
Fe	0.36883	-0.21779	-1.64949
N	0.42228	1.49403	-0.33787
H	4.40891	0.30773	3.24912
C	2.37453	-0.68909	0.67816
C	0.25464	4.07605	0.73444
H	0.18662	5.07845	1.14792
C	3.56860	-0.32112	1.34644
C	1.51161	2.22699	-0.12207
C	1.47883	3.51611	0.43486
N	2.30650	-0.76298	-0.67781
H	2.45589	1.78564	-0.41790
H	2.40504	4.05695	0.59380
C	4.75218	-0.22732	0.56853
C	3.42873	-0.65589	-1.39166
H	5.69311	0.02649	1.04878
H	3.31260	-0.71453	-2.46913
C	4.68684	-0.43324	-0.79734
H	5.57177	-0.37298	-1.42146
O	0.73986	0.86848	-3.03398
H	0.74900	0.51910	-3.94407
Cl	0.15742	-2.20286	-2.67972

^{5}CisbetatranstoquinolylNFOH
Charge: 2+
Energy: -1673078.8032829

H	3.41423	-3.92469	-2.22885
H	5.10110	-2.59500	-0.88911
H	3.94924	-3.40761	0.16440
C	3.15987	-2.94898	-1.80156
C	4.04639	-2.62433	-0.59918
H	3.31038	-2.20433	-2.59479
H	1.57837	-3.77947	-0.62616
H	1.02580	-3.20430	-2.19491
C	1.69661	-2.97470	-1.35882
H	4.30258	-1.00383	0.81386
C	3.64804	-1.25983	-0.02452
H	3.80511	-0.50836	-0.80508
H	2.04528	-1.89242	1.28270
H	-0.28592	-1.46398	-2.95138
C	2.18129	-1.19852	0.45043
C	1.23731	-1.63439	-0.71564
H	-0.64246	-3.79911	-0.03528
H	1.24826	-0.83391	-1.46124
H	4.14667	1.41609	0.35184
H	0.32400	-3.11398	1.31263
H	4.40531	3.35106	-1.13635
H	3.56400	0.39228	2.28525
C	-0.48886	-2.93391	0.61819
H	-2.34758	-1.02441	-4.21495
C	-1.19198	-1.21274	-2.41267
C	3.25840	1.84526	-0.09473
C	3.40904	2.96899	-0.93971
N	-0.16866	-1.76895	-0.25592
N	1.79845	0.15575	1.04694
H	2.18587	-0.46781	3.02913
C	-2.37324	-0.98382	-3.13093
C	2.47616	0.35372	2.37429
C	2.01115	1.30670	0.17215
H	-1.38901	-2.73897	1.19225
C	-1.21983	-1.26984	-1.00753
H	2.41633	4.44613	-2.13899
C	2.30704	3.57901	-1.49461
C	0.85904	1.95692	-0.34603
H	2.11883	1.29510	2.79552
C	1.00698	3.10291	-1.18945
C	-3.58123	-0.77282	-2.47467
Fe	-0.34741	0.15139	1.72845
N	-0.37969	1.51145	0.03447
H	-4.49658	-0.63776	-3.04379
C	-2.42640	-0.86567	-0.32086
C	-0.17001	3.74720	-1.64267
H	-0.08628	4.61675	-2.28863
C	-3.62521	-0.67973	-1.05398
C	-1.45773	2.17844	-0.37146
C	-1.40359	3.28916	-1.22999
N	-2.33259	-0.52925	0.99389
H	-2.41091	1.83295	0.01071
H	-2.32173	3.78175	-1.52999
C	-4.78783	-0.31173	-0.32779
C	-3.43291	-0.15582	1.65036
H	-5.73179	-0.18780	-0.85125
H	-3.29005	0.13385	2.68618
C	-4.69695	-0.08272	1.03258
H	-5.56426	0.20369	1.61734
O	-0.75952	1.45609	2.89696
H	-0.69487	1.31475	3.85855
F	0.03966	-1.29745	2.68581

^{3}CisbetatranstoquinolylNN$_{3}$OH
Charge: 2+
Energy: -1713470.5047022

H	2.58943	-4.05310	-2.74640
H	4.53243	-3.16982	-1.38374
H	3.32796	-3.95279	-0.36755
C	2.51298	-3.11369	-2.19015
C	3.50189	-3.09002	-1.02418
H	2.74418	-2.30589	-2.89784
H	0.87378	-3.80607	-0.99483
H	0.36559	-3.03399	-2.48513
C	1.07921	-2.96251	-1.66261
H	4.04427	-1.76940	0.61018
C	3.34947	-1.78241	-0.23494
H	3.61838	-0.94608	-0.88865
H	1.66713	-2.39723	0.96642
H	-1.02540	-1.86435	-3.07374
C	1.90803	-1.58793	0.27144
C	0.89470	-1.63533	-0.88902
H	-1.25344	-3.41841	-0.49550
H	1.06455	-0.78846	-1.55982
H	4.35490	0.56671	1.39508
H	-0.36513	-3.09334	1.02633
H	5.36801	2.50015	0.27412
H	3.27404	-0.93654	2.49484
C	-1.05899	-2.68861	0.29252
H	-3.05188	-1.12881	-4.24977
C	-1.74374	-1.26168	-2.53511
C	3.73274	1.17187	0.74774
C	4.31955	2.28369	0.09856
N	-0.49991	-1.42729	-0.31522
N	1.74035	-0.31667	1.13023
H	1.60994	-1.32649	2.98414
C	-2.92141	-0.84526	-3.21060
C	2.24368	-0.57674	2.51666
C	2.40306	0.85680	0.54184
H	-2.00142	-2.45241	0.78333
C	-1.54664	-0.92204	-1.21419
H	4.02698	3.92672	-1.25091
C	3.57726	3.07645	-0.74742
C	1.61228	1.68910	-0.27702
H	2.19351	0.35502	3.07969
C	2.19907	2.80519	-0.94391
C	-3.90457	-0.13178	-2.56174
Fe	-0.27689	0.11837	1.12488
N	0.26857	1.42809	-0.35656
H	-4.81880	0.14849	-3.07589
C	-2.50931	-0.11201	-0.56254
C	1.35164	3.61374	-1.73957
H	1.76723	4.46734	-2.26755
C	-3.71644	0.26624	-1.21096
C	-0.50070	2.23284	-1.08547
C	0.00559	3.32292	-1.81395
N	-2.19704	0.36154	0.68654
H	-1.56117	2.02542	-1.09588
H	-0.67509	3.93049	-2.39956
C	-4.63138	1.06102	-0.47157
C	-3.05526	1.13366	1.34586
H	-5.57493	1.35045	-0.92569
H	-2.72441	1.51464	2.30468
C	-4.30940	1.47738	0.80494
H	-4.98514	2.09306	1.38796
O	-0.12546	1.53094	2.16774
H	-0.13712	1.28333	3.11146
N	-0.57639	-1.05291	2.54034
N	-1.70557	-1.17505	3.02611
N	-2.71650	-1.35044	3.52908

^{3}CisbetatranstoquinolylNNCSOH
Charge: 2+
Energy: -1918576.0086836

H	2.63092	0.83875	4.85319
H	4.45632	1.53671	3.24537
H	3.07553	2.62495	3.17169
C	2.56235	0.61243	3.78460
C	3.39987	1.59601	2.96591
H	2.94441	-0.40896	3.65151
H	0.73569	1.70703	3.53827
H	0.48255	0.02694	3.96895
C	1.09175	0.68802	3.35039
H	3.84314	1.99859	0.87960
C	3.26005	1.28464	1.46958
H	3.67707	0.29020	1.27946
H	1.40388	2.32813	1.16708
H	-0.73345	-1.36963	3.52464
C	1.78891	1.31498	1.01778
C	0.92100	0.35026	1.85076
H	-1.41400	1.53281	2.93799
H	1.23893	-0.67983	1.66427
H	4.25753	1.04847	-1.34682
H	-0.64270	2.54332	1.68170
H	5.53418	-0.92133	-2.06310
H	2.92143	2.68548	-1.05121
C	-1.22940	1.64483	1.86781
H	-2.54443	-3.00203	3.81281
C	-1.46320	-1.47359	2.73349
C	3.75604	0.08910	-1.36938
C	4.49498	-1.04622	-1.77778
N	-0.50624	0.43553	1.33584
N	1.60788	1.07824	-0.49373
H	1.20572	3.10793	-0.92833
C	-2.51825	-2.40918	2.90441
C	1.90496	2.33748	-1.24499
C	2.43293	-0.03229	-0.99039
H	-2.18384	1.73106	1.35148
C	-1.39785	-0.70354	1.59255
H	4.47788	-3.16601	-2.11389
C	3.91051	-2.29263	-1.80731
C	1.80154	-1.28925	-1.06967
H	1.78057	2.13502	-2.30838
C	2.54198	-2.44137	-1.46611
C	-3.51683	-2.54227	1.96559
Fe	-0.34207	0.48852	-0.77047
N	0.45471	-1.34564	-0.81478
H	-4.34069	-3.23130	2.12447
C	-2.36930	-0.89852	0.57839
C	1.84925	-3.67366	-1.53926
H	2.38400	-4.57357	-1.82940
C	-3.46161	-1.78885	0.76235
C	-0.16716	-2.51619	-0.93381

C	0.49810	-3.70880	-1.26684
N	-2.16990	-0.25460	-0.61497
H	-1.23526	-2.52579	-0.77534
H	-0.06976	-4.63013	-1.33035
C	-4.39827	-1.89547	-0.29914
C	-3.04587	-0.38936	-1.60309
H	-5.25746	-2.55115	-0.18902
H	-2.80116	0.10922	-2.53321
C	-4.20175	-1.18426	-1.46624
H	-4.89765	-1.25384	-2.29482
O	-0.19529	0.34793	-2.53814
H	-0.48881	1.15808	-2.99247
N	-1.03977	2.22902	-0.90498
C	-1.65063	3.21950	-1.15149
S	-2.44847	4.58234	-1.46619

^{3}CisbetatranstoquinolylNOHBr
Charge: 2+
Energy: -3225734.4175306

H	2.32613	5.24082	0.35612
H	4.37483	3.79698	-0.01775
H	3.35392	3.86878	-1.44915
C	2.27049	4.14884	0.40496
C	3.39479	3.51089	-0.41190
H	2.36958	3.87312	1.46372
H	0.82320	4.02254	-1.17622
H	0.10089	4.18733	0.41240
C	0.90690	3.69520	-0.13420
H	4.06302	1.52558	-0.97603
C	3.27041	1.98101	-0.37502
H	3.40962	1.64039	0.65654
H	1.78037	1.82668	-1.92490
H	-1.34895	3.46494	1.41987
C	1.89411	1.51354	-0.88359
C	0.75528	2.15526	-0.06823
H	-1.30058	3.34918	-1.62923
H	0.81227	1.81962	0.97148
H	4.37336	-0.86892	-0.44416
H	-0.20607	2.30656	-2.59361
H	5.18358	-1.87262	1.64757
H	3.45454	-0.13419	-2.28397
C	-1.00960	2.32272	-1.86101
H	-3.51138	3.44453	2.58408
C	-2.03469	2.65323	1.21970
C	3.66488	-1.04293	0.35602
C	4.13264	-1.61758	1.56144
N	-0.57018	1.63707	-0.59204
N	1.77289	-0.02664	-0.96062
H	1.86017	-0.10683	-3.06803
C	-3.29042	2.64874	1.88045
C	2.42698	-0.49913	-2.22626
C	2.33461	-0.69634	0.21689
H	-1.86068	1.78383	-2.27134
C	-1.72140	1.65866	0.31733
H	3.63226	-2.28293	3.53980
C	3.27319	-1.84650	2.61286
C	1.42922	-0.98138	1.25559
H	2.41496	-1.58723	-2.24335
C	1.89255	-1.54848	2.47820
C	-4.23629	1.68662	1.60527
Fe	-0.26994	-0.39788	-0.96608
N	0.09128	-0.77400	1.01599
H	-5.21269	1.71546	2.07920
C	-2.64377	0.60397	0.10537
C	0.93013	-1.83435	3.47573
H	1.24916	-2.26101	4.42244
C	-3.93191	0.62875	0.70722
C	-0.78654	-1.08726	1.97005
C	-0.40504	-1.59453	3.22209
N	-2.22998	-0.47515	-0.63935
H	-1.83311	-0.95367	1.74070
H	-1.17128	-1.81862	3.95556
C	-4.81920	-0.43345	0.39266
C	-3.07954	-1.46074	-0.91767
H	-5.81966	-0.43627	0.81629
H	-2.69364	-2.28686	-1.50189
C	-4.40403	-1.45427	-0.43837
H	-5.06226	-2.27457	-0.70210
O	-0.41105	-0.15730	-2.68358
H	-0.45956	-0.99324	-3.18919
Br	0.01355	-2.84508	-1.27341

^{5}CisbetatranstoquinolylNOHCl
Charge: 2+
Energy: -1899203.4899398

H	2.82336	4.65185	1.35632
H	4.76271	3.23226	0.55584
H	3.69277	3.67625	-0.76879
C	2.69969	3.58329	1.15330
C	3.75264	3.09164	0.15878
H	2.81278	3.06196	2.11380
H	1.22419	3.90587	-0.36157
H	0.52816	3.74470	1.23902
C	1.30014	3.34584	0.57610
H	4.27679	1.24901	-0.85908
C	3.53508	1.60218	-0.13556
H	3.69059	1.04347	0.79348
H	1.99531	1.80546	-1.63765
H	-0.61171	2.50975	2.36967
C	2.11987	1.30450	-0.67318
C	1.03764	1.84355	0.29267
H	-0.96840	3.55134	-0.82213
H	1.08733	1.27074	1.22446
H	4.37115	-1.11474	-0.23043
H	0.04790	2.72161	-2.04292
H	4.84865	-2.64376	1.63523
H	3.65086	-0.41683	-2.22342
C	-0.74796	2.60077	-1.31268
H	-2.67535	2.40559	3.69056
C	-1.46640	1.99512	1.95046
C	3.54404	-1.48205	0.36463
C	3.82001	-2.36292	1.43514
N	-0.33885	1.59248	-0.27138
N	1.90104	-0.16511	-0.99619
H	2.17301	0.09569	-3.07187
C	-2.66110	1.94052	2.71031
C	2.56677	-0.54212	-2.28180
C	2.24809	-1.08680	0.08129
H	-1.63449	2.24045	-1.82861
C	-1.42287	1.44842	0.68096
H	3.00407	-3.53157	3.04025
C	2.79825	-2.85838	2.21361
C	1.18281	-1.62936	0.83294
H	2.33092	-1.58335	-2.50118
C	1.45339	-2.51821	1.91985
C	-3.80426	1.35450	2.20776
Fe	-0.29696	-0.38792	-1.35013
N	-0.11010	-1.33617	0.46890
H	-4.72672	1.35781	2.78051
C	-2.55855	0.73328	0.20125
C	0.35227	-3.05369	2.62902
H	0.53078	-3.72742	3.46242
C	-3.77280	0.71653	0.93863
C	-1.12176	-1.90140	1.12967
C	-0.93350	-2.74251	2.23591
N	-2.40242	-0.00687	-0.93539
H	-2.11773	-1.70172	0.76265
H	-1.79947	-3.15678	2.73967
C	-4.86659	0.01427	0.36690
C	-3.43447	-0.67807	-1.43828
H	-5.82079	-0.00176	0.88631
H	-3.23720	-1.27355	-2.32364
C	-4.70641	-0.65652	-0.83057
H	-5.52609	-1.19853	-1.28923
O	-0.19784	0.47154	-2.88887
H	-0.30654	-0.09452	-3.67878
Cl	-0.46793	-2.39590	-2.30004

^{3}CisbetatranstoquinolylNOHF
Charge: 2+
Energy: -1673081.3821773

H	-2.09485	4.56868	-2.03439
H	-4.19491	3.40827	-1.23272
H	-3.21278	3.97465	0.11294
C	-2.07016	3.53542	-1.67459
C	-3.23696	3.26385	-0.72379
H	-2.15028	2.89029	-2.56020
H	-0.64052	3.99068	-0.13096
H	0.08923	3.50512	-1.65695
C	-0.72786	3.28863	-0.96735
H	-3.97804	1.62976	0.50474
C	-3.15977	1.82509	-0.19592
H	-3.28011	1.12939	-1.03382
H	-1.72809	2.23941	1.35119
H	1.86748	2.89823	-1.84070
C	-1.81452	1.55991	0.49946
C	-0.62267	1.83811	-0.44685
H	1.35461	3.47547	0.75445
H	-0.65335	1.14695	-1.29197
H	-4.36349	-0.80414	1.15996
H	0.21574	2.79297	1.95601
H	-5.29035	-2.48207	-0.37571
H	-3.35894	0.52794	2.50286
C	1.05127	2.57675	1.29423
H	4.05623	2.40211	-2.82879
C	2.40697	2.03168	-1.48439
C	-3.70640	-1.25087	0.42416
C	-4.24346	-2.21230	-0.46634
N	0.67078	1.50747	0.30063
N	-1.74229	0.16029	1.14507
H	-1.73368	0.89464	3.12374
C	3.68273	1.75671	-2.04065
C	-2.31802	0.19761	2.52669
C	-2.37907	-0.88322	0.33312
H	1.88242	2.21143	1.89327

C	1.88967	1.23158	-0.48614
H	-3.87685	-3.51487	-2.13225
C	-3.46022	-2.78828	-1.44153
C	-1.54743	-1.50780	-0.61516
H	-2.24781	-0.80527	2.94802
C	-2.08470	-2.45214	-1.53653
C	4.45773	0.71831	-1.57317
Fe	0.24343	-0.29595	1.22108
N	-0.20994	-1.20128	-0.58795
H	5.44618	0.53420	-1.98286
C	2.66304	0.13522	-0.02667
C	-1.19666	-3.02156	-2.48059
H	-1.57087	-3.74084	-3.20358
C	3.96075	-0.12805	-0.54758
C	0.59626	-1.76586	-1.48576
C	0.13636	-2.66444	-2.46355
N	2.10302	-0.71199	0.89180
H	1.64625	-1.51437	-1.43600
H	0.84425	-3.08190	-3.17072
C	4.66058	-1.24543	-0.01893
C	2.75686	-1.76907	1.35759
H	5.66116	-1.46409	-0.38151
H	2.20982	-2.39918	2.05019
C	4.06970	-2.05259	0.93454
H	4.58524	-2.91318	1.34589
O	0.51569	0.44596	2.77126
H	0.47430	-0.25738	3.45163
F	-0.08309	-1.85564	1.97862

^{3}CisbetatranstoquinolylNOHN$_{3}$
Charge: 2+
Energy: -1713471.3978427

H	2.34257	5.08219	0.17502
H	4.38393	3.62780	-0.18779
H	3.34300	3.65701	-1.60619
C	2.28544	3.99208	0.25368
C	3.39873	3.32971	-0.55952
H	2.39703	3.74422	1.31812
H	0.82472	3.82484	-1.30775
H	0.11460	4.03556	0.28147
C	0.91510	3.52574	-0.25784
H	4.06032	1.32715	-1.07098
C	3.27489	1.80166	-0.47502
H	3.42780	1.49435	0.56494
H	1.76757	1.58950	-2.00246
H	-1.31394	3.31867	1.35844
C	1.89234	1.31889	-0.95042
C	0.76399	1.98980	-0.14593
H	-1.25012	3.15250	-1.73326
H	0.82995	1.68602	0.90278
H	4.34669	-1.04015	-0.41290
H	-0.22143	2.02305	-2.67675
H	5.16995	-1.96668	1.70986
H	3.40787	-0.35445	-2.32061
C	-1.00364	2.10670	-1.92628
H	-3.47350	3.32747	2.53089
C	-2.01104	2.51530	1.16258
C	3.64341	-1.18291	0.39840
C	4.11902	-1.71212	1.62174
N	-0.56506	1.44866	-0.64388
N	1.75749	-0.21900	-0.95875
H	1.78780	-0.48253	-3.05393
C	-3.26423	2.52504	1.83114
C	2.40103	-0.75961	-2.19910
C	2.31372	-0.83748	0.25201
H	-1.89495	1.60023	-2.29090
C	-1.71384	1.51233	0.26604
H	3.63312	-2.29259	3.63006
C	3.26743	-1.89463	2.68845
C	1.41358	-1.07293	1.31309
H	2.45831	-1.84454	-2.12067
C	1.88800	-1.59275	2.55322
C	-4.21993	1.56747	1.57423
Fe	-0.26063	-0.61723	-0.93002
N	0.07888	-0.85082	1.08607
H	-5.19062	1.60714	2.05890
C	-2.65009	0.46682	0.06691
C	0.93384	-1.82128	3.57489
H	1.26089	-2.20798	4.53597
C	-3.93095	0.49956	0.68228
C	-0.78958	-1.11329	2.05932
C	-0.40092	-1.57517	3.32902
N	-2.24336	-0.60992	-0.68166
H	-1.83713	-0.96680	1.83504
H	-1.15909	-1.75587	4.08265
C	-4.81958	-0.56845	0.39198
C	-3.09045	-1.60715	-0.92075
H	-5.81544	-0.56827	0.82618
H	-2.70874	-2.44511	-1.49262
C	-4.40850	-1.60387	-0.42384
H	-5.06497	-2.43392	-0.66008
O	-0.34841	-0.45526	-2.69947
H	-1.26696	-0.48268	-3.02367
N	-0.05960	-2.44460	-0.98767
N	0.03417	-3.02841	-2.07456
N	0.13432	-3.64204	-3.03028

^{3}CisbetatranstoquinolylNOHNCS
Charge: 2+
Energy: -1918577.5973744

H	1.20772	5.63990	0.27804
H	3.50368	4.62234	-0.04536
H	2.51620	4.48168	-1.49529
C	1.36273	4.55799	0.33526
C	2.60684	4.14615	-0.45359
H	1.49262	4.31185	1.39816
H	0.00077	4.14260	-1.27110
H	-0.77161	4.18138	0.30067
C	0.12355	3.84452	-0.22422
H	3.65606	2.32320	-0.98833
C	2.78049	2.62182	-0.40342
H	2.96773	2.32285	0.63373
H	1.37503	2.16952	-1.97281
H	-2.08386	3.22157	1.25967
C	1.52949	1.89435	-0.92576
C	0.27168	2.30679	-0.14244
H	-1.94525	3.07395	-1.71883
H	0.37317	1.99888	0.90256
H	4.39819	0.04496	-0.46234
H	-0.67056	2.25768	-2.68200
H	5.39907	-0.78050	1.62362
H	3.36435	0.54262	-2.31222
C	-1.46571	2.12187	-1.95317
H	-4.20734	2.79295	2.41038
C	-2.58396	2.28030	1.07956
C	3.74016	-0.26415	0.34025
C	4.31803	-0.73365	1.54400
N	-0.90902	1.51676	-0.68753
N	1.69014	0.36356	-0.97960
H	1.78294	0.25242	-3.08191
C	-3.82029	2.03716	1.73487
C	2.41976	-0.00047	-2.23719
C	2.36789	-0.18046	0.20458
H	-2.19483	1.43335	-2.37294
C	-2.05903	1.34511	0.21398
H	3.96868	-1.45826	3.53373
C	3.52596	-1.11166	2.60492
C	1.53788	-0.62413	1.25783
H	2.61515	-1.07232	-2.23154
C	2.11332	-1.07648	2.48236
C	-4.54555	0.89244	1.49237
Fe	-0.22428	-0.39143	-0.99420
N	0.18399	-0.65508	1.03790
H	-5.51136	0.73511	1.96260
C	-2.74864	0.12090	0.03342
C	1.22966	-1.50379	3.50432
H	1.63297	-1.84295	4.45426
C	-4.01969	-0.10657	0.63023
C	-0.60808	-1.08816	2.01346
C	-0.12815	-1.50012	3.27157
N	-2.11344	-0.86057	-0.68309
H	-1.66855	-1.12488	1.80437
H	-0.83445	-1.82814	4.02600
C	-4.65957	-1.34006	0.34560
C	-2.73172	-2.01099	-0.92873
H	-5.64154	-1.54146	0.76444
H	-2.17793	-2.74667	-1.49995
C	-4.02906	-2.27618	-0.45077
H	-4.49856	-3.22404	-0.68911
O	-0.40126	-0.16685	-2.74151
H	-0.38329	-1.02923	-3.19647
N	0.35873	-2.17464	-1.21523
C	0.81527	-3.27288	-1.19477
S	1.42774	-4.76227	-1.18156

^{6}FeN4PyBr
Charge: 2+
Energy: -3138118.5743244

Fe	0.05780	-0.00029	0.53755
N	-0.15898	-0.00012	-1.69477
N	-1.52336	1.42903	0.16920
N	-1.52397	-1.42881	0.16913
N	1.50785	1.45741	-0.02656
N	1.50775	-1.45796	-0.02682
C	-1.90298	2.43837	0.96918
C	-2.94393	3.29612	0.61617
C	-3.59842	3.09440	-0.59904
C	-3.19863	2.03933	-1.42910
C	-2.15687	1.22567	-1.00665
C	-1.65756	0.00020	-1.76220
C	-2.15741	-1.22508	-1.00671
C	-3.19957	-2.03822	-1.42917
C	-3.59985	-3.09314	-0.59916
C	-2.94543	-3.29524	0.61602
C	-1.90406	-2.43801	0.96906

C	2.42734	1.95591	0.82526
C	3.47000	2.76678	0.39267
C	3.56998	3.05753	-0.96919
C	2.61869	2.53619	-1.84889
C	1.59166	1.74394	-1.34414
C	0.47056	1.23861	-2.22840
C	0.47004	-1.23911	-2.22837
C	1.59153	-1.74421	-1.34449
C	2.61879	-2.53598	-1.84950
C	3.57036	-3.05715	-0.96999
C	3.47040	-2.76673	0.39194
C	2.42749	-1.95632	0.82480
H	-1.36023	2.53902	1.90272
H	-3.23098	4.10011	1.28507
H	-4.41081	3.74773	-0.90198
H	-3.68834	1.85792	-2.38049
H	-2.02353	0.00030	-2.79522
H	-3.68922	-1.85652	-2.38054
H	-4.41256	-3.74606	-0.90212
H	-3.23285	-4.09913	1.28488
H	-1.36134	-2.53898	1.90258
H	2.30572	1.68403	1.86750
H	4.18675	3.15316	1.10901
H	4.37721	3.67968	-1.34329
H	2.66987	2.74717	-2.91253
H	2.66994	-2.74673	-2.91318
H	4.37779	-3.67893	-1.34430
H	4.18735	-3.15302	1.10813
H	2.30588	-1.68469	1.86711
H	0.82816	1.07987	-3.25137
H	-0.29393	2.01968	-2.28217
H	0.82705	-1.08083	-3.25162
H	-0.29459	-2.02009	-2.28134
Br	0.14006	-0.00047	2.93042

^{6}FeN4PyCl
Charge: 2+
Energy: -1811590.5736448

Fe	0.06275	-0.00028	0.77275
N	-0.13554	-0.00022	-1.47551
N	-1.51052	1.42196	0.38548
N	-1.51109	-1.42179	0.38554
N	1.50627	1.45575	0.21198
N	1.50619	-1.45633	0.21186
C	-1.89310	2.42350	1.19289
C	-2.93182	3.28426	0.84030
C	-3.57812	3.09212	-0.38102
C	-3.17505	2.04277	-1.21727
C	-2.13661	1.22496	-0.79500
C	-1.63383	0.00007	-1.55034
C	-2.13713	-1.22455	-0.79493
C	-3.17596	-2.04190	-1.21713
C	-3.57948	-3.09104	-0.38082
C	-2.93324	-3.28342	0.84049
C	-1.89411	-2.42313	1.19301
C	2.40864	1.95316	1.08200
C	3.45241	2.77272	0.66902
C	3.56990	3.07147	-0.68997
C	2.63509	2.54989	-1.58739
C	1.60557	1.74862	-1.10242
C	0.49853	1.23908	-2.00242
C	0.49806	-1.23982	-2.00229
C	1.60548	-1.74903	-1.10260
C	2.63525	-2.54985	-1.58775
C	3.57034	-3.07119	-0.69046
C	3.45284	-2.77266	0.66857
C	2.40881	-1.95351	1.08174
H	-1.35451	2.51393	2.13024
H	-3.22352	4.08296	1.51351
H	-4.38806	3.74852	-0.68391
H	-3.66030	1.86894	-2.17236
H	-1.99624	0.00012	-2.58460
H	-3.66116	-1.86790	-2.17222
H	-4.38973	-3.74708	-0.68366
H	-3.22527	-4.08196	1.51374
H	-1.35553	-2.51376	2.13034
H	2.27083	1.67217	2.12009
H	4.15679	3.15950	1.39731
H	4.37883	3.70052	-1.04859
H	2.70119	2.76751	-2.64887
H	2.70134	-2.76733	-2.64926
H	4.37948	-3.69988	-1.04923
H	4.15742	-3.15928	1.39676
H	2.27099	-1.67270	2.11987
H	0.87166	1.07977	-3.01974
H	-0.26683	2.01842	-2.06898
H	0.87061	-1.08104	-3.01990
H	-0.26745	-2.01907	-2.06799
Cl	0.16331	-0.00035	2.97786

^{6}FeN4PyF
Charge: 2+
Energy: -1585464.6908921

Fe	-0.07427	-0.00028	-0.89306
N	0.13113	-0.00025	1.37575
N	1.50343	1.41827	-0.51646
N	1.50389	-1.41818	-0.51658
N	-1.49239	1.45952	-0.31449
N	-1.49242	-1.46004	-0.31439
C	1.88137	2.42280	-1.32256
C	2.91609	3.28847	-0.97032
C	3.56083	3.09983	0.25246
C	3.16054	2.04976	1.08905
C	2.12742	1.22520	0.66609
C	1.63021	-0.00001	1.42738
C	2.12786	-1.22496	0.66597
C	3.16134	-2.04914	1.08879
C	3.56202	-3.09896	0.25209
C	2.91731	-3.28775	-0.97068
C	1.88222	-2.42248	-1.32280
C	-2.37875	1.95316	-1.20189
C	-3.41424	2.79208	-0.80755
C	-3.53557	3.10941	0.54771
C	-2.61626	2.58701	1.46114
C	-1.59401	1.76534	0.99466
C	-0.49954	1.24041	1.90465
C	-0.49914	-1.24118	1.90450
C	-1.59403	-1.76570	0.99482
C	-2.61658	-2.58688	1.46147
C	-3.53620	-3.10899	0.54817
C	-3.41486	-2.79185	-0.80712
C	-2.37906	-1.95339	-1.20165
H	1.34119	2.51509	-2.25943
H	3.20473	4.08874	-1.64295
H	4.36688	3.76042	0.55663
H	3.64404	1.88045	2.04584
H	2.01102	0.00001	2.45512
H	3.64481	-1.87972	2.04558
H	4.36836	-3.75926	0.55615
H	3.20625	-4.08784	-1.64341
H	1.34203	-2.51489	-2.25965
H	-2.23060	1.64667	-2.23219
H	-4.11003	3.17884	-1.54403
H	-4.33868	3.75386	0.89183
H	-2.69002	2.81867	2.51915
H	-2.69034	-2.81842	2.51951
H	-4.33956	-3.75306	0.89243
H	-4.11088	-3.17840	-1.54351
H	-2.23090	-1.64706	-2.23199
H	-0.88679	1.07835	2.91622
H	0.27020	2.01425	1.98670
H	-0.88579	-1.07963	2.91639
H	0.27071	-2.01500	1.98568
F	-0.37721	-0.00034	-2.62594

^{6}FeN4PyN$_3$
Charge: 2+
Energy: -1625852.8655326

Fe	0.06480	-0.00044	0.67749
N	-0.10218	-0.00018	-1.57590
N	-1.51939	1.43793	0.24672
N	-1.52026	-1.43765	0.24658
N	1.52905	1.45667	0.12585
N	1.52893	-1.45753	0.12541
C	-1.92043	2.45723	1.02161
C	-2.95003	3.31374	0.63456
C	-3.57150	3.10010	-0.59613
C	-3.14821	2.03781	-1.40389
C	-2.11878	1.22691	-0.94440
C	-1.59651	0.00028	-1.68365
C	-2.11958	-1.22607	-0.94449
C	-3.14961	-2.03618	-1.40399
C	-3.57362	-3.09824	-0.59632
C	-2.95224	-3.31245	0.63432
C	-1.92200	-2.45673	1.02140
C	2.43191	1.94742	0.99696
C	3.49060	2.75127	0.59105
C	3.62224	3.04182	-0.76866
C	2.68823	2.52689	-1.66991
C	1.64460	1.74076	-1.18797
C	0.54078	1.23677	-2.09613
C	0.54007	-1.23746	-2.09617
C	1.64442	-1.74119	-1.18855
C	2.68836	-2.52663	-1.67089
C	3.62277	-3.04137	-0.76992
C	3.49119	-2.75131	0.58989
C	2.43216	-1.94810	0.99621
H	-1.39785	2.57521	1.96510
H	-3.25254	4.12645	1.28589
H	-4.37404	3.75137	-0.92827
H	-3.60915	1.84914	-2.36821
H	-1.93776	0.00042	-2.72549
H	-3.61047	-1.84709	-2.36826
H	-4.37665	-3.74891	-0.92847
H	-3.25529	-4.12501	1.28559

H	-1.39945	-2.57519	1.96484
H	2.28368	1.67131	2.03534
H	4.19511	3.13229	1.32225
H	4.44197	3.65854	-1.12411
H	2.76605	2.73681	-2.73217
H	2.76611	-2.73620	-2.73321
H	4.44276	-3.65756	-1.12569
H	4.19599	-3.13222	1.32086
H	2.28397	-1.67239	2.03471
H	0.92031	1.07967	-3.11173
H	-0.21987	2.02040	-2.16571
H	0.91879	-1.08094	-3.11217
H	-0.22082	-2.02095	-2.16469
N	0.13272	-0.00070	2.53047
N	-0.08050	-0.00095	3.72600
N	-0.27333	-0.00118	4.85618

^{6}FeN4PyNCS
Charge: 2+
Energy: -1830961.1271671

Fe	0.07626	-0.00056	0.48039
N	-0.26473	0.00094	-1.75951
N	-1.53548	1.43247	0.17869
N	-1.53601	-1.43250	0.17694
N	1.48997	1.45986	-0.18957
N	1.48999	-1.46005	-0.19160
C	-1.87577	2.44515	0.99022
C	-2.93225	3.30333	0.68811
C	-3.64521	3.09765	-0.49332
C	-3.28592	2.04024	-1.33794
C	-2.22455	1.22685	-0.96384
C	-1.76290	0.00121	-1.74487
C	-2.22502	-1.22520	-0.96532
C	-3.28676	-2.03767	-1.34036
C	-3.64650	-3.09592	-0.49699
C	-2.93361	-3.30333	0.68418
C	-1.87674	-2.44599	0.98728
C	2.45499	1.95186	0.61117
C	3.47799	2.75805	0.12589
C	3.50497	3.04918	-1.23980
C	2.50594	2.53299	-2.06771
C	1.50365	1.74458	-1.50798
C	0.33387	1.23825	-2.32830
C	0.33341	-1.23594	-2.32971
C	1.50361	-1.74293	-1.51042
C	2.50615	-2.53012	-2.07139
C	3.50551	-3.04704	-1.24432
C	3.47859	-2.75785	0.12177
C	2.45531	-1.95276	0.60832
H	-1.28386	2.55286	1.89319
H	-3.18517	4.11105	1.36621
H	-4.47063	3.75083	-0.75903
H	-3.82034	1.85699	-2.26464
H	-2.18853	0.00190	-2.75522
H	-3.82114	-1.85307	-2.26682
H	-4.47222	-3.74841	-0.76345
H	-3.18687	-4.11174	1.36132
H	-1.28485	-2.55504	1.89011
H	2.38584	1.67546	1.65777
H	4.23541	3.14043	0.80136
H	4.29409	3.66756	-1.65638
H	2.50215	2.74366	-3.13266
H	2.50230	-2.73931	-3.13663
H	4.29484	-3.66450	-1.66187
H	4.23625	-3.14086	0.79661
H	2.38618	-1.67786	1.65532
H	0.63429	1.08187	-3.37019
H	-0.43108	2.02081	-2.33904
H	0.63318	-1.07877	-3.37167
H	-0.43161	-2.01843	-2.34053
N	0.32188	-0.00188	2.33282
C	0.42341	-0.00279	3.53971
S	0.56105	-0.00396	5.11160

^{2}FeN4PyOH
Charge: 2+
Energy: -1570381.1011888

Fe	0.03296	-0.00030	-0.62377
N	-0.15551	-0.00012	1.40560
N	-1.41625	-1.35844	-0.49373
N	-1.41697	1.35766	-0.49423
N	1.43420	-1.35298	-0.29957
N	1.43329	1.35333	-0.29961
O	0.23978	-0.00173	-2.39542
C	-1.69413	-2.36240	-1.33708
C	-2.71460	-3.27312	-1.06438
C	-3.44430	-3.13606	0.11713
C	-3.13942	-2.09164	0.99988
C	-2.11732	-1.21963	0.65552
C	-1.67002	-0.00034	1.45020
C	-2.11773	1.21866	0.65522
C	-3.13994	2.09041	0.99995
C	-3.44534	3.13488	0.11746
C	-2.71588	3.27234	-1.06415
C	-1.69528	2.36185	-1.33716
C	2.29035	-1.80150	-1.23337
C	3.32523	-2.67340	-0.90882
C	3.47629	-3.07428	0.41982
C	2.58248	-2.60004	1.38342
C	1.56193	-1.74185	0.98748
C	0.48821	-1.24694	1.93398
C	0.48768	1.24695	1.93405
C	1.56074	1.74273	0.98730
C	2.58049	2.60207	1.38285
C	3.47378	3.07682	0.41903
C	3.32306	2.67529	-0.90946
C	2.28900	1.80230	-1.23364
H	-1.07999	-2.41493	-2.22954
H	-2.92629	-4.07175	-1.76692
H	-4.23954	-3.83527	0.35606
H	-3.68296	-1.96517	1.93056
H	-2.06490	-0.00024	2.47097
H	-3.68317	1.96370	1.93078
H	-4.24070	3.83386	0.35669
H	-2.92781	4.07108	-1.76649
H	-1.08130	2.41512	-2.22970
H	2.11232	-1.43483	-2.23803
H	3.99967	-3.02136	-1.68355
H	4.28005	-3.74569	0.70545
H	2.67395	-2.89563	2.42387
H	2.67175	2.89809	2.42320
H	4.27690	3.74912	0.70437
H	3.99716	3.02357	-1.68433
H	2.11131	1.43495	-2.23811
H	0.88857	-1.07673	2.93776
H	-0.28133	-2.01914	2.02684
H	0.88858	1.07665	2.93759
H	-0.28227	2.01868	2.02752
H	-0.60801	0.00279	-2.87402

^{6}FeTMCBr
Charge: 2+
Energy: -2892574.0507313

Fe	-0.00001	0.00001	0.11306
H	-3.37555	-1.16037	-2.64127
H	-1.72725	-2.82382	-2.23529
H	-1.76625	-3.57287	0.06241
H	-3.44692	-1.48469	-0.93516
C	-2.81604	-1.03589	-1.70683
H	-2.12417	-2.01756	0.85571
C	-1.51070	-1.80488	-1.88782
C	-1.33571	-2.63745	0.43869
H	0.38676	-3.76881	-0.97885
H	-3.29067	-0.46399	0.95959
H	-0.90749	-1.31764	-2.66331
H	-3.60432	0.97768	-1.61766
H	-0.62774	-2.85671	1.23713
N	-0.63372	-1.91893	-0.67195
H	-3.97553	1.15032	0.70282
C	-2.63822	0.46817	-1.50370
C	0.59608	-2.69531	-1.05003
H	0.82222	-2.48659	-2.09670
C	-3.05152	0.59531	0.90567
H	-1.97976	0.84559	-2.29107
H	1.54895	-2.59851	0.88560
N	-2.05624	0.86509	-0.17864
H	-2.64311	0.90796	1.86495
C	1.76570	-2.33488	-0.15264
H	2.65664	-2.89974	-0.45651
H	-2.65672	2.89983	-0.45580
C	-1.76577	2.33491	-0.15208
H	1.97910	-0.84505	-2.29141
N	2.05614	-0.86506	-0.17900
H	-0.82246	2.48689	-2.09618
H	-1.54896	2.59839	0.88618
H	2.64351	-0.90851	1.86443
C	-0.59622	2.69548	-1.04951
C	2.63783	-0.46791	-1.50412
H	0.90725	1.31839	-2.66325
H	3.60383	-0.97752	-1.61845
C	3.05160	-0.59538	0.90516
H	3.97573	-1.15005	0.70190
N	0.63364	1.91907	-0.67168
H	-0.38692	3.76897	-0.97823
C	1.51054	1.80534	-1.88763
H	0.62791	2.85629	1.23769
C	2.81581	1.03618	-1.70694
H	3.29043	0.46397	0.95944
H	3.37523	1.16081	-2.64142
C	1.33573	2.63736	0.43904
H	1.72715	2.82436	-2.23480
H	2.12438	2.01746	0.85570
H	3.44682	1.48474	-0.93524
H	1.76607	3.57297	0.06295
Br	0.00024	-0.00029	2.48971

^{6}FeTMCCl
Charge: 2+
Energy: -1566046.5803286

Fe	0.00001	-0.00001	0.36441
H	3.41830	1.17020	-2.35180
H	1.74935	2.81699	-1.97401
H	1.74917	3.56363	0.33841
H	3.45739	1.49148	-0.64427
C	2.84382	1.03855	-1.42745
H	2.11102	2.00278	1.11955
C	1.53514	1.79683	-1.62871
C	1.32247	2.62081	0.70002
H	-0.37456	3.75326	-0.77245
H	3.28474	0.44352	1.23438
H	0.94630	1.30469	-2.41207
H	3.65346	-0.96428	-1.31049
H	0.60433	2.82459	1.49343
N	0.63983	1.90757	-0.42597
H	3.92969	-1.19473	1.03774
C	2.67746	-0.46741	-1.23007
C	-0.58725	2.67903	-0.82112
H	-0.81199	2.44683	-1.86339
C	3.01537	-0.60920	1.19298
H	2.05110	-0.85438	-2.03871
H	-1.54189	2.61653	1.11606
N	2.05677	-0.87108	0.07437
H	2.55807	-0.88923	2.14033
C	-1.75900	2.33914	0.08165
H	-2.64690	2.90442	-0.22992
H	2.64691	-2.90444	-0.22990
C	1.75903	-2.33915	0.08169
H	-2.05070	0.85427	-2.03875
N	-2.05671	0.87106	0.07432
H	0.81198	-2.44685	-1.86331
H	1.54196	-2.61654	1.11611
H	-2.55825	0.88934	2.14020
C	0.58724	-2.67905	-0.82104
C	-2.67724	0.46740	-1.23019
H	-0.94628	-1.30497	-2.41212
H	-3.65317	0.96438	-1.31079
C	-3.01537	0.60909	1.19284
H	-3.92983	1.19435	1.03742
N	-0.63985	-1.90757	-0.42594
H	0.37455	-3.75328	-0.77237
C	-1.53515	-1.79695	-1.62869
H	-0.60456	-2.82426	1.49365
C	-2.84375	-1.03855	-1.42751
H	-3.28444	-0.44371	1.23435
H	-3.41821	-1.17019	-2.35186
C	-1.32258	-2.62071	0.70008
H	-1.74943	-2.81715	-1.97384
H	-2.11128	-2.00269	1.11934
H	-3.45739	-1.49137	-0.64431
H	-1.74912	-3.56364	0.33856
Cl	-0.00011	0.00011	2.54564

^{6}FeTMCF
Charge: 2+
Energy: -1339923.3402316

Fe	0.00000	-0.00002	0.44099
H	3.62905	1.08579	-2.04812
H	1.97198	2.76308	-1.78210
H	1.75372	3.54177	0.53102
H	3.54334	1.38200	-0.33913
C	2.98128	0.95413	-1.17349
H	2.15582	1.96946	1.26483
C	1.70862	1.74616	-1.46240
C	1.35376	2.57110	0.84637
H	-0.21196	3.71174	-0.84784
H	3.18768	0.25938	1.48936
H	1.16516	1.27527	-2.29008
H	3.74985	-1.05544	-0.97812
H	0.61018	2.71886	1.62889
N	0.73485	1.87018	-0.32304
H	3.67491	-1.44309	1.43575
C	2.77521	-0.55075	-1.01177
C	-0.45997	2.64460	-0.79960
H	-0.68144	2.31783	-1.81824
C	2.81570	-0.76199	1.44144
H	2.24625	-0.92932	-1.89158
H	-1.44175	2.77214	1.12441
N	1.99960	-0.96481	0.20343
H	2.19436	-0.94821	2.31690
C	-1.65378	2.42048	0.11262
H	-2.51809	2.98969	-0.25150
H	2.51813	-2.98969	-0.25143
C	1.65380	-2.42047	0.11265
H	-2.24645	0.92948	-1.89156
N	-1.99960	0.96482	0.20343
H	0.68147	-2.31799	-1.81823
H	1.44175	-2.77209	1.12446
H	-2.19427	0.94805	2.31692
C	0.45999	-2.64466	-0.79956
C	-2.77529	0.55078	-1.01173
H	-1.16494	-1.27486	-2.29003
H	-3.74997	1.05537	-0.97794
C	-2.81567	0.76200	1.44146
H	-3.67480	1.44321	1.43587
N	-0.73483	-1.87018	-0.32306
H	0.21197	-3.71181	-0.84770
C	-1.70847	-1.74597	-1.46251
H	-0.61033	-2.71948	1.62859
C	-2.98121	-0.95410	-1.17354
H	-3.18779	-0.25933	1.48928
H	-3.62900	-1.08577	-2.04816
C	-1.35395	-2.57112	0.84622
H	-1.97172	-2.76284	-1.78247
H	-2.15564	-1.96919	1.26497
H	-3.54318	-1.38210	-0.33917
H	-1.75443	-3.54151	0.53064
F	-0.00002	-0.00010	2.18707

^{6}FeTMCN$_3$
Charge: 2+
Energy: -1380310.9696918

Fe	0.00007	-0.00040	0.21720
H	3.52009	1.15280	-2.40588
H	1.85396	2.80574	-2.08588
H	1.74861	3.58624	0.20557
H	3.49494	1.44540	-0.69368
C	2.90736	1.01228	-1.50774
H	2.13109	2.03128	0.98574
C	1.61518	1.78836	-1.74803
C	1.33439	2.63343	0.55644
H	-0.31071	3.74438	-1.02050
H	3.20711	0.36059	1.17120
H	1.04774	1.30375	-2.55150
H	3.69790	-0.99645	-1.38581
H	0.60154	2.82459	1.34009
N	0.68283	1.90523	-0.57475
H	3.86290	-1.27432	0.96833
C	2.72156	-0.49510	-1.34197
C	-0.53017	2.66990	-1.01836
H	-0.74504	2.38723	-2.05074
C	2.94134	-0.69116	1.08700
H	2.13183	-0.86587	-2.18526
H	-1.51337	2.69929	0.90429
N	2.03552	-0.91714	-0.07743
H	2.43725	-0.99733	2.00307
C	-1.72049	2.38131	-0.12029
H	-2.59568	2.94771	-0.46445
H	2.59808	-2.94407	-0.47477
C	1.72175	-2.37988	-0.12984
H	-2.12367	0.88015	-2.18660
N	-2.03448	0.91827	-0.07818
H	0.75258	-2.37350	-2.06348
H	1.51134	-2.70440	0.89202
H	-2.44335	0.98613	2.00136
C	0.53438	-2.66277	-1.03363
C	-2.71629	0.50421	-1.34764
H	-1.03886	-1.28729	-2.56318
H	-3.69242	1.00594	-1.39165
C	-2.94414	0.68504	1.08180
H	-3.86556	1.26850	0.96346
N	-0.68009	-1.90098	-0.58905
H	0.31496	-3.73721	-1.04334
C	-1.60881	-1.77679	-1.76448
H	-0.60466	-2.83208	1.32030
C	-2.90168	-1.00209	-1.52343
H	-3.20974	-0.36729	1.15894
H	-3.51153	-1.13691	-2.42440
C	-1.33507	-2.63631	0.53550
H	-1.84660	-2.79204	-2.10934
H	-2.13340	-2.03710	0.96590
H	-3.49192	-1.44025	-0.71401
H	-1.74783	-3.58709	0.17747
N	-0.00283	-0.00591	2.04631
N	-0.00883	-0.01286	3.26064
N	-0.01428	-0.01930	4.40640

^{6}FeTMCNCS
Charge: 2+
Energy: -1585420.7873553

Fe	-0.00362	-0.00007	-0.00007
H	-2.61668	3.52934	1.15888
H	-2.30298	1.85777	2.80835
H	-0.00818	1.72990	3.58492
H	-0.90482	3.49440	1.45287
C	-1.72152	2.91256	1.01701
H	0.76544	2.11885	2.02785
C	-1.96890	1.61941	1.78956
C	0.33576	1.32038	2.62746
H	-1.25960	-0.31742	3.73549

H	0.95227	3.21590	0.36413
H	-2.77736	1.05915	1.30511
H	-1.59313	3.71029	-0.98831
H	1.11817	0.58376	2.80859
N	-0.80206	0.67900	1.90109
H	0.76750	3.85830	-1.27818
C	-1.55437	2.73156	-0.49099
C	-1.25108	-0.53472	2.66050
H	-2.28192	-0.74767	2.37053
C	0.87575	2.94107	-0.68597
H	-2.40007	2.14735	-0.86519
H	0.67019	-1.52109	2.69907
N	-0.29287	2.04129	-0.91303
H	1.79081	2.42689	-0.97727
C	-0.35295	-1.72635	2.37539
H	-0.70170	-2.60101	2.93999
H	-0.69014	2.60447	-2.93972
C	-0.34542	1.72807	-2.37534
H	-2.41050	-2.13530	0.86641
N	-0.30276	-2.03987	0.91307
H	-2.27929	0.75914	-2.36960
H	0.67651	1.51775	-2.69962
H	1.77897	-2.43605	0.97629
C	-1.24967	0.54095	-2.66000
C	-1.56797	-2.72376	0.49170
H	-2.78340	-1.04506	-1.30377
H	-1.61138	-3.70230	0.98899
C	0.86116	-2.94558	0.68547
H	0.74856	-3.86222	1.27777
N	-0.80647	-0.67502	-1.90072
H	-1.25975	0.32364	-3.73497
C	-1.97805	-1.60943	-1.78864
H	1.11385	-0.58958	-2.80892
C	-1.73691	-2.90387	-1.01623
H	0.93577	-3.22087	-0.36465
H	-2.63530	-3.51604	-1.15759
C	0.32775	-1.32219	-2.62757
H	-2.31387	-1.84604	-2.80727
H	0.75354	-2.12291	-2.02820
H	-0.92344	-3.48988	-1.45254
H	-0.01865	-1.72987	-3.58494
N	1.83855	-0.00473	-0.00044
C	3.05131	-0.00757	-0.00060
S	4.62530	-0.01124	-0.00081

^{6}FeTMCOH
Charge: 2+
Energy: -1324840.0894085

Fe	-0.00089	-0.00108	0.48697
H	3.56176	1.14868	-2.10486
H	1.88775	2.79784	-1.79870
H	1.75534	3.56046	0.50906
H	3.51424	1.43713	-0.39287
C	2.93786	1.00410	-1.21509
H	2.13609	1.99577	1.26526
C	1.64704	1.77811	-1.46952
C	1.33922	2.60162	0.84055
H	-0.27548	3.73330	-0.77552
H	3.22024	0.31934	1.45168
H	1.08964	1.29697	-2.28168
H	3.73408	-1.00005	-1.06404
H	0.59869	2.78490	1.61965
N	0.69942	1.88980	-0.30715
H	3.79304	-1.35068	1.31524
C	2.75427	-0.50380	-1.05368
C	-0.50725	2.66151	-0.75770
H	-0.72618	2.36404	-1.78518
C	2.89911	-0.71868	1.38422
H	2.19445	-0.88028	-1.91461
H	-1.48954	2.72093	1.16840
N	2.03012	-0.92577	0.18826
H	2.33678	-0.97669	2.28097
C	-1.69812	2.39447	0.14678
H	-2.56843	2.96570	-0.20117
H	2.56770	-2.95321	-0.23290
O	-0.05584	-0.15435	2.25856
C	1.69709	-2.38430	0.11804
H	-2.19241	0.92080	-1.90393
N	-2.02493	0.93533	0.20050
H	0.72914	-2.32556	-1.81571
H	1.47983	-2.71809	1.13487
H	-2.32500	0.91590	2.29837
C	0.50879	-2.63755	-0.79261
C	-2.74990	0.53012	-1.04767
H	-1.07976	-1.24653	-2.29719
H	-3.73033	1.02524	-1.04762
C	-2.89411	0.70544	1.39428
H	-3.77842	1.35227	1.34401
N	-0.69979	-1.87684	-0.33143
H	0.27962	-3.70947	-0.82585
C	-1.64031	-1.74304	-1.49614
H	-0.61279	-2.78914	1.58803
C	-2.93238	-0.97482	-1.23296
H	-3.22501	-0.33015	1.43187
H	-3.55460	-1.10471	-2.12617
C	-1.34478	-2.61109	0.80180
H	-1.87960	-2.75621	-1.84582
H	-2.14392	-2.01362	1.23155
H	-3.50912	-1.42112	-0.41851
H	-1.75045	-3.56570	0.44686
H	0.29938	0.29452	3.04374

^{6}Fe13TMCBr
Charge: 2+
Energy: -2867893.7550729

Fe	-0.06141	-0.02843	0.12384
N	-1.90941	0.88206	-0.72946
N	0.73957	1.96785	-0.09373
N	1.86777	-1.02457	-0.14073
N	-0.75303	-1.66164	-1.13193
C	1.30182	2.44612	1.20815
C	-0.42277	2.84710	-0.46767
C	-1.39104	2.11944	-1.38734
C	-2.91326	1.21705	0.32649
C	1.77673	2.03954	-1.18285
C	2.97637	1.10459	-1.03509
C	2.66981	-0.37903	-1.23446
C	2.66337	-1.07844	1.12516
C	-1.46278	-1.00375	-2.26764
C	-2.51803	-0.04222	-1.74053
C	-1.66700	-2.53017	-0.32696
C	0.42823	-2.45074	-1.59862
C	1.50644	-2.43042	-0.52507
H	-2.16786	-3.25323	-0.98160
H	-1.08902	-3.06152	0.42868
H	-2.41002	-1.92699	0.19234
H	2.09025	-1.59885	1.89116
H	3.60879	-1.60543	0.94933
H	2.87955	-0.07445	1.48333
H	1.64714	3.48202	1.10877
H	0.53119	2.38598	1.97652
H	2.13817	1.82126	1.51297
H	-0.05503	3.76176	-0.94686
H	-0.92252	3.14742	0.45428
H	-2.46820	1.86044	1.08426
H	-3.77716	1.72179	-0.12208
H	-3.23817	0.30055	0.81880
H	-0.89461	1.82548	-2.31681
H	-2.22394	2.78093	-1.65763
H	-2.95933	0.52915	-2.56494
H	-3.33346	-0.58613	-1.26248
H	0.13236	-3.48298	-1.81713
H	0.78731	-2.01798	-2.53429
H	2.40030	-2.96788	-0.86558
H	1.14850	-2.92745	0.37988
H	2.11598	-0.49814	-2.17027
H	3.60769	-0.94032	-1.33887
H	3.67672	1.38332	-1.83123
H	3.51977	1.28695	-0.10453
H	1.26907	1.82605	-2.12962
H	2.12914	3.07808	-1.23128
H	-0.70844	-0.46296	-2.85020
H	-1.91712	-1.75365	-2.92788
Br	-0.60634	-0.44555	2.38465

^{6}Fe13TMCCl
Charge: 2+
Energy: -1541365.8122246

Fe	-0.07692	-0.03422	0.39619
N	-2.05400	0.69174	-0.32297
N	0.58047	1.94723	-0.15121
N	1.85758	-0.97745	0.01198
N	-0.82224	-1.82777	-0.57312
C	1.24918	2.58562	1.02555
C	-0.65927	2.73163	-0.48675
C	-1.69156	1.85824	-1.18250
C	-2.91507	1.11006	0.82498
C	1.49024	1.93201	-1.35058
C	2.75046	1.07549	-1.23275
C	2.51365	-0.43405	-1.22458
C	2.76988	-0.85073	1.19100
C	-1.71054	-1.35048	-1.67271
C	-2.73961	-0.37119	-1.12649
C	-1.56982	-2.62104	0.45145
C	0.33555	-2.61589	-1.09529
C	1.53019	-2.43128	-0.17111
H	-2.10298	-3.44785	-0.03236
H	-0.86887	-3.01780	1.18529
H	-2.27721	-1.98792	0.98466
H	2.28096	-1.26433	2.07217
H	3.70514	-1.38956	0.99783
H	2.99950	0.19444	1.38558
H	1.52031	3.62074	0.78686
H	0.56914	2.56774	1.87748
H	2.14812	2.03629	1.29514

H	-0.39519	3.58786	-1.11777
H	-1.06157	3.13298	0.44425
H	-2.39925	1.84783	1.43819
H	-3.85697	1.53249	0.45556
H	-3.12126	0.24446	1.45440
H	-1.29789	1.47175	-2.12737
H	-2.58723	2.44709	-1.41810
H	-3.31234	0.07748	-1.94589
H	-3.45734	-0.88069	-0.48263
H	0.07147	-3.67720	-1.16552
H	0.55764	-2.27434	-2.10821
H	2.40546	-2.96684	-0.55923
H	1.30988	-2.83702	0.81915
H	1.88221	-0.69418	-2.07916
H	3.46917	-0.95883	-1.35551
H	3.34498	1.28802	-2.12909
H	3.37818	1.39361	-0.39650
H	0.89597	1.58521	-2.20300
H	1.77673	2.97154	-1.55653
H	-1.07065	-0.85947	-2.41432
H	-2.20395	-2.19668	-2.16774
Cl	-0.31497	-0.18846	2.54750

^{6}Fe13TMCF
Charge: 2+
Energy: -1315240.3587762

Fe	0.08056	0.03217	0.50422
N	2.05073	-0.71130	-0.13751
N	-0.58512	-1.92661	-0.08316
N	-1.81705	1.01863	0.11666
N	0.88845	1.82844	-0.38881
C	-1.24203	-2.55704	1.10469
C	0.64062	-2.72467	-0.44543
C	1.71389	-1.83733	-1.05872
C	2.79530	-1.18060	1.07003
C	-1.51181	-1.88143	-1.26927
C	-2.76536	-1.01892	-1.11694
C	-2.53389	0.49182	-1.09293
C	-2.66687	0.90079	1.34324
C	1.85712	1.38535	-1.43413
C	2.82007	0.35864	-0.85117
C	1.55823	2.58844	0.71161
C	-0.24027	2.61859	-0.96678
C	-1.47021	2.46705	-0.08216
H	2.09855	3.44821	0.29888
H	0.81140	2.93595	1.42506
H	2.25124	1.94498	1.25222
H	-2.08304	1.20032	2.21452
H	-3.55351	1.53843	1.24814
H	-2.99031	-0.12867	1.48248
H	-1.51254	-3.59535	0.88055
H	-0.55443	-2.52849	1.95172
H	-2.14013	-2.00744	1.37713
H	0.36827	-3.52750	-1.13919
H	1.01056	-3.20230	0.46252
H	2.20493	-1.91248	1.62048
H	3.75246	-1.62764	0.77715
H	2.97064	-0.33382	1.73408
H	1.36427	-1.40485	-2.00164
H	2.61153	-2.42860	-1.28080
H	3.43889	-0.07734	-1.64327
H	3.50191	0.82443	-0.13870
H	0.03830	3.67507	-1.05644
H	-0.43319	2.24819	-1.97625
H	-2.32534	3.00077	-0.51402
H	-1.28648	2.89522	0.90575
H	-1.94876	0.77516	-1.97319
H	-3.49846	1.01149	-1.16360
H	-3.37883	-1.21908	-2.00339
H	-3.37765	-1.34795	-0.27323
H	-0.92320	-1.52518	-2.12244
H	-1.81117	-2.91424	-1.48979
H	1.27460	0.94371	-2.24975
H	2.40511	2.24285	-1.84480
F	0.23689	0.12571	2.23417

^{6}Fe13TMCN$_3$
Charge: 2+
Energy: -1355629.8687442

Fe	-0.09821	-0.04707	0.23414
N	-1.90322	0.83129	-0.72652
N	0.71259	1.94655	-0.05100
N	1.84442	-1.05200	0.07827
N	-0.74087	-1.72980	-0.99161
C	1.19324	2.47773	1.25989
C	-0.42014	2.80892	-0.53642
C	-1.36448	2.02744	-1.43859
C	-2.90835	1.21919	0.30448
C	1.81401	1.96852	-1.07636
C	3.00744	1.05150	-0.80828
C	2.73474	-0.44402	-0.96570
C	2.53192	-1.07196	1.40342
C	-1.44387	-1.13169	-2.16314
C	-2.50237	-0.14137	-1.69514
C	-1.65148	-2.58089	-0.16994
C	0.46412	-2.50893	-1.40674
C	1.50789	-2.46491	-0.29870
H	-2.12005	-3.35112	-0.79419
H	-1.08019	-3.05902	0.62588
H	-2.42305	-1.97062	0.29844
H	1.86990	-1.52151	2.14367
H	3.46132	-1.65111	1.34247
H	2.76957	-0.05956	1.72440
H	1.54295	3.51118	1.14938
H	0.37450	2.44396	1.97995
H	2.00909	1.86694	1.64087
H	-0.02322	3.68194	-1.06727
H	-0.95285	3.18544	0.33799
H	-2.45950	1.88802	1.03870
H	-3.76803	1.71609	-0.16105
H	-3.24585	0.32407	0.82848
H	-0.83949	1.67786	-2.33284
H	-2.18560	2.67405	-1.77447
H	-2.93547	0.38589	-2.55288
H	-3.32367	-0.65968	-1.19848
H	0.19229	-3.54717	-1.63019
H	0.85204	-2.07524	-2.33083
H	2.41536	-3.00116	-0.60363
H	1.12586	-2.95636	0.59937
H	2.26821	-0.61317	-1.94075
H	3.68548	-0.99374	-0.96269
H	3.76017	1.30650	-1.56358
H	3.48283	1.27879	0.14959
H	1.36413	1.70230	-2.03935
H	2.16706	3.00489	-1.15965
H	-0.68645	-0.62089	-2.76785
H	-1.89568	-1.91217	-2.78898
N	-0.59220	-0.30443	1.96950
N	-0.96015	-0.41340	3.12260
N	-1.30690	-0.51943	4.20866

^{6}Fe13TMCNCS
Charge: 2+
Energy: -1560739.4847512

Fe	0.03431	0.02147	0.01146
N	0.01938	2.20137	-0.44043
N	-0.98537	-0.12427	-1.89820
N	-0.93298	-1.75579	0.86271
N	-0.35508	0.82667	1.99738
C	-0.22794	-1.06139	-2.78087
C	-0.95576	1.24893	-2.51105
C	-1.07181	2.33356	-1.44930
C	1.33529	2.62209	-1.00076
C	-2.41743	-0.56076	-1.75045
C	-2.64983	-1.89131	-1.03364
C	-2.37472	-1.88671	0.46998
C	-0.17392	-2.98528	0.48799
C	-1.06322	2.12164	1.78496
C	-0.29535	2.98771	0.79407
C	0.96223	1.01649	2.67302
C	-1.19423	-0.14843	2.75525
C	-0.82350	-1.56835	2.34706
H	0.83213	1.55971	3.61680
H	1.41046	0.04348	2.87427
H	1.64574	1.56532	2.02588
H	0.87051	-2.86330	0.77556
H	-0.59536	-3.86293	0.99323
H	-0.21657	-3.14527	-0.58771
H	-0.67859	-1.09501	-3.78011
H	0.80643	-0.72302	-2.85580
H	-0.22842	-2.06401	-2.35826
H	-1.76430	1.34763	-3.24456
H	-0.01763	1.35081	-3.05834
H	1.58895	2.01469	-1.86930
H	1.31233	3.67977	-1.29006
H	2.10959	2.46538	-0.24882
H	-2.02766	2.25316	-0.92248
H	-1.04051	3.32516	-1.91953
H	-0.87509	3.88369	0.54400
H	0.64316	3.33291	1.22994
H	-1.05724	-0.01651	3.83498
H	-2.24381	0.06158	2.53857
H	-1.45836	-2.29607	2.86815
H	0.21145	-1.78279	2.62429
H	-2.91983	-1.05285	0.92220
H	-2.76657	-2.80988	0.91778
H	-3.71712	-2.11429	-1.14886
H	-2.13514	-2.71403	-1.53707
H	-2.94355	0.23572	-1.21245
H	-2.85279	-0.61353	-2.75714
H	-2.05806	1.88536	1.39200
H	-1.20064	2.65331	2.73550
N	1.79507	-0.45922	-0.15531
C	2.96302	-0.76752	-0.27870
S	4.47564	-1.16548	-0.43807

^{6}Fe13TMCOH
Charge: 2+
Energy: -1300158.3944165

Fe	0.08584	0.03595	0.54124
N	2.07404	-0.68447	-0.15179
N	-0.57468	-1.92459	-0.09027
N	-1.83421	0.99892	0.11781
N	0.86659	1.84575	-0.37891
C	-1.26498	-2.58996	1.05772
C	0.66605	-2.70655	-0.42406
C	1.72707	-1.81943	-1.05827
C	2.87885	-1.14640	1.01634
O	0.14601	-0.01095	2.30987
C	-1.46281	-1.87439	-1.30335
C	-2.72618	-1.02225	-1.18039
C	-2.49891	0.48804	-1.12687
C	-2.73862	0.85491	1.29911
C	1.80359	1.40231	-1.45194
C	2.80032	0.39258	-0.89668
C	1.56772	2.61165	0.69359
C	-0.27326	2.64155	-0.92720
C	-1.49816	2.45216	-0.04246
H	2.11464	3.45883	0.26287
H	0.83656	2.98459	1.41144
H	2.26554	1.96688	1.22829
H	-2.20867	1.17707	2.19507
H	-3.64361	1.45770	1.15759
H	-3.02614	-0.18579	1.43125
H	-1.51568	-3.62538	0.79897
H	-0.60829	-2.56793	1.92756
H	-2.17772	-2.05590	1.31097
H	0.41361	-3.53568	-1.09496
H	1.04027	-3.14863	0.50029
H	2.31877	-1.87915	1.59603
H	3.82538	-1.58753	0.68172
H	3.08764	-0.29517	1.66586
H	1.36325	-1.39725	-1.99999
H	2.62366	-2.40923	-1.28905
H	3.39957	-0.03576	-1.70809
H	3.49963	0.87440	-0.21193
H	-0.00642	3.70313	-0.98671
H	-0.46727	2.30290	-1.94704
H	-2.35785	2.99541	-0.45427
H	-1.31080	2.85206	0.95711
H	-1.87767	0.77911	-1.97912
H	-3.46022	1.00806	-1.23414
H	-3.30936	-1.21187	-2.08927
H	-3.36328	-1.36525	-0.36113
H	-0.85451	-1.50188	-2.13515
H	-1.74722	-2.90654	-1.54679
H	1.19700	0.94469	-2.24083
H	2.32693	2.26082	-1.89228
H	0.61592	0.34176	3.08324

^{2}Fe13TMCOOCCH33Br
Charge: 1+
Energy: -3061586.4423401

Fe	-0.25444	-0.07659	0.01509
N	-0.39466	-1.53497	1.45778
N	-0.65644	1.28481	1.57168
N	-0.21070	1.24014	-1.58347
N	-0.22541	-1.60147	-1.36845
C	0.55551	1.98154	2.09129
C	-1.23817	0.46103	2.71277
C	-1.43491	-1.03848	2.40900
C	0.86545	-1.75888	2.21801
O	1.48123	0.14202	0.41562
O	2.53769	-0.27520	-0.47157
C	3.83936	0.10956	0.06945
C	4.09041	-0.58473	1.40953
C	-1.62872	2.35674	1.14032
C	-1.28075	3.08338	-0.16623
C	-1.29509	2.27860	-1.47532
C	1.08879	1.96391	-1.70229
C	-1.05700	-2.68372	-0.73463
C	-0.74631	-2.83404	0.76374
C	1.08375	-2.18788	-1.75998
C	-0.88897	-1.00985	-2.57659
C	-0.35851	0.39995	-2.83674
C	4.78143	-0.42732	-1.01370
C	3.95806	1.62962	0.20300
H	0.91240	-3.03443	-2.43650
H	1.69810	-1.44036	-2.25255
H	1.61872	-2.52362	-0.87364
H	1.89133	1.24234	-1.80757
H	1.05734	2.63371	-2.57085
H	1.27935	2.54453	-0.80459
H	0.27939	2.62823	2.93325
H	1.29997	1.25751	2.41116
H	0.99863	2.58837	1.30542
H	-2.20478	0.88114	3.00200
H	-0.57232	0.57836	3.57051
H	1.14584	-0.85365	2.75066
H	0.71511	-2.57124	2.94023
H	1.66916	-2.00970	1.53141
H	-2.40784	-1.20837	1.96133
H	-1.37687	-1.60503	3.34836
H	-1.60190	-3.29891	1.26290
H	0.10515	-3.50434	0.89594
H	-0.69925	-1.63691	-3.45752
H	-1.95931	-0.98274	-2.39643
H	-1.01427	0.91134	-3.54946
H	0.62933	0.33998	-3.29705
H	-2.25184	1.77834	-1.59883
H	-1.16140	2.97907	-2.31148
H	-2.05308	3.85363	-0.28467
H	-0.34268	3.63800	-0.06536
H	-2.60629	1.89437	1.04709
H	-1.67837	3.10120	1.94688
H	-2.10209	-2.43080	-0.87272
H	-0.86419	-3.63980	-1.23712
H	5.10973	-0.37921	1.75127
H	3.39808	-0.22455	2.17453
H	3.97780	-1.66921	1.30981
H	4.95071	1.89086	0.58312
H	3.82690	2.12425	-0.76382
H	3.21433	2.01690	0.90306
H	5.81839	-0.20902	-0.74079
H	4.67403	-1.51130	-1.12139
H	4.57429	0.04457	-1.97968
Br	-3.05940	-0.20836	-0.23440

^{2}Fe13TMCOOCCH33Cl
Charge: 1+
Energy: -1735063.1380731

Fe	0.51548	-0.11508	0.03054
N	0.66641	-1.63668	-1.34531
N	1.04245	1.17083	-1.55767
N	0.44746	1.27444	1.56936
N	0.35301	-1.58327	1.47221
C	-0.10518	1.91882	-2.14387
C	1.61061	0.27468	-2.64755
C	1.76752	-1.20913	-2.26126
C	-0.56480	-1.85048	-2.15239
O	-1.19083	0.15347	-0.46029
O	-2.29916	-0.16668	0.40572
C	-3.55917	0.23099	-0.21349
C	-3.78039	-0.53383	-1.52026
C	2.06556	2.18929	-1.11818
C	1.70998	2.98582	0.14618
C	1.60101	2.23672	1.48461
C	-0.80867	2.07793	1.58478
C	1.17952	-2.71582	0.92606
C	0.94447	-2.91408	-0.58224
C	-0.99357	-2.11047	1.81497
C	0.97277	-0.95847	2.68680
C	0.47175	0.47578	2.85602
C	-4.56839	-0.20315	0.85520
C	-3.61173	1.74373	-0.44238
H	-0.88901	-2.93459	2.53192
H	-1.60771	-1.32428	2.24281
H	-1.49215	-2.46412	0.91416
H	-1.65759	1.40847	1.66726
H	-0.78711	2.77890	2.42893
H	-0.91201	2.63329	0.65715
H	0.23655	2.51867	-2.99673
H	-0.87946	1.22687	-2.46466
H	-0.53927	2.57728	-1.39545
H	2.58643	0.65717	-2.95952
H	0.94964	0.35843	-3.51276
H	-0.79685	-0.95597	-2.72486
H	-0.41034	-2.69175	-2.84009
H	-1.40408	-2.05274	-1.49266
H	2.71083	-1.37285	-1.75261
H	1.74778	-1.81947	-3.17459
H	1.81126	-3.42143	-1.01653
H	0.08307	-3.56740	-0.73411
H	0.71725	-1.53831	3.58342
H	2.05110	-0.97059	2.56217
H	1.08475	0.99332	3.60229
H	-0.55072	0.46063	3.23765
H	2.51494	1.68340	1.68200
H	1.46679	2.97987	2.28321
H	2.52755	3.70604	0.27599
H	0.81949	3.59949	-0.02190
H	3.00423	1.66625	-0.96544
H	2.19952	2.90033	-1.94543
H	2.22349	-2.49397	1.11418
H	0.92395	-3.64520	1.45027
H	-4.77623	-0.31471	-1.91826
H	-3.04325	-0.24486	-2.27343
H	-3.71170	-1.61351	-1.35145
H	-4.57481	2.01869	-0.88406
H	-3.50430	2.29081	0.49888

H	-2.82137	2.05965	-1.12691
H	-5.58312	0.03812	0.52418
H	-4.51010	-1.28210	1.03051
H	-4.38315	0.31722	1.80056
Cl	2.94942	-0.32202	0.38225

^{2}Fe13TMCOOCCH33F
Charge: 1+
Energy: -1508957.8265178

Fe	0.53927	0.18770	-0.02226
N	0.20139	1.71720	1.27586
N	1.31044	-0.89551	1.61294
N	1.05947	-1.19968	-1.50172
N	0.25178	1.57596	-1.52382
C	0.46180	-2.00850	2.10609
C	1.43120	0.13214	2.71623
C	1.35660	1.57713	2.21327
C	-1.07977	1.63079	2.02396
O	-1.05415	-0.60840	0.20599
O	-2.25494	0.06177	-0.24676
C	-3.42587	-0.72620	0.10219
C	-3.56556	-0.85525	1.62177
C	2.67952	-1.41224	1.27556
C	2.76061	-2.30765	0.03596
C	2.47736	-1.64065	-1.31408
C	0.16946	-2.38434	-1.59319
C	0.79067	2.83075	-0.90561
C	0.21211	3.00546	0.49790
C	-1.10436	1.82397	-2.07153
C	1.15411	1.06074	-2.60208
C	0.91361	-0.43097	-2.78690
C	-4.55878	0.12185	-0.48555
C	-3.36123	-2.10181	-0.56593
H	-1.04689	2.55873	-2.88544
H	-1.53827	0.89491	-2.43365
H	-1.75900	2.19270	-1.28560
H	-0.85336	-2.04965	-1.73755
H	0.48157	-3.02626	-2.42791
H	0.20204	-2.95727	-0.67012
H	0.89852	-2.45510	3.00904
H	-0.53656	-1.63255	2.31768
H	0.36851	-2.77580	1.34054
H	2.37031	-0.01574	3.26067
H	0.62654	-0.05266	3.42961
H	-1.13437	0.69253	2.56979
H	-1.16209	2.47277	2.72325
H	-1.90048	1.63682	1.31184
H	2.25717	1.84066	1.66636
H	1.23305	2.25638	3.06784
H	0.77287	3.77157	1.04535
H	-0.82190	3.34956	0.43551
H	0.96666	1.58797	-3.54641
H	2.17984	1.24474	-2.29423
H	1.59409	-0.83596	-3.54683
H	-0.10428	-0.59637	-3.14523
H	3.10710	-0.75988	-1.41901
H	2.72094	-2.34797	-2.11998
H	3.79655	-2.66579	-0.01087
H	2.15451	-3.21047	0.16149
H	3.31537	-0.54307	1.12861
H	3.04603	-1.97730	2.14474
H	1.86965	2.73327	-0.85293
H	0.53643	3.70214	-1.52294
H	-4.47270	-1.41567	1.86962
H	-2.71133	-1.39084	2.04389
H	-3.63564	0.12917	2.09478
H	-4.28810	-2.65544	-0.38469
H	-3.23452	-1.99453	-1.64882
H	-2.52831	-2.68594	-0.16671
H	-5.52248	-0.35832	-0.28978
H	-4.57394	1.11891	-0.03287
H	-4.44114	0.23049	-1.56853
F	2.28765	0.80055	-0.15297

^{2}Fe13TMCOOCCH33N_3
Charge: 1+
Energy: -1549326.5642470

Fe	0.39864	-0.09721	0.09031
N	0.65032	-1.78986	-1.05925
N	1.06627	0.97113	-1.58910
N	0.19712	1.48296	1.43066
N	0.14538	-1.37500	1.69810
C	-0.02867	1.62442	-2.35954
C	1.72943	-0.05427	-2.49466
C	1.83534	-1.47524	-1.90471
C	-0.49676	-2.11877	-1.94647
O	-1.28135	0.06610	-0.54484
O	-2.43046	-0.10141	0.31434
C	-3.65582	0.16446	-0.42802
C	-3.80778	-0.82861	-1.58271
C	2.05145	2.04507	-1.19968
C	1.62122	2.98234	-0.06214
C	1.38942	2.38936	1.33626
C	-1.02807	2.30771	1.23834
C	1.04959	-2.52269	1.35060
C	0.85330	-2.94854	-0.11116
C	-1.20646	-1.90696	2.00607
C	0.65789	-0.57346	2.85552
C	0.08754	0.84191	2.79499
C	-4.72191	-0.07455	0.64660
C	-3.69195	1.60936	-0.93370
H	-1.13384	-2.64903	2.81152
H	-1.86810	-1.10015	2.30525
H	-1.63666	-2.36417	1.11667
H	-1.89895	1.66827	1.32780
H	-1.05777	3.10943	1.98770
H	-1.03842	2.74409	0.24353
H	0.37865	2.10454	-3.25822
H	-0.77912	0.88859	-2.63669
H	-0.51618	2.37488	-1.74148
H	2.73361	0.28681	-2.76207
H	1.15342	-0.09116	-3.42137
H	-0.67111	-1.30686	-2.64873
H	-0.27916	-3.04012	-2.50210
H	-1.39577	-2.24067	-1.34938
H	2.73608	-1.59629	-1.31364
H	1.90366	-2.19250	-2.73428
H	1.70585	-3.55459	-0.43596
H	-0.03271	-3.58126	-0.18972
H	0.36956	-1.04364	3.80468
H	1.74193	-0.54654	2.78907
H	0.57891	1.47337	3.54475
H	-0.97433	0.81567	3.04544
H	2.26060	1.82455	1.65980
H	1.23315	3.21943	2.03983
H	2.44247	3.70166	0.04721
H	0.76013	3.58391	-0.36837
H	3.00002	1.57763	-0.95576
H	2.23346	2.65986	-2.09232
H	2.07263	-2.20424	1.51958
H	0.84006	-3.37949	2.00391
H	-4.78399	-0.70243	-2.06153
H	-3.03515	-0.66974	-2.33898
H	-3.73974	-1.85805	-1.21499
H	-4.62452	1.79097	-1.47737
H	-3.64156	2.32071	-0.10387
H	-2.85797	1.80062	-1.61289
H	-5.71715	0.09732	0.22534
H	-4.67744	-1.10369	1.01721
H	-4.58434	0.60906	1.49085
N	2.31807	-0.17795	0.68165
N	3.43309	-0.21167	0.22773
N	4.51878	-0.24047	-0.17520

^{2}Fe13TMCOOCCH33NCS
Charge: 1+
Energy: -1754439.4714031

Fe	-0.18825	-0.07912	0.02564
N	-0.37752	-1.62637	1.37395
N	-0.63882	1.19319	1.64620
N	-0.12936	1.34917	-1.48201
N	-0.16540	-1.52534	-1.44794
C	0.53215	1.93533	2.18687
C	-1.16352	0.28932	2.74614
C	-1.44641	-1.15487	2.30441
C	0.85366	-1.91980	2.15437
O	1.54598	0.08627	0.44955
O	2.57361	-0.17769	-0.52594
C	3.88834	0.09660	0.04247
C	4.14894	-0.81569	1.24299
C	-1.69273	2.19669	1.25364
C	-1.40776	3.00986	-0.01758
C	-1.30509	2.27707	-1.36506
C	1.10914	2.17679	-1.51092
C	-1.05507	-2.60042	-0.88959
C	-0.74180	-2.86618	0.59140
C	1.12878	-2.13815	-1.84336
C	-0.78351	-0.82345	-2.61867
C	-0.16675	0.56418	-2.77112
C	4.80821	-0.25858	-1.13036
C	4.02156	1.57290	0.42572
H	0.94647	-2.95079	-2.55796
H	1.77863	-1.39172	-2.28850
H	1.63604	-2.52624	-0.96126
H	1.96753	1.52182	-1.60888
H	1.06347	2.88257	-2.35030
H	1.21439	2.73083	-0.58232
H	0.23592	2.51969	3.06733
H	1.32103	1.23544	2.45202
H	0.92807	2.60764	1.42924
H	-2.07594	0.71755	3.17277
H	-0.41954	0.28422	3.54493
H	1.15982	-1.04224	2.71867
H	0.66489	-2.75190	2.84483
H	1.66281	-2.17168	1.47396

H	-2.40121	-1.22983	1.79575
H	-1.48002	-1.79908	3.19386
H	-1.59572	-3.36633	1.05987
H	0.10601	-3.54971	0.66604
H	-0.62061	-1.39840	-3.53959
H	-1.85381	-0.74991	-2.44718
H	-0.70579	1.13111	-3.53963
H	0.86615	0.46571	-3.10934
H	-2.20886	1.70663	-1.55971
H	-1.20793	3.03337	-2.15667
H	-2.25324	3.70171	-0.11742
H	-0.53418	3.65231	0.12986
H	-2.63467	1.66720	1.14903
H	-1.80275	2.90182	2.08959
H	-2.08619	-2.29005	-1.01071
H	-0.91513	-3.53048	-1.45484
H	5.18017	-0.69560	1.58969
H	3.48057	-0.57110	2.07208
H	4.00265	-1.86515	0.96573
H	5.01832	1.76315	0.83612
H	3.88605	2.22115	-0.44539
H	3.28287	1.84342	1.18367
H	5.85129	-0.08995	-0.84584
H	4.69354	-1.31038	-1.41141
H	4.58636	0.36483	-2.00281
N	-2.14436	-0.16028	-0.21033
C	-3.33181	-0.19305	-0.28014
S	-4.93684	-0.22419	-0.36170

[2]Fe13TMCOOCCH33OH
Charge: 1+
Energy: -1493857.7023604

Fe	-0.61547	0.13936	0.08975
N	-0.80023	1.83175	-1.07626
N	-1.34211	-0.91459	-1.59063
N	-0.49901	-1.44060	1.43033
N	-0.32405	1.41446	1.68150
C	-0.29478	-1.65849	-2.34220
C	-1.91989	0.14384	-2.50960
C	-2.01828	1.54548	-1.87909
C	0.34321	2.10533	-1.98376
O	1.07309	-0.11449	-0.54894
O	2.22417	0.00193	0.32603
C	3.43642	-0.30900	-0.40879
C	3.63348	0.68283	-1.55886
C	-2.40644	-1.89402	-1.18051
C	-2.04160	-2.84665	-0.03373
C	-1.76038	-2.24384	1.35149
C	0.66551	-2.34602	1.24051
C	-1.19040	2.58492	1.31927
C	-0.94441	3.00208	-0.13485
C	1.04432	1.89451	1.99254
C	-0.88111	0.63479	2.83104
C	-0.34433	-0.79240	2.78349
C	4.51260	-0.12209	0.66626
C	3.41298	-1.75223	-0.92275
H	0.99914	2.64616	2.79158
H	1.67349	1.06464	2.29875
H	1.49722	2.32455	1.10069
H	1.57615	-1.76005	1.30648
H	0.65366	-3.13563	2.00372
H	0.63649	-2.79970	0.25357
H	-0.72485	-2.11570	-3.24302
H	0.51266	-0.98160	-2.60934
H	0.12917	-2.43587	-1.71105
H	-2.90923	-0.16622	-2.86350
H	-1.28214	0.19434	-3.39359
H	0.49199	1.27376	-2.66819
H	0.15240	3.02268	-2.55657
H	1.25102	2.20663	-1.39567
H	-2.87613	1.63524	-1.21742
H	-2.13477	2.28744	-2.68192
H	-1.75224	3.66070	-0.47353
H	-0.01913	3.57735	-0.20260
H	-0.60237	1.10201	3.78493
H	-1.96310	0.63403	2.73531
H	-0.83560	-1.40408	3.55037
H	0.72325	-0.78953	3.01013
H	-2.57727	-1.58825	1.64431
H	-1.68087	-3.06801	2.07509
H	-2.91050	-3.50522	0.09010
H	-1.22751	-3.51032	-0.33944
H	-3.30470	-1.33889	-0.91179
H	-2.66781	-2.49495	-2.06339
H	-2.22196	2.27742	1.44718
H	-0.97605	3.43499	1.98040
H	4.60487	0.52165	-2.03735
H	2.85491	0.55961	-2.31564
H	3.60402	1.71189	-1.18425
H	4.33592	-1.97320	-1.46858
H	3.33138	-2.46334	-0.09471
H	2.56866	-1.90375	-1.59932
H	5.50040	-0.33594	0.24643
H	4.51218	0.90649	1.04142
H	4.34289	-0.80182	1.50792
O	-2.41100	0.32843	0.64120
H	-3.09719	0.16900	-0.01453

[6]FeBQENBrOH
Charge: 3+
Energy: -3127442.9520008

Fe	0.08781	0.23666	-0.89289
N	-1.80740	-0.76817	-0.74213
N	-0.78100	0.31836	1.66694
N	2.01236	0.85454	-0.03774
C	-2.29017	-1.30856	-1.87698
C	-3.62140	-1.71739	-2.02357
C	-4.50177	-1.50703	-0.97149
C	-4.02740	-0.90510	0.21821
C	-4.90959	-0.51884	1.26745
C	-4.43770	0.22266	2.35839
C	-3.09010	0.55712	2.45015
C	-2.15237	0.08834	1.49703
C	-2.64271	-0.58618	0.31519
H	-1.58120	-1.38685	-2.69451
H	-3.95101	-2.15538	-2.96002
H	-5.55241	-1.76960	-1.06417
H	-5.96489	-0.76945	1.19450
H	-5.12114	0.52104	3.14753
H	-2.74737	1.10897	3.31794
C	2.44089	2.13201	-0.02375
C	3.77265	2.48705	0.22763
C	4.70969	1.47931	0.44977
C	4.28317	0.13171	0.43039
C	5.18749	-0.95625	0.57130
C	4.72954	-2.28939	0.46992
C	3.38553	-2.55499	0.23582
C	2.44263	-1.50445	0.14275
C	2.90248	-0.13992	0.20307
H	1.69178	2.88532	-0.24089
H	4.05977	3.53388	0.22481
H	5.75584	1.72041	0.62134
H	6.24334	-0.75827	0.74103
H	5.43263	-3.10882	0.58787
H	3.05798	-3.58635	0.16962
N	1.04758	-1.74900	-0.04810
C	0.27395	-2.01035	1.22489
C	0.10796	-0.80689	2.13315
H	-0.69134	-2.40695	0.91094
H	0.77832	-2.79832	1.79793
H	-0.28762	-1.15945	3.09436
H	1.07681	-0.34696	2.33401
C	0.80821	-2.86225	-1.02054
H	1.39213	-2.67992	-1.92166
H	-0.24877	-2.84858	-1.28200
H	1.03943	-3.84136	-0.58845
C	-0.42810	1.57595	2.37193
H	-1.08196	2.38094	2.03941
H	0.59817	1.82864	2.10002
H	-0.47734	1.45779	3.46114
O	0.58865	-0.25437	-2.53977
H	0.63168	0.31732	-3.32967
Br	-0.91438	2.43183	-1.08300

[4]FeBQENClOH
Charge: 3+
Energy: -1800914.4317935

Fe	0.03266	0.32180	-0.67524
N	-1.83404	-0.31040	-0.94767
N	-0.65518	0.51801	1.35990
N	1.86180	0.95968	-0.23816
C	-2.33285	-0.68363	-2.13455
C	-3.69945	-0.94283	-2.31807
C	-4.57516	-0.78776	-1.24632
C	-4.06511	-0.38307	0.00956
C	-4.87388	-0.17997	1.16156
C	-4.29746	0.24068	2.37042
C	-2.91787	0.46783	2.46452
C	-2.09999	0.28364	1.34545
C	-2.66566	-0.14976	0.11856
H	-1.61994	-0.77205	-2.94603
H	-4.05453	-1.25052	-3.29644
H	-5.63994	-0.96767	-1.37111
H	-5.94548	-0.35168	1.10046
H	-4.92673	0.39418	3.24186
H	-2.50119	0.79479	3.41143
C	2.33439	2.20912	-0.36615
C	3.69455	2.51448	-0.20436
C	4.59402	1.49574	0.08184
C	4.12005	0.16848	0.21422
C	4.96611	-0.93791	0.49990
C	4.43483	-2.22478	0.61554
C	3.05787	-2.44464	0.45150
C	2.20621	-1.37922	0.16210
C	2.72492	-0.06529	0.04511

H	1.61190	2.97815	-0.61118
H	4.02100	3.54326	-0.31696
H	5.65359	1.70841	0.19910
H	6.03255	-0.77332	0.62859
H	5.08885	-3.06349	0.83307
H	2.67131	-3.45403	0.54811
N	0.76353	-1.54509	-0.02881
C	0.07197	-1.84107	1.27741
C	0.05291	-0.58475	2.11977
H	-0.93999	-2.17698	1.03753
H	0.58196	-2.65770	1.79888
H	-0.44048	-0.75723	3.08158
H	1.06649	-0.22816	2.32084
C	0.47240	-2.62364	-1.03182
H	1.02942	-2.42224	-1.94500
H	-0.59724	-2.61407	-1.24098
H	0.74471	-3.60262	-0.62773
C	-0.33384	1.84785	1.99008
H	-0.94815	2.62279	1.53565
H	0.71915	2.06047	1.80971
H	-0.50696	1.80795	3.06915
O	0.51991	-0.10984	-2.28789
H	0.60937	0.65590	-2.89477
Cl	-0.75792	2.33443	-1.19299

^{6}FeBQENFOH
Charge: 3+
Energy: -1574791.0393937

Fe	-0.03213	-0.23469	1.17164
N	1.88770	-0.87916	0.45057
N	0.93516	1.50640	-0.85323
N	-1.88531	0.75021	0.69503
C	2.35337	-2.01353	1.00902
C	3.69670	-2.40351	0.94995
C	4.60684	-1.55197	0.34388
C	4.15182	-0.33372	-0.21505
C	5.06452	0.64420	-0.70607
C	4.61026	1.90605	-1.10339
C	3.25178	2.20020	-1.07585
C	2.28804	1.21727	-0.72495
C	2.75575	-0.04804	-0.19004
H	1.61867	-2.60812	1.54180
H	4.00866	-3.33569	1.40939
H	5.66626	-1.79386	0.32184
H	6.12637	0.41298	-0.73197
H	5.31491	2.65038	-1.46144
H	2.92202	3.17043	-1.42930
C	-2.29592	1.80198	1.42722
C	-3.61622	2.27242	1.39013
C	-4.54650	1.60995	0.59301
C	-4.13160	0.49167	-0.16895
C	-5.03680	-0.32956	-0.89895
C	-4.58718	-1.51051	-1.52414
C	-3.24907	-1.88709	-1.45740
C	-2.29657	-1.04964	-0.82927
C	-2.76184	0.11477	-0.11533
H	-1.54133	2.24461	2.06981
H	-3.90284	3.12175	2.00213
H	-5.58548	1.92912	0.57124
H	-6.09023	-0.06265	-0.93986
H	-5.29141	-2.12478	-2.07767
H	-2.93381	-2.79442	-1.95973
N	-0.90998	-1.33255	-0.83499
C	-0.07335	-0.66580	-1.91381
C	0.05985	0.84945	-1.87999
H	0.90193	-1.14730	-1.86701
H	-0.51873	-0.92583	-2.88180
H	0.45289	1.14992	-2.86096
H	-0.91944	1.31682	-1.77651
C	-0.60704	-2.79345	-0.79958
H	-1.20036	-3.26213	-0.01554
H	0.44849	-2.90743	-0.55699
H	-0.78426	-3.26988	-1.77032
C	0.53546	2.91088	-0.61589
H	1.13087	3.33004	0.19387
H	-0.51178	2.90783	-0.30967
H	0.62466	3.51849	-1.52493
O	-0.55595	-1.66089	2.11651
H	-0.62135	-1.71209	3.08905
F	0.52684	1.18604	2.04455

^{4}FeBQENN$_3$OH
Charge: 3+
Energy: -1615185.3928187

Fe	0.02536	0.61702	-0.20659
N	-1.81249	0.26903	-0.86101
N	-0.62926	-0.57050	1.45217
N	1.90229	0.82589	0.42566
C	-2.31127	0.71160	-2.02481
C	-3.66738	0.56370	-2.35494
C	-4.52943	-0.04634	-1.44700
C	-4.02018	-0.51033	-0.21085
C	-4.82181	-1.12953	0.78753
C	-4.24919	-1.55439	1.99503
C	-2.87966	-1.38166	2.23611
C	-2.06425	-0.77455	1.27485
C	-2.63152	-0.33424	0.04768
H	-1.60277	1.19963	-2.68571
H	-4.02652	0.93647	-3.30878
H	-5.58545	-0.16068	-1.67827
H	-5.88456	-1.27102	0.60904
H	-4.87195	-2.02431	2.75009
H	-2.46305	-1.72457	3.17756
C	2.38484	1.85592	1.13668
C	3.74961	1.99521	1.43317
C	4.64725	1.03949	0.97376
C	4.16441	-0.06412	0.23119
C	4.99916	-1.10192	-0.26727
C	4.44966	-2.17026	-0.97848
C	3.06552	-2.23972	-1.21067
C	2.22424	-1.23046	-0.74497
C	2.76414	-0.13733	-0.02272
H	1.66030	2.58568	1.47884
H	4.08240	2.84967	2.01338
H	5.70987	1.13121	1.18313
H	6.06952	-1.05929	-0.08487
H	5.09448	-2.95848	-1.35442
H	2.66687	-3.08701	-1.75915
N	0.77395	-1.23408	-0.95217
C	0.12112	-2.31384	-0.12588
C	0.10872	-1.88340	1.32611
H	-0.89373	-2.44344	-0.51038
H	0.64869	-3.26486	-0.25075
H	-0.35253	-2.64615	1.96206
H	1.12429	-1.71043	1.69253
C	0.45005	-1.41505	-2.40707
H	0.94878	-0.63613	-2.98067
H	-0.62801	-1.32015	-2.53044
H	0.76011	-2.40530	-2.75171
C	-0.32776	0.05706	2.78322
H	-0.94518	0.94476	2.91140
H	0.72455	0.34333	2.78662
H	-0.50510	-0.64845	3.59964
O	0.39553	1.43992	-1.73409
H	1.29442	1.81623	-1.79165
N	-0.58674	2.09877	0.67528
N	-0.86528	3.13089	0.04167
N	-1.15484	4.10520	-0.46985

^{6}FeBQENNCSOH
Charge: 3+
Energy: -1820298.1371612

Fe	0.08900	0.35946	-0.65129
N	-1.81759	-0.53916	-0.96380
N	-0.59907	-0.31289	1.50780
N	2.00517	0.90540	0.15451
C	-2.35131	-0.64767	-2.19022
C	-3.65896	-1.10828	-2.40721
C	-4.44077	-1.45238	-1.31249
C	-3.90391	-1.33408	-0.00683
C	-4.65309	-1.61546	1.16725
C	-4.08198	-1.43607	2.43154
C	-2.76211	-0.98335	2.55858
C	-1.98110	-0.72707	1.42618
C	-2.55972	-0.87967	0.12604
H	-1.70748	-0.34335	-3.00890
H	-4.04270	-1.17904	-3.41955
H	-5.46087	-1.80232	-1.44787
H	-5.67952	-1.96052	1.07619
H	-4.66093	-1.65968	3.32219
H	-2.34122	-0.86457	3.55149
C	2.38083	2.14477	0.49775
C	3.70994	2.48677	0.78909
C	4.68983	1.50846	0.69522
C	4.32724	0.19269	0.31908
C	5.27243	-0.85874	0.17778
C	4.85837	-2.13178	-0.21698
C	3.50352	-2.39125	-0.47442
C	2.54469	-1.38730	-0.33187
C	2.94998	-0.07551	0.06155
H	1.59111	2.88690	0.53563
H	3.95445	3.50530	1.07124
H	5.73087	1.74514	0.89873
H	6.32204	-0.66304	0.37932
H	5.58610	-2.93049	-0.32020
H	3.20940	-3.39180	-0.77366
N	1.13132	-1.62046	-0.57625
C	0.48417	-2.36922	0.56152
C	0.32145	-1.48012	1.77927
H	-0.48525	-2.71972	0.19921
H	1.08170	-3.25108	0.81788
H	-0.05854	-2.06546	2.62428
H	1.28355	-1.05461	2.07520
C	0.90156	-2.33575	-1.87133
H	1.42084	-1.80370	-2.66712

H	-0.17018	-2.32418	-2.07462
H	1.23666	-3.37641	-1.82353
C	-0.38752	0.74572	2.53703
H	-1.13897	1.52545	2.41263
H	0.60486	1.17247	2.37952
H	-0.43473	0.34751	3.55620
O	0.39795	0.69031	-2.38581
H	0.94123	1.26257	-2.95625
N	-0.79575	2.28455	-0.25564
C	-1.37428	3.31829	-0.29130
S	-2.15526	4.74726	-0.35036

^{6}FeBQENOHBr
Charge: 3+
Energy: -3127444.1359856

Fe	0.08008	-0.75660	0.81962
N	2.17107	-1.02141	0.26054
N	1.05376	1.27550	1.16438
N	-1.91823	0.18740	1.08660
C	2.72817	-2.22013	-0.00889
C	4.03356	-2.35042	-0.49758
C	4.78098	-1.19949	-0.74968
C	4.21312	0.06834	-0.46684
C	4.87834	1.29487	-0.70382
C	4.24288	2.52514	-0.40358
C	2.96691	2.55519	0.15876
C	2.29046	1.35501	0.44247
C	2.89733	0.10131	0.07798
H	2.09810	-3.08704	0.15851
H	4.44090	-3.33812	-0.68906
H	5.78765	-1.26949	-1.15445
H	5.88398	1.29546	-1.11755
H	4.77526	3.45517	-0.58126
H	2.53292	3.51222	0.42789
C	-2.50543	-0.11695	2.26131
C	-3.89220	-0.10488	2.45869
C	-4.71462	0.13430	1.36927
C	-4.12841	0.43209	0.11587
C	-4.90371	0.51443	-1.07797
C	-4.28163	0.64606	-2.32508
C	-2.90369	0.80775	-2.41034
C	-2.10678	0.89381	-1.23490
C	-2.71224	0.54204	0.03758
H	-1.83434	-0.42198	3.05617
H	-4.29898	-0.33846	3.43709
H	-5.79565	0.06900	1.46061
H	-5.98529	0.42694	-1.01476
H	-4.88129	0.67243	-3.22964
H	-2.45788	0.99240	-3.38077
N	-0.80648	1.33728	-1.29910
C	-0.36933	2.54176	-0.51924
C	0.08458	2.38242	0.93465
H	0.44142	2.97227	-1.11049
H	-1.18628	3.27046	-0.52592
H	0.49939	3.34665	1.25545
H	-0.76129	2.17457	1.58541
C	-0.05866	1.14066	-2.55848
H	-0.30879	0.17132	-2.98853
H	1.00698	1.14631	-2.31790
H	-0.25669	1.94585	-3.27633
C	1.36125	1.16603	2.65376
H	2.01671	0.31303	2.82682
H	0.42129	0.99545	3.17899
H	1.82989	2.09000	3.00556
O	0.11279	-1.61022	2.38414
H	-0.04997	-2.54431	2.61427
Br	-0.62310	-2.18298	-1.02326

^{4}FeBQENOHCl
Charge: 3+
Energy: -1800914.4326532

Fe	0.03264	0.32165	-0.67534
N	1.86176	0.95961	-0.23842
N	0.76364	-1.54512	-0.02857
N	-1.83403	-0.31072	-0.94756
C	2.33428	2.20905	-0.36664
C	3.69442	2.51451	-0.20489
C	4.59395	1.49587	0.08148
C	4.12004	0.16861	0.21413
C	4.96614	-0.93766	0.50012
C	4.43490	-2.22451	0.61615
C	3.05795	-2.44447	0.45216
C	2.20624	-1.37916	0.16240
C	2.72493	-0.06526	0.04507
H	1.61175	2.97798	-0.61185
H	4.02080	3.54330	-0.31764
H	5.65351	1.70860	0.19866
H	6.03257	-0.77301	0.62874
H	5.08893	-3.06313	0.83394
H	2.67143	-3.45384	0.54907
C	-2.33282	-0.68434	-2.13431
C	-3.69943	-0.94361	-2.31775
C	-4.57514	-0.78814	-1.24607
C	-4.06509	-0.38304	0.00968
C	-4.87385	-0.17953	1.16162
C	-4.29741	0.24149	2.37033
C	-2.91781	0.46854	2.46440
C	-2.09992	0.28394	1.34540
C	-2.66565	-0.14975	0.11863
H	-1.61993	-0.77296	-2.94577
H	-4.05450	-1.25164	-3.29601
H	-5.63993	-0.96803	-1.37080
H	-5.94546	-0.35119	1.10058
H	-4.92667	0.39534	3.24171
H	-2.50113	0.79576	3.41122
N	-0.65510	0.51812	1.35975
C	0.05285	-0.58465	2.11988
C	0.07195	-1.84103	1.27761
H	1.06642	-0.22809	2.32105
H	-0.44075	-0.75699	3.08161
H	0.58186	-2.65767	1.79914
H	-0.94000	-2.17687	1.03764
C	-0.33365	1.84805	1.98983
H	-0.94779	2.62298	1.53515
H	0.71939	2.06046	1.80960
H	-0.50697	1.80829	3.06886
C	0.47262	-2.62371	-1.03157
H	1.02949	-2.42216	-1.94481
H	-0.59705	-2.61438	-1.24060
H	0.74523	-3.60265	-0.62757
O	0.51974	-0.10995	-2.28801
H	0.60940	0.65562	-2.89504
Cl	-0.75812	2.33417	-1.19330

^{4}FeBQENOHF
Charge: 3+
Energy: -1574791.0579115

Fe	0.01784	-0.10209	-0.79155
N	1.81877	0.64977	-0.81290
N	0.72466	-1.22324	0.82774
N	-1.86885	-0.74176	-0.72435
C	2.25577	1.57195	-1.68142
C	3.61188	1.92643	-1.75012
C	4.52702	1.29645	-0.91232
C	4.07908	0.30917	-0.00032
C	4.93267	-0.40501	0.88431
C	4.40755	-1.37527	1.74272
C	3.03114	-1.66356	1.74983
C	2.17221	-0.98187	0.89111
C	2.68903	0.00714	0.01797
H	1.50376	2.01459	-2.32539
H	3.92745	2.68007	-2.46431
H	5.58284	1.55095	-0.95962
H	5.99840	-0.19269	0.88717
H	5.06836	-1.91684	2.41247
H	2.65602	-2.42389	2.42739
C	-2.36775	-1.71873	-1.49346
C	-3.74242	-1.99924	-1.54145
C	-4.62315	-1.23819	-0.77606
C	-4.11096	-0.20266	0.04022
C	-4.91975	0.62753	0.86470
C	-4.33640	1.63370	1.65203
C	-2.95144	1.84347	1.63359
C	-2.13468	1.05383	0.81732
C	-2.70559	0.02037	0.03120
H	-1.64873	-2.28247	-2.07701
H	-4.09890	-2.80336	-2.17730
H	-5.69207	-1.43404	-0.80405
H	-5.99598	0.47617	0.88562
H	-4.96541	2.25886	2.27854
H	-2.52875	2.63079	2.24935
N	-0.68663	1.24308	0.71025
C	0.01101	0.83283	1.98493
C	0.03256	-0.68058	2.05683
H	1.02327	1.24282	1.94074
H	-0.48912	1.26623	2.85678
H	0.54026	-1.02953	2.96154
H	-0.98078	-1.09103	2.05901
C	-0.37593	2.67033	0.35024
H	-0.89494	2.91838	-0.57438
H	0.70020	2.75428	0.20320
H	-0.67709	3.34532	1.15562
C	0.42511	-2.68771	0.66401
H	0.98465	-3.07220	-0.18688
H	-0.64433	-2.79494	0.48083
H	0.68841	-3.23473	1.57326
O	0.49584	-1.39216	-1.85635
H	0.58358	-1.08479	-2.78492
F	-0.49213	1.05294	-1.99410

^{4}FeBQENOHN$_{3}$
Charge: 3+
Energy: -1615185.3907479

Fe	0.02509	0.61719	-0.20610

N	1.90253	0.82492	0.42672
N	0.77371	-1.23422	-0.95187
N	-1.81252	0.26997	-0.86052
C	2.38513	1.85437	1.13857
C	3.74998	1.99347	1.43483
C	4.64757	1.03826	0.97419
C	4.16459	-0.06474	0.23081
C	4.99922	-1.10207	-0.26883
C	4.44947	-2.16992	-0.98076
C	3.06526	-2.23936	-1.21239
C	2.22408	-1.23056	-0.74547
C	2.76423	-0.13785	-0.02265
H	1.66059	2.58376	1.48154
H	4.08292	2.84741	2.01573
H	5.71025	1.12995	1.18330
H	6.06966	-1.05961	-0.08684
H	5.09430	-2.95773	-1.35757
H	2.66642	-3.08628	-1.76131
C	-2.31101	0.71293	-2.02434
C	-3.66703	0.56507	-2.35487
C	-4.52932	-0.04538	-1.44744
C	-4.02037	-0.50992	-0.21138
C	-4.82213	-1.12995	0.78644
C	-4.24971	-1.55566	1.99370
C	-2.88019	-1.38292	2.23522
C	-2.06483	-0.77487	1.27463
C	-2.63184	-0.33382	0.04767
H	-1.60238	1.20123	-2.68490
H	-4.02586	0.93818	-3.30870
H	-5.58525	-0.15971	-1.67910
H	-5.88482	-1.27149	0.60762
H	-4.87255	-2.02624	2.74827
H	-2.46375	-1.72657	3.17649
N	-0.62983	-0.57033	1.45234
C	0.10861	-1.88292	1.32683
C	0.12124	-2.31384	-0.12497
H	1.12403	-1.70948	1.69343
H	-0.35243	-2.64569	1.96293
H	0.64906	-3.26476	-0.24947
H	-0.89357	-2.44389	-0.50948
C	-0.32921	0.05749	2.78347
H	-0.94623	0.94558	2.91076
H	0.72330	0.34301	2.78786
H	-0.50781	-0.64767	3.59993
C	0.44887	-1.41530	-2.40647
H	0.94738	-0.63655	-2.98052
H	-0.62926	-1.32030	-2.52917
H	0.75847	-2.40564	-2.75133
O	0.39598	1.43995	-1.73355
H	1.29571	1.81426	-1.79121
N	-0.58588	2.09954	0.67513
N	-0.86362	3.13192	0.04135
N	-1.15212	4.10630	-0.47060

^{6}FeBQENOHNCS
Charge: 3+
Energy: -1820298.1377636

Fe	0.08907	0.35954	-0.65120
N	2.00518	0.90538	0.15470
N	1.13133	-1.62039	-0.57638
N	-1.81759	-0.53904	-0.96378
C	2.38080	2.14471	0.49811
C	3.70991	2.48670	0.78947
C	4.68982	1.50842	0.69543
C	4.32726	0.19270	0.31910
C	5.27246	-0.85868	0.17758
C	4.85841	-2.13166	-0.21739
C	3.50356	-2.39113	-0.47483
C	2.54471	-1.38722	-0.33206
C	2.95000	-0.07549	0.06156
H	1.59106	2.88681	0.53609
H	3.95441	3.50519	1.07176
H	5.73086	1.74510	0.89895
H	6.32208	-0.66300	0.37910
H	5.58615	-2.93033	-0.32078
H	3.20945	-3.39163	-0.77423
C	-2.35134	-0.64741	-2.19020
C	-3.65899	-1.10800	-2.40722
C	-4.44078	-1.45223	-1.31253
C	-3.90389	-1.33411	-0.00686
C	-4.65301	-1.61570	1.16719
C	-4.08186	-1.43653	2.43149
C	-2.76199	-0.98381	2.55854
C	-1.98104	-0.72730	1.42616
C	-2.55970	-0.87971	0.12602
H	-1.70753	-0.34300	-3.00886
H	-4.04275	-1.17865	-3.41956
H	-5.46088	-1.80217	-1.44793
H	-5.67945	-1.96076	1.07611
H	-4.66076	-1.66031	3.32212
H	-2.34106	-0.86519	3.55146
N	-0.59903	-0.31305	1.50778
C	0.32155	-1.48024	1.77918
C	0.48427	-2.36925	0.56137
H	1.28363	-1.05470	2.07512
H	-0.05840	-2.06565	2.62417
H	1.08183	-3.25111	0.81764
H	-0.48516	-2.71974	0.19908
C	-0.38758	0.74554	2.53706
H	-1.13901	1.52527	2.41259
H	0.60482	1.17227	2.37967
H	-0.43493	0.34730	3.55622
C	0.90150	-2.33559	-1.87150
H	1.42072	-1.80349	-2.66728
H	-0.17026	-2.32400	-2.07473
H	1.23659	-3.37625	-1.82380
O	0.39808	0.69062	-2.38565
H	0.94039	1.26336	-2.95652
N	-0.79597	2.28453	-0.25548
C	-1.37451	3.31826	-0.29105
S	-2.15545	4.74725	-0.35035

^{2}FeBnTPENOH
Charge: 2+
Energy: -1570381.1023559

Fe	-0.03302	-0.00035	-0.62382
N	0.15555	-0.00034	1.40557
N	1.41633	1.35809	-0.49393
N	1.41700	-1.35795	-0.49395
N	-1.43394	1.35258	-0.29956
N	-1.43371	-1.35345	-0.29951
O	-0.24007	-0.00053	-2.39541
C	1.69413	2.36224	-1.33708
C	2.71429	3.27323	-1.06417
C	3.44377	3.13630	0.11750
C	3.13894	2.09177	1.00011
C	2.11716	1.21948	0.65548
C	1.67000	0.00015	1.45023
C	2.11796	-1.21878	0.65533
C	3.14060	-2.09016	0.99967
C	3.44616	-3.13438	0.11693
C	2.71655	-3.27189	-1.06459
C	1.69554	-2.36178	-1.33724
C	-2.28982	1.80133	-1.23354
C	-3.32415	2.67396	-0.90928
C	-3.47491	3.07544	0.41922
C	-2.58140	2.60096	1.38297
C	-1.56143	1.74193	0.98736
C	-0.48831	1.24632	1.93418
C	-0.48744	-1.24759	1.93385
C	-1.56108	-1.74278	0.98745
C	-2.58130	-2.60139	1.38327
C	-3.47524	-3.07548	0.41971
C	-3.32462	-2.67404	-0.90880
C	-2.29001	-1.80180	-1.23328
H	1.08015	2.41491	-2.22964
H	2.92594	4.07195	-1.76662
H	4.23878	3.83570	0.35665
H	3.68227	1.96541	1.93093
H	2.06485	0.00020	2.47102
H	3.68405	-1.96337	1.93036
H	4.24185	-3.83308	0.35586
H	2.92873	-4.07040	-1.76711
H	1.08143	-2.41486	-2.22970
H	-2.11200	1.43419	-2.23805
H	-3.99842	3.02204	-1.68410
H	-4.27821	3.74749	0.70464
H	-2.67267	2.89700	2.42333
H	-2.67246	-2.89740	2.42365
H	-4.27874	-3.74722	0.70530
H	-3.99919	-3.02182	-1.68349
H	-2.11232	-1.43470	-2.23783
H	-0.88938	1.07556	2.93757
H	0.28127	2.01835	2.02805
H	-0.88766	-1.07778	2.93774
H	0.28252	-2.01941	2.02639
H	0.60750	-0.00003	-2.87440

^{6}FeBnTPENBr
Charge: 2+
Energy: -3138118.5743997

Fe	0.05781	-0.00029	0.53755
N	-0.15897	-0.00012	-1.69478
N	-1.52335	1.42902	0.16921
N	-1.52397	-1.42880	0.16914
N	1.50785	1.45741	-0.02656
N	1.50775	-1.45798	-0.02684
C	-1.90298	2.43836	0.96920
C	-2.94392	3.29612	0.61619
C	-3.59841	3.09441	-0.59903
C	-3.19862	2.03934	-1.42909
C	-2.15686	1.22568	-1.00664
C	-1.65756	0.00020	-1.76219
C	-2.15741	-1.22507	-1.00670
C	-3.19957	-2.03821	-1.42916

C	-3.59986	-3.09313	-0.59915
C	-2.94544	-3.29522	0.61604
C	-1.90408	-2.43800	0.96907
C	2.42733	1.95593	0.82525
C	3.46997	2.76683	0.39267
C	3.56994	3.05760	-0.96919
C	2.61866	2.53623	-1.84890
C	1.59165	1.74395	-1.34415
C	0.47056	1.23860	-2.22841
C	0.47004	-1.23912	-2.22838
C	1.59152	-1.74423	-1.34450
C	2.61876	-2.53602	-1.84951
C	3.57032	-3.05721	-0.97000
C	3.47038	-2.76678	0.39193
C	2.42748	-1.95634	0.82479
H	-1.36023	2.53901	1.90274
H	-3.23097	4.10010	1.28509
H	-4.41080	3.74774	-0.90197
H	-3.68832	1.85794	-2.38049
H	-2.02353	0.00031	-2.79522
H	-3.68922	-1.85651	-2.38054
H	-4.41258	-3.74604	-0.90211
H	-3.23287	-4.09910	1.28490
H	-1.36135	-2.53896	1.90259
H	2.30573	1.68404	1.86749
H	4.18671	3.15323	1.10901
H	4.37715	3.67977	-1.34329
H	2.66984	2.74722	-2.91253
H	2.66990	-2.74677	-2.91319
H	4.37774	-3.67900	-1.34431
H	4.18732	-3.15308	1.10812
H	2.30588	-1.68471	1.86709
H	0.82818	1.07986	-3.25137
H	-0.29392	2.01967	-2.28221
H	0.82705	-1.08083	-3.25163
H	-0.29461	-2.02008	-2.28135
Br	0.14009	-0.00047	2.93042

^{6}FeBnTPENCl
Charge: 2+
Energy: -1811590.5737515

Fe	0.06275	-0.00028	0.77275
N	-0.13554	-0.00022	-1.47551
N	-1.51052	1.42196	0.38548
N	-1.51110	-1.42179	0.38554
N	1.50627	1.45575	0.21198
N	1.50619	-1.45634	0.21186
C	-1.89310	2.42350	1.19289
C	-2.93182	3.28427	0.84030
C	-3.57811	3.09213	-0.38102
C	-3.17504	2.04278	-1.21727
C	-2.13661	1.22496	-0.79500
C	-1.63383	0.00008	-1.55034
C	-2.13713	-1.22455	-0.79493
C	-3.17596	-2.04190	-1.21713
C	-3.57948	-3.09104	-0.38082
C	-2.93324	-3.28342	0.84049
C	-1.89411	-2.42312	1.19301
C	2.40864	1.95317	1.08200
C	3.45240	2.77274	0.66902
C	3.56989	3.07149	-0.68997
C	2.63508	2.54990	-1.58739
C	1.60557	1.74863	-1.10242
C	0.49853	1.23908	-2.00242
C	0.49806	-1.23982	-2.00229
C	1.60548	-1.74904	-1.10261
C	2.63525	-2.54986	-1.58775
C	3.57033	-3.07120	-0.69047
C	3.45283	-2.77267	0.66856
C	2.40880	-1.95352	1.08173
H	-1.35451	2.51392	2.13024
H	-3.22351	4.08296	1.51351
H	-4.38805	3.74853	-0.68391
H	-3.66029	1.86895	-2.17237
H	-1.99624	0.00012	-2.58460
H	-3.66115	-1.86790	-2.17222
H	-4.38973	-3.74707	-0.68366
H	-3.22528	-4.08195	1.51374
H	-1.35554	-2.51375	2.13035
H	2.27083	1.67218	2.12008
H	4.15677	3.15952	1.39731
H	4.37882	3.70054	-1.04859
H	2.70119	2.76752	-2.64887
H	2.70133	-2.76734	-2.64926
H	4.37947	-3.69990	-1.04923
H	4.15740	-3.15929	1.39676
H	2.27099	-1.67271	2.11987
H	0.87167	1.07977	-3.01974
H	-0.26683	2.01841	-2.06899
H	0.87061	-1.08104	-3.01990
H	-0.26745	-2.01907	-2.06799
Cl	0.16332	-0.00036	2.97786

^{6}FeBnTPENF
Charge: 2+
Energy: -1585464.6908357

Fe	-0.07426	-0.00028	-0.89306
N	0.13113	-0.00025	1.37575
N	1.50343	1.41827	-0.51645
N	1.50389	-1.41819	-0.51656
N	-1.49240	1.45952	-0.31449
N	-1.49242	-1.46003	-0.31439
C	1.88137	2.42279	-1.32256
C	2.91609	3.28846	-0.97033
C	3.56085	3.09981	0.25245
C	3.16055	2.04975	1.08905
C	2.12743	1.22519	0.66610
C	1.63021	-0.00001	1.42739
C	2.12786	-1.22496	0.66598
C	3.16134	-2.04913	1.08879
C	3.56202	-3.09895	0.25208
C	2.91730	-3.28775	-0.97069
C	1.88220	-2.42247	-1.32280
C	-2.37876	1.95315	-1.20189
C	-3.41425	2.79207	-0.80755
C	-3.53558	3.10940	0.54772
C	-2.61626	2.58700	1.46114
C	-1.59401	1.76533	0.99466
C	-0.49954	1.24042	1.90464
C	-0.49914	-1.24117	1.90450
C	-1.59403	-1.76570	0.99481
C	-2.61658	-2.58688	1.46147
C	-3.53621	-3.10898	0.54817
C	-3.41487	-2.79185	-0.80713
C	-2.37907	-1.95338	-1.20166
H	1.34117	2.51508	-2.25942
H	3.20474	4.08872	-1.64297
H	4.36690	3.76041	0.55660
H	3.64406	1.88045	2.04583
H	2.01102	0.00001	2.45512
H	3.64483	-1.87973	2.04557
H	4.36836	-3.75925	0.55614
H	3.20624	-4.08783	-1.64342
H	1.34200	-2.51488	-2.25964
H	-2.23061	1.64667	-2.23219
H	-4.11005	3.17883	-1.54403
H	-4.33869	3.75385	0.89183
H	-2.69002	2.81867	2.51915
H	-2.69033	-2.81842	2.51950
H	-4.33956	-3.75306	0.89243
H	-4.11089	-3.17839	-1.54351
H	-2.23091	-1.64705	-2.23200
H	-0.88679	1.07835	2.91622
H	0.27020	2.01426	1.98670
H	-0.88580	-1.07963	2.91638
H	0.27070	-2.01499	1.98568
F	-0.37718	-0.00033	-2.62594

^{6}FeBnTPENN$_3$
Charge: 2+
Energy: -1625852.8656706

Fe	0.06479	-0.00045	0.67749
N	-0.10219	-0.00018	-1.57594
N	-1.51937	1.43792	0.24672
N	-1.52026	-1.43763	0.24658
N	1.52903	1.45666	0.12584
N	1.52892	-1.45753	0.12539
C	-1.92039	2.45723	1.02162
C	-2.94998	3.31375	0.63457
C	-3.57145	3.10013	-0.59612
C	-3.14818	2.03784	-1.40389
C	-2.11877	1.22692	-0.94441
C	-1.59653	0.00028	-1.68366
C	-2.11957	-1.22608	-0.94449
C	-3.14961	-2.03620	-1.40398
C	-3.57361	-3.09825	-0.59630
C	-2.95222	-3.31245	0.63434
C	-1.92199	-2.45672	1.02141
C	2.43189	1.94740	0.99696
C	3.49059	2.75125	0.59105
C	3.62222	3.04182	-0.76865
C	2.68822	2.52691	-1.66991
C	1.64458	1.74077	-1.18799
C	0.54077	1.23678	-2.09614
C	0.54004	-1.23750	-2.09618
C	1.64440	-1.74121	-1.18856
C	2.68834	-2.52665	-1.67089
C	3.62277	-3.04137	-0.76992
C	3.49119	-2.75129	0.58988
C	2.43215	-1.94809	0.99621
H	-1.39781	2.57519	1.96511
H	-3.25247	4.12646	1.28591
H	-4.37398	3.75142	-0.92826
H	-3.60913	1.84918	-2.36820
H	-1.93779	0.00042	-2.72550

H	-3.61047	-1.84711	-2.36825
H	-4.37663	-3.74892	-0.92845
H	-3.25527	-4.12500	1.28562
H	-1.39944	-2.57516	1.96486
H	2.28366	1.67127	2.03533
H	4.19510	3.13227	1.32225
H	4.44195	3.65854	-1.12409
H	2.76603	2.73684	-2.73216
H	2.76609	-2.73624	-2.73321
H	4.44276	-3.65756	-1.12569
H	4.19600	-3.13219	1.32086
H	2.28396	-1.67236	2.03469
H	0.92030	1.07970	-3.11175
H	-0.21988	2.02041	-2.16573
H	0.91875	-1.08102	-3.11219
H	-0.22085	-2.02099	-2.16467
N	0.13270	-0.00070	2.53048
N	-0.08050	-0.00095	3.72601
N	-0.27328	-0.00117	4.85620

[6]FeBnTPENNCS
Charge: 2+
Energy: -1830961.1270667

Fe	0.07639	-0.00077	0.48037
N	-0.26479	0.00129	-1.75945
N	-1.53544	1.43242	0.17921
N	-1.53615	-1.43249	0.17682
N	1.49002	1.45980	-0.18935
N	1.49005	-1.46005	-0.19215
C	-1.87576	2.44495	0.99092
C	-2.93215	3.30326	0.68895
C	-3.64503	3.09794	-0.49258
C	-3.28574	2.04071	-1.33741
C	-2.22447	1.22713	-0.96340
C	-1.76296	0.00164	-1.74473
C	-2.22512	-1.22490	-0.96542
C	-3.28690	-2.03722	-1.34070
C	-3.64678	-3.09563	-0.49759
C	-2.93397	-3.30331	0.68357
C	-1.87704	-2.44613	0.98690
C	2.45500	1.95169	0.61152
C	3.47781	2.75826	0.12647
C	3.50466	3.04987	-1.23912
C	2.50569	2.53378	-2.06716
C	1.50358	1.74500	-1.50766
C	0.33379	1.23874	-2.32802
C	0.33326	-1.23549	-2.33003
C	1.50357	-1.74269	-1.51103
C	2.50603	-2.52981	-2.07221
C	3.50542	-3.04694	-1.24531
C	3.47860	-2.75802	0.12084
C	2.45541	-1.95296	0.60762
H	-1.28391	2.55244	1.89398
H	-3.18505	4.11081	1.36726
H	-4.47038	3.75125	-0.75821
H	-3.82006	1.85770	-2.26422
H	-2.18867	0.00258	-2.75505
H	-3.82115	-1.85238	-2.26718
H	-4.47253	-3.74801	-0.76425
H	-3.18732	-4.11182	1.36057
H	-1.28522	-2.55545	1.88974
H	2.38597	1.67487	1.65802
H	4.23519	3.14054	0.80204
H	4.29363	3.66856	-1.65552
H	2.50181	2.74480	-3.13204
H	2.50210	-2.73877	-3.13750
H	4.29469	-3.66436	-1.66304
H	4.23628	-3.14120	0.79555
H	2.38639	-1.67822	1.65466
H	0.63420	1.08251	-3.36994
H	-0.43119	2.02127	-2.33864
H	0.63284	-1.07807	-3.37201
H	-0.43179	-2.01795	-2.34089
N	0.32220	-0.00257	2.33288
C	0.42374	-0.00381	3.53979
S	0.56144	-0.00540	5.11164

[2]FeBnTPENOH
Charge: 2+
Energy: -1570381.1023936

Fe	-0.03296	-0.00012	-0.62387
N	0.15567	-0.00005	1.40546
N	1.41676	1.35794	-0.49411
N	1.41648	-1.35826	-0.49390
N	-1.43352	1.35315	-0.29954
N	-1.43388	-1.35301	-0.29954
C	1.69485	2.36213	-1.33712
C	2.71536	3.27272	-1.06424
C	3.44501	3.13534	0.11728
C	3.13990	2.09080	0.99978
C	2.11772	1.21895	0.65521
C	1.67020	-0.00014	1.45007
C	2.11755	-1.21936	0.65534
C	3.13965	-2.09133	0.99977
C	3.44453	-3.13586	0.11718
C	2.71480	-3.27307	-1.06431
C	1.69436	-2.36235	-1.33708
C	-2.28961	1.80171	-1.23339
C	-3.32396	2.67430	-0.90905
C	-3.47455	3.07588	0.41944
C	-2.58085	2.60153	1.38308
C	-1.56088	1.74256	0.98739
C	-0.48761	1.24697	1.93401
C	-0.48784	-1.24697	1.93398
C	-1.56138	-1.74218	0.98745
C	-2.58170	-2.60067	1.38330
C	-3.47560	-3.07481	0.41973
C	-3.32485	-2.67352	-0.90882
C	-2.29015	-1.80139	-1.23330
H	1.08079	2.41519	-2.22961
H	2.92713	4.07150	-1.76659
H	4.24032	3.83440	0.35641
H	3.68334	1.96409	1.93048
H	2.06504	-0.00010	2.47086
H	3.68321	-1.96473	1.93043
H	4.23977	-3.83504	0.35620
H	2.92646	-4.07181	-1.76673
H	1.08025	-2.41509	-2.22955
H	-2.11198	1.43447	-2.23790
H	-3.99837	3.02225	-1.68381
H	-4.27784	3.74790	0.70493
H	-2.67201	2.89760	2.42344
H	-2.67296	-2.89655	2.42369
H	-4.27917	-3.74646	0.70535
H	-3.99938	-3.02134	-1.68352
H	-2.11236	-1.43444	-2.23789
H	-0.88836	1.07661	2.93760
H	0.28227	2.01877	2.02739
H	-0.88838	-1.07664	2.93765
H	0.28186	-2.01897	2.02710
O	-0.24006	-0.00072	-2.39546
H	0.60752	0.00140	-2.87443

[1]FetpenaBr
Charge: 2+
Energy: -3209716.9508974

Fe	-0.03549	-0.07879	0.25160
N	-1.20941	1.56013	-0.01668
N	-0.04499	-0.13875	-1.86680
N	-1.77684	-1.02007	0.08602
N	2.51521	-1.87636	-0.88491
N	1.77699	1.01318	0.18757
C	-1.96749	2.15800	0.92559
H	-1.76798	1.86075	1.94797
C	-2.94711	3.09274	0.60555
H	-3.52448	3.55314	1.39993
C	-3.17425	3.40347	-0.73458
H	-3.94153	4.11735	-1.01755
C	-2.40022	2.77337	-1.71181
H	-2.54613	2.98927	-2.76534
C	-1.42551	1.86365	-1.31717
C	-0.47022	1.23431	-2.29062
H	-0.88013	1.21593	-3.30726
H	0.43173	1.85500	-2.31424
C	-2.62625	-1.27159	1.09990
H	-2.27414	-1.00682	2.08852
C	-3.87904	-1.83666	0.88158
H	-4.53051	-2.03158	1.72637
C	-4.26994	-2.13213	-0.42377
H	-5.24644	-2.56044	-0.62712
C	-3.38197	-1.87379	-1.47041
H	-3.64692	-2.10353	-2.49764
C	-2.13591	-1.32938	-1.17762
C	-1.06850	-1.16826	-2.22845
H	-0.55478	-2.12939	-2.31204
H	-1.50076	-0.95023	-3.21227
C	1.25006	-0.42550	-2.57274
H	1.89973	0.43299	-2.41201
H	1.04522	-0.47234	-3.65139
C	2.03440	-1.71698	-2.25233
H	1.45580	-2.60832	-2.50087
H	2.90223	-1.70532	-2.92991
C	2.38667	-3.15521	-0.19295
H	3.28615	-3.42665	0.36514
H	2.14081	-3.96965	-0.87867
C	1.19881	-2.81860	0.72644
O	0.65324	-3.37778	1.62252
O	0.80817	-1.61894	0.23323
C	3.39853	-0.89491	-0.26432
H	4.37265	-0.95976	-0.76899
H	3.55542	-1.22232	0.76893
C	3.00574	0.58325	-0.19769
C	4.06476	1.47829	-0.37728
H	5.03163	1.10407	-0.69866
C	3.89755	2.83618	-0.11124

H	4.72080	3.53096	-0.24459
C	2.65732	3.26242	0.35088
H	2.46774	4.29812	0.61089
C	1.63898	2.32484	0.48017
H	0.66931	2.62350	0.84665
Br	0.06060	0.12845	2.62792

^{5}FetpenaCl
Charge: 2+
Energy: -1883214.4248495

Fe	0.03867	0.09692	0.81546
N	-1.15322	1.78314	0.01687
N	0.11748	-0.27385	-1.57610
N	-1.81527	-0.87546	0.38050
N	2.47426	-2.09434	-0.51155
N	2.03655	0.92736	0.40563
C	-1.94881	2.54277	0.79700
H	-1.74015	2.51416	1.85905
C	-2.98349	3.31536	0.27772
H	-3.58941	3.91917	0.94452
C	-3.22198	3.28179	-1.09536
H	-4.03046	3.85922	-1.53305
C	-2.39998	2.49220	-1.90395
H	-2.54994	2.45128	-2.97809
C	-1.37016	1.76509	-1.31575
C	-0.35526	1.02657	-2.14730
H	-0.72967	0.87628	-3.16826
H	0.52310	1.67692	-2.22215
C	-2.77128	-0.95645	1.32396
H	-2.50668	-0.56989	2.30219
C	-4.02029	-1.50421	1.05360
H	-4.76595	-1.56364	1.83878
C	-4.28178	-1.96487	-0.23773
H	-5.24890	-2.39090	-0.48604
C	-3.28294	-1.87743	-1.21025
H	-3.45533	-2.23900	-2.21906
C	-2.04865	-1.33573	-0.86343
C	-0.87610	-1.35669	-1.82035
H	-0.37291	-2.31754	-1.67638
H	-1.22610	-1.33496	-2.86140
C	1.41055	-0.55183	-2.27043
H	2.04896	0.31358	-2.10300
H	1.23654	-0.61281	-3.35567
C	2.19878	-1.82944	-1.92100
H	1.71154	-2.71769	-2.32621
H	3.16202	-1.73353	-2.44163
C	1.95299	-3.24788	0.08572
H	2.57064	-3.61614	0.91011
H	1.72168	-4.03643	-0.62749
C	0.52458	-2.81865	0.82740
O	-0.38193	-3.60310	0.72312
O	0.65080	-1.67459	1.37193
C	3.31239	-1.21430	0.31702
H	4.35368	-1.51145	0.13144
H	3.08532	-1.45151	1.35941
C	3.20386	0.28912	0.13464
C	4.35668	1.00311	-0.19202
H	5.27851	0.47026	-0.40214
C	4.32973	2.39971	-0.22290
H	5.22562	2.96135	-0.46873
C	3.13748	3.04864	0.08390
H	3.06365	4.13065	0.09625
C	2.02091	2.27536	0.39029
H	1.07592	2.74103	0.64244
Cl	-0.05531	0.87775	2.89827

^{5}FetpenaF
Charge: 2+
Energy: -1657091.7515190

Fe	-0.03370	0.08749	-0.90739
N	1.08182	1.80433	-0.16558
N	-0.08937	-0.19866	1.51616
N	1.82067	-0.85408	-0.43059
N	-2.41741	-2.07008	0.49858
N	-2.04130	0.90329	-0.57043
C	1.80301	2.55248	-1.02504
H	1.55915	2.42411	-2.07300
C	2.80324	3.41498	-0.58825
H	3.35474	4.01049	-1.30765
C	3.08302	3.47838	0.77756
H	3.86837	4.12816	1.15139
C	2.34050	2.69157	1.66259
H	2.53157	2.72303	2.73058
C	1.33809	1.87080	1.15479
C	0.39492	1.11326	2.05484
H	0.83751	0.97420	3.04955
H	-0.48738	1.74889	2.18808
C	2.76705	-0.93831	-1.38274
H	2.48146	-0.57652	-2.36507
C	4.02902	-1.45433	-1.10933
H	4.77022	-1.51962	-1.89823
C	4.30967	-1.87559	0.19180
H	5.28729	-2.27588	0.44189
C	3.31921	-1.78118	1.17303
H	3.50916	-2.11078	2.18957
C	2.07189	-1.27294	0.82337
C	0.90126	-1.27978	1.78307
H	0.39719	-2.24240	1.65349
H	1.25134	-1.24231	2.82353
C	-1.38664	-0.45520	2.21058
H	-2.02965	0.39706	1.99586
H	-1.22728	-0.46956	3.29962
C	-2.15719	-1.75345	1.90116
H	-1.66333	-2.62085	2.34183
H	-3.12659	-1.65153	2.40898
C	-1.88322	-3.23646	-0.05920
H	-2.51289	-3.65856	-0.84832
H	-1.61251	-3.98538	0.68201
C	-0.48635	-2.81667	-0.87120
O	0.42678	-3.59362	-0.76589
O	-0.63715	-1.69654	-1.45524
C	-3.29073	-1.24669	-0.35022
H	-4.32233	-1.54522	-0.11867
H	-3.08997	-1.53656	-1.38460
C	-3.19913	0.26649	-0.25613
C	-4.36174	0.98207	0.02770
H	-5.27411	0.45008	0.27739
C	-4.35813	2.37798	-0.03705
H	-5.26244	2.94016	0.17437
C	-3.17824	3.02382	-0.39278
H	-3.12250	4.10350	-0.47946
C	-2.04854	2.24997	-0.64531
H	-1.11087	2.71635	-0.92131
F	0.24516	0.70055	-2.53854

^{5}FetpenaN_3
Charge: 2+
Energy: -1697480.1661066

Fe	-0.08854	-0.13004	0.20553
N	-0.28059	1.92737	0.62592
N	-0.76097	0.71168	-1.79113
N	-2.23071	-0.41342	0.27636
N	0.23620	-1.91205	-1.11032
N	1.97838	0.14891	-0.38256
C	-0.39550	2.43631	1.86869
H	-0.29554	1.73060	2.68634
C	-0.61061	3.79324	2.08816
H	-0.69462	4.17079	3.10134
C	-0.71589	4.63989	0.98325
H	-0.88950	5.70303	1.11901
C	-0.60141	4.10619	-0.30526
H	-0.68327	4.74281	-1.18056
C	-0.37787	2.74231	-0.45380
C	-0.17449	2.07883	-1.80171
H	-0.59519	2.69069	-2.60885
H	0.89809	1.98244	-1.99212
C	-2.84420	-1.03612	1.30943
H	-2.20824	-1.31588	2.14125
C	-4.20397	-1.31522	1.29988
H	-4.65829	-1.81546	2.14817
C	-4.95422	-0.95266	0.17727
H	-6.01655	-1.17140	0.12876
C	-4.32145	-0.30135	-0.88178
H	-4.87944	0.00298	-1.76211
C	-2.95655	-0.03151	-0.79221
C	-2.25219	0.78351	-1.85291
H	-2.60140	0.49625	-2.85127
H	-2.55137	1.82795	-1.71239
C	-0.19296	-0.18805	-2.83329
H	0.87384	0.02789	-2.91976
H	-0.64807	0.00301	-3.81320
C	-0.40529	-1.64592	-2.42577
H	-1.47355	-1.85226	-2.32183
H	-0.01606	-2.31891	-3.19966
C	-0.39389	-3.00648	-0.32452
H	-0.03699	-3.99708	-0.62375
H	-1.47586	-2.97591	-0.47776
C	-0.13978	-2.77391	1.17565
O	-0.22348	-3.64454	1.99838
O	0.12140	-1.48190	1.46297
C	1.70825	-2.13617	-1.19435
H	1.95791	-2.66850	-2.11978
H	1.99443	-2.79139	-0.36424
C	2.53672	-0.88262	-1.04958
C	3.85840	-0.83714	-1.49266
H	4.27790	-1.68003	-2.03280
C	4.63024	0.28896	-1.21129
H	5.66372	0.34101	-1.53969
C	4.05661	1.34459	-0.49532
H	4.62570	2.23317	-0.24471
C	2.72950	1.23772	-0.10488
H	2.23660	2.02375	0.45370
N	2.00703	0.30525	2.89268
N	2.56983	-0.68444	2.55889
N	3.11480	-1.66376	2.19487

[1]FetpenaNCS
Charge: 2+
Energy: -1902563.9067230

Fe	-0.07936	0.07026	0.25993
N	-1.03745	1.65457	-0.56227
N	-0.46371	-0.82689	-1.63157
N	-1.90706	-0.53066	0.66530
N	1.96414	-2.60814	-0.50733
N	1.88466	0.59975	-0.37013
C	-1.43464	2.74687	0.12515
H	-1.02211	2.85244	1.12028
C	-2.33128	3.66845	-0.40137
H	-2.61484	4.53579	0.18483
C	-2.86297	3.44237	-1.67225
H	-3.57816	4.13438	-2.10583
C	-2.46506	2.30525	-2.37571
H	-2.85607	2.09514	-3.36616
C	-1.54569	1.43788	-1.79193
C	-0.97075	0.26692	-2.53200
H	-1.68355	-0.14045	-3.25786
H	-0.11422	0.63768	-3.10485
C	-2.61020	-0.15469	1.74776
H	-2.09414	0.49278	2.44491
C	-3.91810	-0.58154	1.95136
H	-4.45258	-0.26727	2.84103
C	-4.51411	-1.40810	0.99870
H	-5.53592	-1.75145	1.12610
C	-3.77678	-1.79423	-0.12291
H	-4.20638	-2.44484	-0.87787
C	-2.46731	-1.34534	-0.25223
C	-1.54387	-1.82119	-1.34270
H	-1.06869	-2.73792	-0.98478
H	-2.09119	-2.07985	-2.25721
C	0.66793	-1.46308	-2.39311
H	1.40092	-0.67641	-2.56387
H	0.28457	-1.77057	-3.37622
C	1.38000	-2.70930	-1.82899
H	0.71711	-3.57678	-1.84083
H	2.17918	-2.92351	-2.55671
C	1.50349	-3.50557	0.54044
H	2.30355	-3.74090	1.24884
H	1.12304	-4.44554	0.13502
C	0.39817	-2.68252	1.22662
O	-0.52928	-3.03869	1.90083
O	0.67975	-1.42139	0.89008
C	3.06387	-1.69609	-0.24785
H	3.94963	-2.07906	-0.77434
H	3.28126	-1.74850	0.82233
C	2.96020	-0.19927	-0.61256
C	4.15038	0.34455	-1.11082
H	4.99073	-0.31297	-1.30905
C	4.28055	1.71418	-1.32812
H	5.21049	2.12730	-1.70614
C	3.19068	2.52811	-1.04009
H	3.22564	3.60397	-1.17274
C	2.02743	1.92779	-0.57492
H	1.16303	2.53353	-0.34630
N	0.18877	1.01467	1.84533
C	1.01195	1.42284	2.61733
S	2.04872	1.98425	3.68987

[5]FetpenaOH
Charge: 2+
Energy: -1642001.1183859

Fe	-0.01744	0.11915	-0.73795
N	0.99081	1.82484	-0.18925
N	-0.01303	-0.24184	1.46138
N	1.92082	-0.80360	-0.42915
N	-2.33902	-2.13574	0.48257
N	-2.12543	0.83951	-0.48606
C	1.59692	2.63177	-1.08083
H	1.30033	2.48760	-2.11353
C	2.55266	3.56352	-0.68972
H	3.01382	4.20644	-1.43142
C	2.91035	3.63302	0.65775
H	3.66665	4.33626	0.99271
C	2.28647	2.78306	1.57549
H	2.54125	2.81722	2.62989
C	1.31979	1.89461	1.11731
C	0.49117	1.05442	2.05004
H	1.02693	0.85568	2.98516
H	-0.38911	1.65118	2.31103
C	2.89080	-0.79813	-1.35656
H	2.61100	-0.39576	-2.32428
C	4.16932	-1.27401	-1.07947
H	4.93076	-1.26745	-1.85172
C	4.44134	-1.74960	0.20452
H	5.43002	-2.12057	0.45625
C	3.42765	-1.74543	1.16742
H	3.60965	-2.11478	2.17170
C	2.17108	-1.27133	0.80614
C	0.96925	-1.34492	1.71712
H	0.46797	-2.29441	1.51172
H	1.26417	-1.35614	2.77396
C	-1.30834	-0.50713	2.17306
H	-1.95587	0.34098	1.96199
H	-1.12187	-0.51377	3.25672
C	-2.06911	-1.81264	1.87955
H	-1.56170	-2.67180	2.32135
H	-3.03274	-1.71539	2.39852
C	-1.74453	-3.25595	-0.09922
H	-2.36524	-3.71442	-0.87524
H	-1.40188	-3.99151	0.62535
C	-0.39857	-2.75115	-0.97387
O	0.52849	-3.52044	-0.93353
O	-0.60861	-1.62908	-1.52364
C	-3.28344	-1.35894	-0.33123
H	-4.29023	-1.71707	-0.07572
H	-3.09428	-1.62742	-1.37338
C	-3.26679	0.15460	-0.22379
C	-4.47063	0.81488	0.02278
H	-5.36777	0.24209	0.23479
C	-4.52306	2.21016	-0.02857
H	-5.45720	2.73217	0.15403
C	-3.35794	2.90814	-0.33084
H	-3.34446	3.99031	-0.40264
C	-2.18801	2.18323	-0.54656
H	-1.26004	2.68953	-0.78314
O	0.16053	0.64526	-2.41969
H	-0.14728	-0.06832	-3.01203

[6]FePhIOTf3BrOH
Charge: 0
Energy: -4645979.4985462

Fe	-0.43646	0.40800	-1.18087
O	-2.28069	-0.00671	-1.05096
S	-3.12482	-1.31345	-1.21947
O	-2.28451	-2.52295	-1.17841
O	-4.12786	-1.17215	-2.26112
C	-3.99153	-1.25954	0.43376
F	-3.07657	-1.41300	1.39982
F	-4.62193	-0.10418	0.58861
F	-4.86323	-2.26759	0.49158
O	1.01256	1.68135	-1.27532
S	2.51551	1.56979	-0.83639
O	2.71796	0.71367	0.32518
O	3.09897	2.90269	-0.90151
C	3.21075	0.62775	-2.30349
F	2.57761	1.00397	-3.42983
F	3.04351	-0.68729	-2.13883
O	-0.21452	0.29103	0.73176
S	-0.89182	0.90010	1.98753
O	-0.94976	-0.10784	3.04496
O	-2.10249	1.67257	1.66752
F	4.50855	0.89477	-2.42215
C	0.41512	2.12978	2.51425
F	1.49649	1.47149	2.93431
F	-0.07773	2.86158	3.51291
F	0.73694	2.92248	1.49443
O	0.38259	-1.31919	-1.36660
I	0.32849	-2.71348	0.01360
C	2.12035	-2.23552	1.03253
C	3.34361	-2.50102	0.41274
H	3.39186	-2.98649	-0.55541
C	4.50670	-2.10614	1.06975
H	5.47153	-2.29474	0.60881
C	4.42985	-1.46132	2.30801
H	5.34185	-1.14813	2.80747
C	3.19272	-1.20394	2.90078
H	3.13476	-0.68090	3.84987
C	2.01306	-1.58014	2.25983
H	1.04913	-1.34533	2.69627
O	-0.55119	0.61616	-2.93039
H	0.26968	1.05383	-3.24128
Br	-2.03621	3.30047	-0.54796

[6]FePhIOTf3FOH
Charge: 0
Energy: -3093320.7314838

Fe	0.51279	0.10574	1.31726
O	2.51351	0.14335	1.78356
S	3.64077	-0.71264	1.20708
O	3.15580	-1.98883	0.59386
O	4.76822	-0.82777	2.12199
C	4.22785	0.30706	-0.25716
F	3.51757	-0.00508	-1.34462
F	4.09853	1.60204	0.00944
F	5.51302	0.02109	-0.48507
O	-1.88758	-0.25203	0.54264
S	-3.09665	0.58258	0.43055
O	-3.77815	0.48253	-0.92714
O	-3.03123	1.98861	0.84376
C	-4.29826	-0.24880	1.58626

F	-3.78670	-0.25377	2.81636
F	-4.49568	-1.51421	1.18642
O	0.39240	1.78975	0.47398
S	0.28550	2.19941	-1.03858
O	-0.91409	1.64368	-1.67392
O	1.56742	2.10969	-1.72788
F	-5.46093	0.39870	1.58188
C	-0.06713	4.00784	-0.74132
F	-1.18153	4.14686	-0.02955
F	-0.22012	4.59857	-1.93133
F	0.95554	4.56700	-0.09676
O	0.89203	-0.56044	-0.38474
I	0.95826	-2.44745	-0.78103
C	-1.03144	-2.26159	-1.54030
C	-2.05977	-3.04491	-0.98175
H	-1.83434	-3.81898	-0.25564
C	-3.37239	-2.78711	-1.35184
H	-4.18122	-3.36965	-0.92442
C	-3.64881	-1.73365	-2.23338
H	-4.67306	-1.50957	-2.50914
C	-2.59950	-0.95264	-2.76948
H	-2.82294	-0.11704	-3.42205
C	-1.27418	-1.22243	-2.42815
H	-0.48180	-0.57785	-2.78585
O	0.21270	-1.56400	1.87032
H	-0.00849	-1.52381	2.82081
F	-0.02623	0.73596	2.82748

[6]FePhIOTf3OHNCS
Charge: 0
Energy: -3338829.4447117

Fe	-0.57739	0.24379	-0.94223
O	0.81527	1.31025	-0.04329
S	1.59207	2.59795	-0.41423
O	2.10115	3.25350	0.78458
O	0.84947	3.39692	-1.41274
C	3.05023	1.88089	-1.33357
F	3.73721	1.07220	-0.53487
F	2.59998	1.21009	-2.39423
F	3.83064	2.88487	-1.73700
O	-2.46060	-0.10764	-0.79796
S	-3.25693	-0.97373	0.22576
O	-2.75076	-0.82330	1.60592
O	-3.55400	-2.30638	-0.27787
C	-4.83715	0.01923	0.18907
F	-5.34837	0.00679	-1.03885
F	-4.58764	1.27960	0.55691
O	0.33235	-0.84826	-2.23161
S	1.46763	-1.91282	-2.00713
O	2.41083	-1.50395	-0.96720
O	1.94893	-2.34185	-3.31400
F	-5.70264	-0.52700	1.04378
C	0.50358	-3.38829	-1.30139
F	0.81673	-3.56461	-0.00622
F	0.85795	-4.48244	-1.97274
F	-0.80823	-3.20154	-1.41366
O	-0.22451	-1.05341	0.32783
I	-0.02319	-0.72198	2.23363
C	2.08378	-0.53908	2.26464
C	2.62252	0.71862	2.54448
H	1.99253	1.58402	2.70962
C	4.01042	0.84715	2.54821
H	4.45113	1.81855	2.74812
C	4.81761	-0.25419	2.25258
H	5.89769	-0.14141	2.24041
C	4.24890	-1.49369	1.94553
H	4.87976	-2.33744	1.68452
C	2.86459	-1.65177	1.94724
H	2.41371	-2.59430	1.66314
O	-0.96130	1.50084	-2.08709
H	-0.30296	2.24577	-2.13160
N	-1.70365	2.24285	1.16378
C	-2.01779	3.11209	0.42130
S	-2.41902	4.30297	-0.61904

[5]FeiPrBIPO2BrOHC
Charge: 0
Energy: -3459232.3576671

Fe	-0.03425	0.06930	0.09007
C	-2.37843	-1.31879	1.46779
C	-1.14203	-1.80914	2.15064
C	-1.15381	-2.68348	3.24381
H	-2.08757	-3.06521	3.63906
C	0.06150	-3.04967	3.82042
H	0.08097	-3.72485	4.67040
C	1.25105	-2.54174	3.30179
H	2.20280	-2.81387	3.74192
C	1.18969	-1.67650	2.20182
C	2.39267	-1.07162	1.55422
C	-3.71670	-1.80479	1.95817
H	-4.52285	-1.36580	1.37029
H	-3.85994	-1.53432	3.01104
H	-3.77781	-2.89696	1.88192
C	3.73506	-1.29418	2.20022
H	3.97128	-2.36330	2.24764
H	3.72307	-0.90938	3.22694
H	4.52156	-0.78597	1.64303
C	-3.29875	0.08423	-0.21635
C	-3.79319	-0.57075	-1.36062
C	-4.85176	0.03519	-2.04736
H	-5.25010	-0.45018	-2.93386
C	-5.39198	1.24610	-1.62362
H	-6.21379	1.69832	-2.17223
C	-4.86536	1.88285	-0.50285
H	-5.27825	2.83496	-0.18149
C	-3.80281	1.32642	0.21718
C	-3.19697	-1.87384	-1.87494
H	-2.39185	-2.17465	-1.20149
C	-4.23765	-3.00824	-1.89750
H	-4.67133	-3.17480	-0.90341
H	-3.77354	-3.94464	-2.22927
H	-5.06238	-2.78495	-2.58459
C	-2.55346	-1.66610	-3.25864
H	-3.30873	-1.41288	-4.01276
H	-2.04232	-2.58093	-3.57987
H	-1.81570	-0.85990	-3.22253
C	-3.22345	2.05608	1.42161
H	-2.33522	1.51656	1.75834
C	-2.74206	3.46734	1.03696
H	-2.05049	3.41889	0.18885
H	-2.22610	3.93287	1.88556
H	-3.57568	4.12141	0.75429
C	-4.23042	2.10328	2.58520
H	-5.13708	2.65442	2.30687
H	-3.78821	2.60095	3.45666
H	-4.53783	1.09471	2.88893
C	3.26774	0.25936	-0.20478
C	3.60147	1.58727	0.13399
C	4.64285	2.19752	-0.57419
H	4.91891	3.21836	-0.32589
C	5.32748	1.52455	-1.58136
H	6.13238	2.01805	-2.11940
C	4.97589	0.21549	-1.89670
H	5.51410	-0.30904	-2.68057
C	3.93995	-0.44488	-1.22553
C	2.89883	2.34537	1.25228
H	2.05756	1.74679	1.60692
C	2.29120	3.66678	0.74804
H	3.06227	4.37642	0.42410
H	1.71812	4.14399	1.55264
H	1.61949	3.48329	-0.09650
C	3.85292	2.58696	2.43744
H	4.70319	3.21598	2.14623
H	4.25830	1.64440	2.82584
H	3.32545	3.09217	3.25548
C	3.60563	-1.88707	-1.58720
H	2.66130	-2.14995	-1.10506
C	4.69347	-2.85059	-1.07209
H	5.66140	-2.63063	-1.53852
H	4.43271	-3.88879	-1.31090
H	4.82717	-2.77394	0.01276
C	3.39758	-2.06865	-3.10126
H	4.33518	-1.94461	-3.65624
H	2.67003	-1.34706	-3.47957
H	3.01935	-3.07616	-3.30821
N	2.18384	-0.37935	0.49365
N	0.01302	-1.34118	1.66212
N	-2.20107	-0.49374	0.50343
O	-0.17061	-1.50567	-1.10505
O	0.59767	-1.59040	-2.12591
O	-0.08017	1.36298	1.41930
H	-0.21121	2.23344	1.00801
Br	-0.18945	1.70546	-1.75897

[5]FeiPrBIPO2Cl2C
Charge: 0
Energy: -2373919.7727615

Fe	-0.00009	-0.31745	-0.14050
C	2.38927	0.12283	1.75449
C	1.16907	0.18262	2.61654
C	1.20584	0.19604	4.01582
H	2.14926	0.18481	4.54798
C	0.00006	0.20780	4.71517
H	0.00006	0.21357	5.80088
C	-1.20571	0.19646	4.01581
H	-2.14915	0.18551	4.54794
C	-1.16893	0.18307	2.61653
C	-2.38912	0.12378	1.75441
C	3.73682	0.13266	2.42699
H	4.53848	0.13004	1.68884
H	3.83791	-0.76147	3.05477
H	3.84996	1.00918	3.07457
C	-3.73669	0.13340	2.42688
H	-3.84955	1.00916	3.07552
H	-3.83810	-0.76148	3.05356

H	-4.53833	0.13193	1.68870
C	3.29428	0.03277	-0.43835
C	3.81529	1.26889	-0.87875
C	4.87218	1.24307	-1.79644
H	5.29570	2.18233	-2.14024
C	5.38504	0.04264	-2.27870
H	6.20191	0.04676	-2.99530
C	4.84150	-1.16104	-1.84148
H	5.23459	-2.09940	-2.22197
C	3.79145	-1.19574	-0.91699
C	3.28133	2.61147	-0.39250
H	2.36642	2.42964	0.17747
C	4.28578	3.30958	0.54559
H	4.52723	2.68967	1.41570
H	3.87991	4.26238	0.90684
H	5.22500	3.52119	0.02106
C	2.91216	3.53530	-1.56800
H	3.80448	3.86677	-2.11155
H	2.39745	4.43094	-1.20065
H	2.25402	3.02548	-2.27671
C	3.22524	-2.52969	-0.45942
H	2.45265	-2.34275	0.28695
C	2.53033	-3.26067	-1.62191
H	1.74415	-2.63393	-2.05250
H	2.06404	-4.18152	-1.25594
H	3.24443	-3.52129	-2.41387
C	4.30171	-3.40920	0.20198
H	5.08868	-3.69532	-0.50657
H	3.84750	-4.32990	0.58564
H	4.78334	-2.89097	1.04104
C	-3.29418	0.03433	-0.43841
C	-3.79286	-1.19403	-0.91580
C	-4.84298	-1.15891	-1.84021
H	-5.23721	-2.09715	-2.21984
C	-5.38516	0.04500	-2.27844
H	-6.20215	0.04942	-2.99492
C	-4.87079	1.24528	-1.79740
H	-5.29326	2.18472	-2.14198
C	-3.81368	1.27066	-0.87997
C	-3.22796	-2.52825	-0.45736
H	-2.45533	-2.34162	0.28905
C	-2.53345	-3.26037	-1.61938
H	-3.24763	-3.52069	-2.41137
H	-2.06805	-4.18148	-1.25292
H	-1.74663	-2.63450	-2.05007
C	-4.30534	-3.40650	0.20422
H	-5.09237	-3.69234	-0.50438
H	-4.78675	-2.88744	1.04288
H	-3.85201	-4.32740	0.58846
C	-3.27797	2.61283	-0.39460
H	-2.36220	2.43012	0.17364
C	-4.28034	3.31143	0.54533
H	-5.22031	3.52360	0.02237
H	-3.87329	4.26394	0.90602
H	-4.52070	2.69156	1.41578
C	-2.91004	3.53667	-1.57042
H	-3.80286	3.86893	-2.11268
H	-2.25317	3.02657	-2.28012
H	-2.39420	4.43188	-1.20360
N	-2.19246	0.02941	0.48827
N	0.00007	0.19884	1.96477
N	2.19262	0.02803	0.48837
O	0.00224	2.02341	-0.19730
O	0.00030	2.68170	-1.23187
Cl	-0.00095	-2.54857	0.78595
Cl	-0.00118	-0.32881	-2.39144

^{5}FeiPrBIPO2ClOHC
Charge: 0
Energy: -2132703.1801437

Fe	-0.03986	0.19642	-0.06119
C	-2.39268	-0.50271	1.75327
C	-1.16267	-0.63560	2.59126
C	-1.18265	-0.92419	3.96079
H	-2.11950	-1.09186	4.47860
C	0.02794	-0.98182	4.64952
H	0.04138	-1.19918	5.71315
C	1.22060	-0.75386	3.96566
H	2.16887	-0.78867	4.48827
C	1.16754	-0.48143	2.59281
C	2.37505	-0.23362	1.74917
C	-3.73480	-0.75264	2.38841
H	-4.53437	-0.62214	1.65908
H	-3.89869	-0.05651	3.21967
H	-3.78526	-1.77150	2.79018
C	3.71497	-0.13920	2.43048
H	3.94108	-1.05764	2.98337
H	3.70506	0.68881	3.14967
H	4.50691	0.03752	1.70303
C	-3.28637	0.02802	-0.38642
C	-3.78106	-1.07484	-1.10918
C	-4.82406	-0.83968	-2.01315
H	-5.22511	-1.67356	-2.58240
C	-5.34723	0.43656	-2.20088
H	-6.15703	0.59494	-2.90802
C	-4.82058	1.51146	-1.48890
H	-5.22174	2.50890	-1.64518
C	-3.77410	1.33560	-0.57796
C	-3.21093	-2.47861	-0.95159
H	-2.38850	-2.43935	-0.23408
C	-4.26734	-3.45915	-0.40873
H	-4.67467	-3.12042	0.55200
H	-3.82744	-4.45285	-0.26198
H	-5.10835	-3.56677	-1.10396
C	-2.60608	-2.97881	-2.27626
H	-3.37527	-3.08805	-3.05041
H	-2.13123	-3.95586	-2.12911
H	-1.84357	-2.28413	-2.63746
C	-3.19936	2.52479	0.17949
H	-2.32234	2.18722	0.73693
C	-2.69730	3.61397	-0.78562
H	-1.98375	3.19010	-1.49989
H	-2.20001	4.41364	-0.22280
H	-3.51828	4.06848	-1.35326
C	-4.21949	3.08841	1.18572
H	-5.11716	3.46154	0.67749
H	-3.78251	3.91989	1.75171
H	-4.54058	2.32099	1.90140
C	3.25166	0.13396	-0.42666
C	3.62399	1.46036	-0.72574
C	4.66483	1.65267	-1.64151
H	4.97059	2.66657	-1.88369
C	5.31079	0.57616	-2.24135
H	6.11652	0.74820	-2.94997
C	4.91875	-0.72336	-1.93172
H	5.42606	-1.56085	-2.40099
C	3.88041	-0.97695	-1.02816
C	2.95606	2.66176	-0.07001
H	2.12679	2.30856	0.54642
C	2.33272	3.60138	-1.11819
H	3.09381	4.05417	-1.76540
H	1.79579	4.41628	-0.61660
H	1.62536	3.05509	-1.74977
C	3.94385	3.41574	0.84027
H	4.78300	3.82945	0.26759
H	4.36355	2.75693	1.61061
H	3.43862	4.24847	1.34411
C	3.49575	-2.41385	-0.69394
H	2.52737	-2.39662	-0.18832
C	4.52686	-3.05092	0.25926
H	5.51691	-3.09043	-0.21112
H	4.23347	-4.07632	0.51514
H	4.62870	-2.48409	1.19101
C	3.32608	-3.28174	-1.95335
H	4.28644	-3.46930	-2.44866
H	2.65309	-2.80231	-2.66745
H	2.89926	-4.25362	-1.68109
N	2.16913	-0.09206	0.49072
N	-0.00466	-0.43585	1.95000
N	-2.20425	-0.16000	0.53329
O	-0.16492	-1.70207	-0.56614
O	0.56588	-2.10255	-1.54549
O	-0.04158	1.90932	0.64625
H	-0.15711	2.53203	-0.09126
Cl	-0.22845	0.94222	-2.21185

^{5}FeiPrBIPO2FOHC
Charge: 0
Energy: -1906574.9552307

Fe	-0.07520	0.41779	0.07853
C	-2.38286	-0.84227	1.59784
C	-1.17085	-1.04402	2.44374
C	-1.20216	-1.53653	3.75334
H	-2.14108	-1.81522	4.21720
C	-0.00175	-1.65190	4.45232
H	0.00320	-2.02407	5.47224
C	1.19257	-1.28382	3.83436
H	2.13434	-1.36515	4.36401
C	1.15074	-0.80841	2.51847
C	2.35930	-0.42166	1.73327
C	-3.72742	-1.27144	2.12052
H	-4.50308	-1.08749	1.37652
H	-3.97481	-0.71280	3.03148
H	-3.72264	-2.33788	2.37392
C	3.71365	-0.55419	2.37608
H	3.91222	-1.58965	2.67380
H	3.75380	0.06612	3.27996
H	4.49653	-0.22765	1.69114
C	-3.20497	-0.02598	-0.48479
C	-3.52649	-1.01636	-1.43255
C	-4.53369	-0.71957	-2.35830
H	-4.81180	-1.46901	-3.09409
C	-5.17533	0.51667	-2.35766
H	-5.95413	0.72585	-3.08619
C	-4.80307	1.49110	-1.43404
H	-5.28719	2.46368	-1.45277

C	-3.80362	1.24790	-0.48613
C	-2.81590	-2.36453	-1.46676
H	-1.99669	-2.33717	-0.74385
C	-3.77320	-3.50429	-1.06932
H	-4.20720	-3.33788	-0.07569
H	-3.24470	-4.46513	-1.05478
H	-4.60331	-3.58913	-1.78102
C	-2.16567	-2.63022	-2.83622
H	-2.91224	-2.67570	-3.63817
H	-1.63605	-3.59034	-2.81729
H	-1.43762	-1.85058	-3.07401
C	-3.36466	2.34023	0.48053
H	-2.55356	1.94959	1.10116
C	-2.76770	3.53342	-0.28918
H	-1.94093	3.18459	-0.91382
H	-2.39235	4.28638	0.41570
H	-3.51514	4.01742	-0.92979
C	-4.51246	2.77245	1.40980
H	-5.34556	3.20789	0.84465
H	-4.16260	3.52767	2.12373
H	-4.90833	1.92216	1.97949
C	3.17643	0.27098	-0.39729
C	3.47755	1.61522	-0.69530
C	4.44598	1.86809	-1.67148
H	4.69686	2.89748	-1.91170
C	5.08668	0.82742	-2.33863
H	5.83443	1.04329	-3.09705
C	4.76223	-0.49181	-2.03492
H	5.25974	-1.29940	-2.56428
C	3.80084	-0.80682	-1.06753
C	2.79418	2.76791	0.02852
H	2.10397	2.35165	0.76739
C	1.94196	3.60609	-0.94354
H	2.55732	4.05016	-1.73548
H	1.45449	4.42730	-0.40148
H	1.16560	2.98844	-1.40482
C	3.81383	3.63782	0.78638
H	4.51497	4.12978	0.10148
H	4.40331	3.03863	1.49135
H	3.29702	4.42123	1.35330
C	3.47699	-2.27242	-0.78509
H	2.63153	-2.31274	-0.09166
C	4.67692	-2.98733	-0.13030
H	5.52850	-3.02502	-0.81993
H	4.41384	-4.01990	0.12956
H	5.01645	-2.48124	0.77932
C	3.03917	-3.02857	-2.05447
H	3.84778	-3.07110	-2.79388
H	2.17158	-2.54468	-2.50822
H	2.77324	-4.06160	-1.79760
N	2.13794	0.00671	0.54567
N	-0.01175	-0.71104	1.86065
N	-2.16949	-0.28793	0.46331
O	0.12612	-1.12394	-1.07927
O	0.79252	-0.80775	-2.15539
O	-0.13279	1.84624	1.23560
H	-0.18481	2.62355	0.65358
F	-0.49186	1.48171	-1.30893

^{5}FeiPrBIPO2N$_3$OHC
Charge: 0
Energy: -1946967.1768868

Fe	-0.01852	0.30631	0.14767
C	-2.31229	-1.06862	1.63131
C	-1.06909	-1.37421	2.40054
C	-1.06245	-2.02604	3.63919
H	-1.98634	-2.37104	4.08812
C	0.15556	-2.20966	4.29101
H	0.18961	-2.70368	5.25723
C	1.32940	-1.75110	3.69591
H	2.28411	-1.88045	4.19138
C	1.25057	-1.12400	2.44654
C	2.44129	-0.63371	1.68940
C	-3.63569	-1.57129	2.14307
H	-4.44184	-1.27556	1.47110
H	-3.83938	-1.16078	3.13929
H	-3.62676	-2.66422	2.22717
C	3.79433	-0.70192	2.34647
H	4.04300	-1.72546	2.64672
H	3.79093	-0.08092	3.25095
H	4.56743	-0.33408	1.67152
C	-3.21604	0.03940	-0.27957
C	-3.63440	-0.81532	-1.31815
C	-4.65824	-0.35654	-2.15632
H	-5.00281	-0.99552	-2.96418
C	-5.22842	0.90096	-1.98310
H	-6.01917	1.23624	-2.64866
C	-4.77156	1.73594	-0.96520
H	-5.21083	2.72161	-0.84041
C	-3.74982	1.33170	-0.10107
C	-3.01280	-2.18792	-1.54815
H	-2.17114	-2.30382	-0.86121
C	-4.02778	-3.31065	-1.25902
H	-4.41743	-3.25087	-0.23549
H	-3.56033	-4.29406	-1.38952
H	-4.88436	-3.25448	-1.94140
C	-2.43103	-2.31568	-2.96769
H	-3.21502	-2.25160	-3.73169
H	-1.93157	-3.28536	-3.07958
H	-1.69686	-1.52998	-3.15902
C	-3.25616	2.24816	1.01100
H	-2.35075	1.81008	1.43914
C	-2.85033	3.63366	0.47950
H	-2.09183	3.53031	-0.30260
H	-2.43196	4.23801	1.29393
H	-3.70376	4.18384	0.06551
C	-4.30781	2.36208	2.13082
H	-5.23579	2.81242	1.75741
H	-3.93365	2.98737	2.95041
H	-4.56176	1.37721	2.54238
C	3.24677	0.24366	-0.37091
C	3.60859	1.60423	-0.40926
C	4.59524	1.98991	-1.32413
H	4.89456	3.03344	-1.36765
C	5.19541	1.06376	-2.17188
H	5.95935	1.38288	-2.87580
C	4.81148	-0.27438	-2.11863
H	5.28309	-0.99123	-2.78391
C	3.82592	-0.71714	-1.22990
C	2.97947	2.63197	0.52267
H	2.20930	2.13739	1.11965
C	2.26200	3.74301	-0.26528
H	2.95976	4.31537	-0.88860
H	1.78316	4.44521	0.42896
H	1.48765	3.31662	-0.91061
C	4.02575	3.21480	1.49116
H	4.81071	3.76146	0.95447
H	4.51358	2.42449	2.07521
H	3.55096	3.91180	2.19202
C	3.44625	-2.19503	-1.17763
H	2.50256	-2.28155	-0.63129
C	4.52329	-3.00443	-0.42618
H	5.48054	-2.95910	-0.95970
H	4.23066	-4.05868	-0.34860
H	4.69530	-2.62356	0.58567
C	3.20695	-2.80442	-2.57039
H	4.12197	-2.81624	-3.17435
H	2.43199	-2.25244	-3.10521
H	2.87379	-3.84392	-2.46373
N	2.20493	-0.16869	0.51948
N	0.07150	-0.95817	1.83483
N	-2.14514	-0.36327	0.57659
O	-0.03894	-1.17167	-1.09039
O	0.77515	-0.91634	-2.08353
O	0.01516	1.63992	1.42223
H	-0.14980	2.46989	0.94283
N	-0.44939	1.64272	-1.16277
N	-0.83553	1.36765	-2.28578
N	-1.21446	1.18070	-3.35525

^{5}FeiPrBIPO2NCSOHC
Charge: 0
Energy: -2152073.6716367

Fe	0.04752	0.04136	-0.29600
C	-2.10803	2.19476	-0.27666
C	-0.82580	2.88052	-0.61502
C	-0.73902	4.22630	-0.98932
H	-1.62400	4.85078	-1.01659
C	0.50675	4.74428	-1.33884
H	0.60172	5.78266	-1.64119
C	1.62944	3.91951	-1.30037
H	2.60501	4.30493	-1.57123
C	1.47262	2.58687	-0.90084
C	2.60489	1.62373	-0.76672
C	-3.38033	2.99802	-0.23777
H	-4.22105	2.36755	0.05236
H	-3.58901	3.43063	-1.22362
H	-3.29081	3.82372	0.47779
C	3.98751	2.07823	-1.14904
H	4.30730	2.93289	-0.54306
H	3.99154	2.39396	-2.19951
H	4.70595	1.26820	-1.02210
C	-3.16352	0.12045	0.22003
C	-3.54965	-0.08238	1.55770
C	-4.66280	-0.89813	1.79150
H	-4.98366	-1.07091	2.81470
C	-5.34960	-1.50319	0.74343
H	-6.20571	-2.13954	0.94902
C	-4.91864	-1.31541	-0.56728
H	-5.44054	-1.81096	-1.38084
C	-3.81168	-0.51249	-0.85886
C	-2.78962	0.53536	2.72387
H	-1.92847	1.07735	2.32576
C	-3.66592	1.53937	3.49582
H	-4.03609	2.33704	2.83942
H	-3.09379	2.00327	4.30821

H	-4.53856	1.04669	3.94086
C	-2.22352	-0.55282	3.65402
H	-3.02421	-1.13342	4.12704
H	-1.62235	-0.09338	4.44744
H	-1.58196	-1.24111	3.09823
C	-3.33253	-0.34404	-2.29516
H	-2.39172	0.21213	-2.28298
C	-3.01735	-1.70349	-2.94583
H	-2.30126	-2.26489	-2.33804
H	-2.58946	-1.55152	-3.94448
H	-3.91528	-2.32185	-3.05840
C	-4.34939	0.45382	-3.13212
H	-5.31034	-0.07103	-3.19523
H	-3.97804	0.60122	-4.15345
H	-4.54128	1.44091	-2.69334
C	3.28137	-0.53012	-0.00317
C	3.47368	-1.60218	-0.89800
C	4.38194	-2.60216	-0.53650
H	4.55108	-3.43201	-1.21675
C	5.06927	-2.54911	0.67270
H	5.76691	-3.33824	0.93963
C	4.86136	-1.47966	1.53927
H	5.40341	-1.44256	2.47964
C	3.96686	-0.44776	1.23172
C	2.76756	-1.65666	-2.24606
H	2.05935	-0.82646	-2.30072
C	1.94297	-2.94550	-2.41073
H	2.57750	-3.83983	-2.40776
H	1.40420	-2.92566	-3.36650
H	1.20977	-3.04024	-1.60458
C	3.77679	-1.48353	-3.39727
H	4.50557	-2.30297	-3.41802
H	4.33638	-0.54486	-3.29916
H	3.25693	-1.47054	-4.36263
C	3.80103	0.71178	2.21249
H	2.97274	1.33982	1.86999
C	5.08045	1.57407	2.25697
H	5.91978	0.99680	2.66244
H	4.93341	2.44724	2.90414
H	5.37926	1.92878	1.26557
C	3.44040	0.24249	3.63504
H	4.23516	-0.37557	4.06866
H	2.51046	-0.32873	3.62889
H	3.30910	1.11376	4.28868
N	2.29890	0.45775	-0.33099
N	0.26747	2.10801	-0.56736
N	-2.02007	0.93509	-0.06288
O	0.18331	0.21810	1.62257
O	0.92142	-0.75414	2.07184
O	-0.02883	-0.00739	-2.13518
H	-0.28248	-0.91391	-2.37904
N	-0.54509	-1.79036	-0.17056
C	-1.20875	-2.69464	0.23211
S	-2.09975	-3.94244	0.72929

[5]FeiPrBIPO2OHBrC
Charge: 0
Energy: -3459236.0082913

Fe	-0.00055	-0.27516	-0.24662
C	2.38725	-0.07492	1.71209
C	1.16834	-0.20914	2.56537
C	1.20443	-0.44193	3.94400
H	2.14964	-0.54134	4.46398
C	-0.00086	-0.55834	4.63436
H	-0.00145	-0.74813	5.70335
C	-1.20535	-0.43603	3.94375
H	-2.15116	-0.53089	4.46351
C	-1.16796	-0.20327	2.56508
C	-2.38605	-0.06313	1.71170
C	3.74184	-0.11882	2.36632
H	4.52831	0.05705	1.63181
H	3.89666	-1.10916	2.81299
H	3.82518	0.62468	3.16636
C	-3.74142	-0.10841	2.36429
H	-3.82365	0.62857	3.17045
H	-3.89963	-1.10207	2.80233
H	-4.52655	0.07580	1.63036
C	3.20810	0.35035	-0.48488
C	3.57319	1.70216	-0.67933
C	4.54845	1.97477	-1.64575
H	4.85811	3.00307	-1.80779
C	5.12448	0.95808	-2.40353
H	5.87645	1.19594	-3.15117
C	4.72928	-0.36153	-2.20366
H	5.17277	-1.15363	-2.80033
C	3.76410	-0.69508	-1.24680
C	2.97040	2.84403	0.13586
H	2.09496	2.45907	0.66670
C	3.98003	3.36420	1.17927
H	4.32626	2.56893	1.84747
H	3.53028	4.15465	1.79244
H	4.86386	3.78427	0.68429
C	2.47350	4.00383	-0.74607
H	3.29927	4.49697	-1.27200
H	1.98446	4.76102	-0.12121
H	1.74850	3.65240	-1.48344
C	3.34590	-2.14351	-1.04586
H	2.60456	-2.18075	-0.24520
C	2.65348	-2.70275	-2.30143
H	1.77228	-2.10286	-2.54546
H	2.32093	-3.72986	-2.11507
H	3.33457	-2.71106	-3.16241
C	4.53646	-3.01883	-0.61366
H	5.30411	-3.07353	-1.39524
H	4.19614	-4.04004	-0.40735
H	5.01419	-2.62771	0.29363
C	-3.20491	0.36901	-0.48452
C	-3.77631	-0.67635	-1.23478
C	-4.74095	-0.33910	-2.19108
H	-5.19593	-1.13073	-2.77969
C	-5.12100	0.98340	-2.40080
H	-5.87292	1.22381	-3.14766
C	-4.52987	1.99972	-1.65405
H	-4.82807	3.03016	-1.82362
C	-3.55406	1.72331	-0.68944
C	-3.37331	-2.12789	-1.02488
H	-2.63138	-2.16815	-0.22489
C	-2.68789	-2.70156	-2.27787
H	-3.37014	-2.70773	-3.13796
H	-2.36570	-3.73097	-2.08601
H	-1.80109	-2.11184	-2.52630
C	-4.57245	-2.98838	-0.58672
H	-5.34109	-3.04015	-1.36749
H	-5.04575	-2.58706	0.31845
H	-4.24244	-4.01177	-0.37450
C	-2.93449	2.86202	0.11733
H	-2.05332	2.47201	0.63489
C	-3.92651	3.38415	1.17651
H	-4.81724	3.80571	0.69528
H	-3.46573	4.17353	1.78284
H	-4.26353	2.58923	1.84987
C	-2.44546	4.02116	-0.76944
H	-3.27642	4.52130	-1.28037
H	-1.73462	3.66732	-1.51944
H	-1.94128	4.77337	-0.15069
N	-2.16806	0.06861	0.45633
N	0.00059	-0.08641	1.91832
N	2.17071	0.05170	0.45591
O	0.01619	1.64596	-0.58071
O	0.00754	2.09253	-1.78801
O	-0.01646	-0.58295	-1.99590
H	-0.01404	0.29665	-2.43634
Br	-0.00992	-2.76088	0.40221

[5]FeiPrBIPO2OHClC
Charge: 0
Energy: -2132706.7317657

Fe	-0.00122	-0.43267	-0.15962
C	2.38697	0.04891	1.75295
C	1.16738	0.04947	2.61635
C	1.20401	0.01718	4.01457
H	2.14927	-0.00790	4.54338
C	-0.00113	0.00371	4.71466
H	-0.00168	-0.02851	5.79993
C	-1.20554	0.02284	4.01352
H	-2.15137	0.00211	4.54148
C	-1.16762	0.05516	2.61530
C	-2.38646	0.06039	1.75098
C	3.74103	0.10456	2.40809
H	4.52905	0.15412	1.65614
H	3.89118	-0.79930	3.01192
H	3.82691	0.96915	3.07524
C	-3.74129	0.11330	2.40483
H	-3.82611	0.97140	3.08041
H	-3.89466	-0.79622	2.99930
H	-4.52801	0.17218	1.65215
C	3.21142	0.10762	-0.48218
C	3.61419	1.40300	-0.87863
C	4.59416	1.49724	-1.87397
H	4.93249	2.47977	-2.19007
C	5.13875	0.36114	-2.46746
H	5.89595	0.46100	-3.24056
C	4.70465	-0.90117	-2.07196
H	5.12311	-1.78704	-2.54135
C	3.73164	-1.05715	-1.07872
C	3.04280	2.67286	-0.25208
H	2.17017	2.39588	0.34670
C	4.07715	3.34002	0.67711
H	4.42549	2.65859	1.46020
H	3.64799	4.22606	1.16060
H	4.95710	3.66153	0.10711
C	2.54851	3.67952	-1.30691
H	3.37156	4.05632	-1.92522
H	2.08995	4.54274	-0.80931
H	1.79881	3.22610	-1.95902
C	3.26937	-2.44464	-0.65971

H	2.51034	-2.33559	0.11744
C	2.58623	-3.18224	-1.82467
H	1.72599	-2.60811	-2.17984
H	2.22367	-4.15832	-1.48334
H	3.28094	-3.34616	-2.65871
C	4.42962	-3.26471	-0.06610
H	5.21322	-3.45375	-0.81013
H	4.06301	-4.23519	0.28779
H	4.89579	-2.74587	0.78128
C	-3.20987	0.12682	-0.48398
C	-3.74791	-1.03661	-1.06675
C	-4.72160	-0.87674	-2.05890
H	-5.15333	-1.76123	-2.51876
C	-5.13949	0.38747	-2.46551
H	-5.89772	0.49005	-3.23725
C	-4.57725	1.52193	-1.88523
H	-4.90328	2.50578	-2.20989
C	-3.59518	1.42350	-0.89253
C	-3.30129	-2.42630	-0.63799
H	-2.54207	-2.32056	0.13943
C	-2.62399	-3.17729	-1.79792
H	-3.31975	-3.33906	-2.63152
H	-2.27112	-4.15488	-1.45076
H	-1.75827	-2.61319	-2.15575
C	-4.47061	-3.23131	-0.04169
H	-5.25465	-3.41746	-0.78595
H	-4.93337	-2.70294	0.80165
H	-4.11416	-4.20319	0.31869
C	-3.00380	2.68907	-0.27619
H	-2.12336	2.40451	0.30743
C	-4.01716	3.36222	0.67154
H	-4.90603	3.68736	0.11761
H	-3.57473	4.24635	1.14655
H	-4.35401	2.68282	1.46145
C	-2.51980	3.69311	-1.33788
H	-3.35000	4.07973	-1.94036
H	-1.78639	3.23364	-2.00420
H	-2.04344	4.55051	-0.84714
N	-2.17033	-0.00437	0.49051
N	0.00027	0.08493	1.95932
N	2.17210	-0.02200	0.49257
O	0.01623	1.41714	-0.73654
O	0.00927	1.70320	-1.99496
O	-0.01574	-0.96249	-1.85329
H	-0.01184	-0.14454	-2.40117
Cl	-0.01120	-2.59877	0.75886

^{5}FeiPrBIPO2OHFC
Charge: 0
Energy: -1906580.1057908

Fe	-0.00122	0.24420	-0.08403
C	-2.39124	-0.65789	1.65397
C	-1.16743	-1.01086	2.43982
C	-1.20457	-1.51727	3.74505
H	-2.14941	-1.69890	4.24302
C	0.00047	-1.77635	4.39551
H	0.00067	-2.17026	5.40740
C	1.20521	-1.51444	3.74568
H	2.15018	-1.69388	4.24419
C	1.16763	-1.00811	2.44039
C	2.39113	-0.65278	1.65510
C	-3.74167	-0.87143	2.28613
H	-4.53600	-0.56750	1.60401
H	-3.82177	-0.27823	3.20541
H	-3.88840	-1.92363	2.55518
C	3.74155	-0.86523	2.28769
H	3.89001	-1.91772	2.55462
H	3.81994	-0.27382	3.20827
H	4.53583	-0.55848	1.60679
C	-3.23953	0.20424	-0.39542
C	-3.83308	-0.78632	-1.20558
C	-4.85059	-0.38142	-2.07840
H	-5.33473	-1.12476	-2.70549
C	-5.24414	0.95157	-2.16434
H	-6.03574	1.24210	-2.84996
C	-4.60685	1.91341	-1.38369
H	-4.89689	2.95681	-1.47078
C	-3.58659	1.56645	-0.49214
C	-3.39076	-2.24621	-1.17064
H	-2.49128	-2.31708	-0.55170
C	-4.47782	-3.14777	-0.55360
H	-4.75103	-2.82602	0.45728
H	-4.13219	-4.18717	-0.49969
H	-5.39019	-3.12919	-1.16184
C	-2.99838	-2.75422	-2.57010
H	-3.85831	-2.76804	-3.25020
H	-2.60960	-3.77700	-2.50179
H	-2.21642	-2.12695	-3.00418
C	-2.86777	2.63379	0.32164
H	-2.11290	2.15074	0.94391
C	-2.08401	3.58356	-0.60279
H	-1.38040	3.01335	-1.21530
H	-1.51015	4.29823	-0.00170
H	-2.75611	4.14922	-1.26130
C	-3.83683	3.39574	1.24243
H	-4.59307	3.94653	0.66960
H	-3.28721	4.12291	1.85185
H	-4.36682	2.71385	1.91983
C	3.23916	0.20953	-0.39427
C	3.58084	1.57273	-0.49669
C	4.60124	1.91999	-1.38792
H	4.88734	2.96416	-1.47880
C	5.24371	0.95740	-2.16335
H	6.03526	1.24812	-2.84895
C	4.85544	-0.37677	-2.07217
H	5.34349	-1.12083	-2.69536
C	3.83838	-0.78219	-1.19903
C	2.85737	2.64056	0.31227
H	2.10041	2.15770	0.93216
C	2.07678	3.58863	-0.61649
H	2.75092	4.15498	-1.27231
H	1.49909	4.30287	-0.01856
H	1.37680	3.01700	-1.23190
C	3.82210	3.40437	1.23611
H	4.58084	3.95419	0.66562
H	4.34915	2.72372	1.91706
H	3.26962	4.13245	1.84184
C	3.40228	-2.24388	-1.15965
H	2.50482	-2.31746	-0.53809
C	4.49479	-3.14002	-0.54432
H	5.40485	-3.11992	-1.15594
H	4.15297	-4.18049	-0.48670
H	4.77067	-2.81495	0.46474
C	3.00814	-2.75604	-2.55719
H	3.86610	-2.76612	-3.23984
H	2.22148	-2.13364	-2.98973
H	2.62522	-3.78087	-2.48623
N	2.18215	-0.15176	0.49625
N	0.00002	-0.79717	1.82089
N	-2.18242	-0.15736	0.49494
O	0.00316	-1.49931	-0.91275
O	0.00275	-1.59393	-2.21394
O	-0.00338	1.02873	-1.67387
H	-0.00126	0.29548	-2.33264
F	-0.00358	1.73586	0.94855

^{5}FeiPrBIPO2OHN$_3$C
Charge: 0
Energy: -1946970.1247506

Fe	0.00678	0.47564	0.02059
C	-2.37961	-0.30602	1.76338
C	-1.16654	-0.38578	2.62893
C	-1.20181	-0.55022	4.01792
H	-2.14705	-0.60202	4.54526
C	0.00430	-0.63984	4.71170
H	0.00599	-0.76082	5.79061
C	1.20784	-0.57409	4.01149
H	2.15482	-0.64459	4.53350
C	1.16841	-0.40851	2.62243
C	2.37789	-0.34828	1.75112
C	-3.73482	-0.50396	2.38731
H	-4.51652	-0.47048	1.62804
H	-3.92165	0.29172	3.11937
H	-3.79132	-1.46170	2.91608
C	3.73517	-0.55016	2.36947
H	3.78524	-1.49922	2.91438
H	3.93616	0.25621	3.08590
H	4.51167	-0.53808	1.60418
C	-3.17623	-0.14219	-0.47613
C	-3.54955	-1.40631	-0.98567
C	-4.53244	-1.43277	-1.98206
H	-4.84638	-2.39061	-2.38684
C	-5.10768	-0.26106	-2.46729
H	-5.87071	-0.30874	-3.23959
C	-4.69153	0.97162	-1.97120
H	-5.13040	1.88533	-2.36153
C	-3.71024	1.05963	-0.97810
C	-2.92808	-2.71290	-0.49836
H	-2.08382	-2.46905	0.15207
C	-3.94570	-3.54390	0.30838
H	-4.35438	-2.98407	1.15658
H	-3.47724	-4.45710	0.69502
H	-4.79051	-3.84354	-0.32333
C	-2.35207	-3.54673	-1.65817
H	-3.13933	-3.88333	-2.34326
H	-1.85696	-4.44122	-1.26052
H	-1.61510	-2.97093	-2.22229
C	-3.25926	2.41543	-0.45296
H	-2.43335	2.24827	0.24389
C	-2.71991	3.30524	-1.58692
H	-1.85947	2.82394	-2.06033
H	-2.38576	4.26616	-1.18349
H	-3.48842	3.50031	-2.34488
C	-4.39062	3.11002	0.32802
H	-5.24863	3.32270	-0.32132
H	-4.03829	4.06137	0.74321

H	-4.74880	2.48573	1.15656
C	3.16821	-0.18926	-0.49099
C	3.74270	1.01019	-0.95122
C	4.71960	0.92164	-1.94884
H	5.18828	1.83247	-2.31034
C	5.09392	-0.30751	-2.48560
H	5.85460	-0.35517	-3.26023
C	4.48112	-1.47524	-2.03747
H	4.76531	-2.42955	-2.47137
C	3.49903	-1.44742	-1.04052
C	3.33646	2.36197	-0.38070
H	2.50609	2.20008	0.31206
C	2.82280	3.30495	-1.48329
H	3.59984	3.51188	-2.22946
H	2.50709	4.25767	-1.04612
H	1.95578	2.85940	-1.97881
C	4.49185	2.99483	0.41745
H	5.35481	3.19950	-0.22790
H	4.83183	2.33416	1.22519
H	4.17241	3.94408	0.86312
C	2.83932	-2.74441	-0.57920
H	1.98475	-2.48575	0.05195
C	3.82113	-3.59645	0.24964
H	4.67995	-3.90201	-0.36015
H	3.32932	-4.50582	0.61590
H	4.21205	-3.04806	1.11370
C	2.27512	-3.56242	-1.75503
H	3.06947	-3.91017	-2.42615
H	1.55907	-2.97104	-2.33013
H	1.75555	-4.44951	-1.37258
N	2.14937	-0.12583	0.50940
N	-0.00018	-0.32667	1.97157
N	-2.15591	-0.07503	0.52218
O	-0.04339	-1.27647	-0.90326
O	-0.03410	-1.24639	-2.21583
O	0.05832	1.33103	-1.54537
H	0.03289	0.60986	-2.21532
N	0.03794	2.13717	1.02741
N	0.01575	3.23749	0.50272
N	0.00093	4.31560	0.10168

^{5}FeiPrBIPO2OHNCSC
Charge: 0
Energy: -2152081.0831133

Fe	0.07227	0.02596	-0.33713
C	2.40379	-0.60630	1.58807
C	1.16170	-0.85385	2.37958
C	1.15636	-1.44375	3.64756
H	2.08402	-1.72447	4.13146
C	-0.06782	-1.68256	4.27015
H	-0.10090	-2.14770	5.25033
C	-1.24849	-1.35124	3.61142
H	-2.20964	-1.56583	4.06163
C	-1.17085	-0.75465	2.34752
C	-2.36905	-0.37452	1.53700
C	3.73507	-0.94967	2.20099
H	4.54810	-0.70024	1.51891
H	3.77515	-2.02480	2.41536
H	3.88479	-0.41609	3.14604
C	-3.73930	-0.68371	2.07585
H	-3.88171	-0.26354	3.07737
H	-3.85720	-1.77213	2.14423
H	-4.50945	-0.28930	1.41211
C	3.31149	0.20441	-0.46143
C	3.91138	1.47635	-0.33377
C	4.93486	1.79986	-1.23307
H	5.42330	2.76654	-1.15101
C	5.33407	0.91245	-2.22908
H	6.12893	1.18820	-2.91684
C	4.70617	-0.32498	-2.34572
H	5.01050	-1.01206	-3.13020
C	3.68156	-0.70458	-1.47243
C	3.49639	2.48090	0.73801
H	2.58250	2.11505	1.21572
C	4.58702	2.61805	1.81956
H	4.82706	1.65642	2.28499
H	4.26384	3.30827	2.60811
H	5.51366	3.01350	1.38668
C	3.16009	3.86059	0.14309
H	4.03910	4.32856	-0.31511
H	2.80436	4.53079	0.93480
H	2.37335	3.78097	-0.61047
C	2.99893	-2.05668	-1.62360
H	2.25183	-2.15432	-0.83338
C	2.23069	-2.14134	-2.95489
H	1.49098	-1.33825	-3.01654
H	1.70181	-3.09913	-3.01999
H	2.91133	-2.06726	-3.81269
C	3.99886	-3.21637	-1.46508
H	4.75577	-3.20883	-2.25867
H	3.47361	-4.17713	-1.51434
H	4.52538	-3.16349	-0.50384
C	-3.14286	0.68203	-0.45625
C	-3.74953	-0.15817	-1.40978
C	-4.68469	0.41709	-2.27864
H	-5.15989	-0.20906	-3.02822
C	-5.00923	1.76825	-2.20281
H	-5.73994	2.19271	-2.88609
C	-4.39259	2.57734	-1.25043
H	-4.65270	3.62990	-1.19467
C	-3.44017	2.05972	-0.36651
C	-3.38765	-1.63035	-1.53226
H	-2.76427	-1.90124	-0.67982
C	-2.54639	-1.87526	-2.79917
H	-3.13219	-1.65499	-3.70097
H	-2.22959	-2.92369	-2.84248
H	-1.65337	-1.24415	-2.79799
C	-4.62403	-2.54470	-1.48664
H	-5.27300	-2.39942	-2.35845
H	-5.22509	-2.36140	-0.58767
H	-4.30759	-3.59346	-1.47592
C	-2.79461	2.94342	0.69591
H	-1.87408	2.45193	1.02335
C	-3.72200	3.07777	1.92067
H	-4.66405	3.56433	1.64017
H	-3.24710	3.68219	2.70318
H	-3.97142	2.10087	2.34911
C	-2.39393	4.33011	0.16782
H	-3.26766	4.93618	-0.09937
H	-1.74693	4.24167	-0.70861
H	-1.84173	4.87582	0.94174
N	-2.11997	0.16846	0.40366
N	0.01590	-0.49411	1.78096
N	2.22774	-0.14815	0.40420
O	0.25177	1.90461	0.03831
O	0.24387	2.77113	-0.91682
O	0.04544	0.36871	-2.07775
H	0.09010	1.34612	-2.18258
N	-0.10594	-1.95998	-0.52187
C	-0.57530	-2.89386	0.04305
S	-1.24882	-4.12894	0.85122

^{3}FeiPrBIPSPhO2ClA
Charge: 0
Energy: -2480403.2177514

Fe	0.01556	0.11679	0.02551
C	2.38268	-1.16093	1.46269
C	1.23176	-1.28805	2.38948
C	1.31081	-1.73560	3.71341
H	2.26844	-1.97754	4.15972
C	0.13191	-1.87074	4.44542
H	0.16505	-2.21153	5.47549
C	-1.09399	-1.58175	3.84152
H	-2.02058	-1.70631	4.38970
C	-1.09923	-1.13645	2.51673
C	-2.31788	-0.87156	1.71135
C	3.74409	-1.60141	1.92625
H	4.45987	-1.57839	1.10431
H	3.69713	-2.61937	2.32962
H	4.10883	-0.94209	2.72268
C	-3.66455	-1.17166	2.31337
H	-3.78216	-0.63972	3.26418
H	-3.76080	-2.24525	2.51752
H	-4.46752	-0.87196	1.64027
C	3.08457	-0.53470	-0.72933
C	4.00541	0.53188	-0.68028
C	4.90303	0.65678	-1.74976
H	5.62057	1.47238	-1.74139
C	4.88720	-0.23165	-2.81945
H	5.59502	-0.11349	-3.63558
C	3.95511	-1.26846	-2.84937
H	3.94347	-1.95195	-3.69213
C	3.02945	-1.43361	-1.81755
C	4.03317	1.55679	0.44843
H	3.24507	1.31327	1.16589
C	5.38443	1.55457	1.18935
H	5.64106	0.56222	1.57612
H	5.35414	2.25337	2.03364
H	6.20012	1.86973	0.52787
C	3.71058	2.96689	-0.07822
H	4.48434	3.32163	-0.77007
H	3.64627	3.67611	0.75466
H	2.75104	2.98047	-0.59826
C	2.03450	-2.58643	-1.81456
H	1.17771	-2.27338	-1.20829
C	1.49067	-2.93029	-3.20784
H	1.06919	-2.04055	-3.68339
H	0.69632	-3.67989	-3.11952
H	2.26519	-3.35104	-3.86037
C	2.65886	-3.82569	-1.14338
H	3.53811	-4.16579	-1.70359
H	1.93852	-4.65138	-1.10540
H	2.98018	-3.60998	-0.11767
C	-3.20057	-0.34282	-0.42325
C	-3.68838	-1.52617	-1.02094
C	-4.72987	-1.40309	-1.94750

H	-5.11939	-2.29239	-2.43283
C	-5.26633	-0.15946	-2.26795
H	-6.07917	-0.08694	-2.98562
C	-4.74613	0.99375	-1.68566
H	-5.15365	1.95958	-1.96302
C	-3.69409	0.93261	-0.76572
C	-3.03436	-2.88171	-0.77129
H	-2.53441	-2.85742	0.20144
C	-1.94072	-3.12146	-1.83117
H	-2.38475	-3.17487	-2.83221
H	-1.41236	-4.06295	-1.63775
H	-1.21532	-2.30268	-1.83636
C	-4.03205	-4.04985	-0.72220
H	-4.48845	-4.24093	-1.69974
H	-4.83967	-3.85976	-0.00551
H	-3.51511	-4.96905	-0.42281
C	-3.09240	2.18664	-0.14894
H	-2.01658	2.01053	-0.05935
C	-3.62196	2.44557	1.27427
H	-4.70339	2.63139	1.25951
H	-3.12170	3.32230	1.69964
H	-3.42930	1.60076	1.94205
C	-3.26614	3.44272	-1.01219
H	-4.31407	3.76612	-1.05669
H	-2.91054	3.27347	-2.03353
H	-2.68230	4.26194	-0.58459
N	-2.11653	-0.44554	0.50940
N	0.04823	-0.98114	1.83824
N	2.09882	-0.70144	0.29185
O	-0.14114	-3.78451	0.69651
O	0.69549	-4.15932	1.49308
S	0.36572	1.97448	1.48445
C	0.06437	3.49871	0.61239
C	-0.32681	4.63576	1.34342
H	-0.45737	4.55456	2.41911
H	-0.83946	6.72337	1.28842
C	-0.54039	5.85713	0.70260
C	-0.37483	5.97042	-0.68052
H	-0.54282	6.92174	-1.17828
H	0.12080	4.90876	-2.49405
C	0.00050	4.84295	-1.41546
C	0.21663	3.61995	-0.78085
H	0.48319	2.74610	-1.36603
Cl	-0.10221	0.25227	-2.24821

[5]FeiPrBIPSPhO2ClB
Charge: 0
Energy: -2480422.9994164

Fe	-0.04905	-0.56715	0.38284
C	-2.45610	-1.99167	-0.90345
C	-1.24619	-2.79687	-1.25940
C	-1.29259	-4.05855	-1.86137
H	-2.23996	-4.53068	-2.09330
C	-0.09019	-4.70393	-2.15061
H	-0.09672	-5.68726	-2.61074
C	1.11956	-4.08287	-1.84548
H	2.05913	-4.57527	-2.06564
C	1.09177	-2.81795	-1.24433
C	2.31466	-2.04392	-0.87065
C	-3.80510	-2.48719	-1.35007
H	-4.59147	-1.80117	-1.03483
H	-4.00198	-3.47212	-0.90990
H	-3.84130	-2.59632	-2.43974
C	3.65634	-2.65056	-1.18667
H	3.74778	-2.87038	-2.25571
H	3.76456	-3.59760	-0.64458
H	4.46530	-1.98335	-0.88997
C	-3.24395	0.06558	0.04210
C	-3.66787	0.94727	-0.97864
C	-4.57310	1.95832	-0.62597
H	-4.91289	2.64916	-1.39204
C	-5.03294	2.10307	0.67780
H	-5.73091	2.89860	0.92483
C	-4.59006	1.22772	1.66831
H	-4.94592	1.34792	2.68603
C	-3.68681	0.20229	1.37810
C	-3.17935	0.87492	-2.42297
H	-2.39225	0.11925	-2.48742
C	-4.31947	0.47030	-3.37955
H	-4.77947	-0.48148	-3.09498
H	-3.94359	0.37579	-4.40557
H	-5.11160	1.22826	-3.38407
C	-2.55418	2.20754	-2.88119
H	-3.31026	2.99885	-2.94877
H	-2.11167	2.08942	-3.87765
H	-1.77097	2.53878	-2.19730
C	-3.23200	-0.78073	2.44325
H	-2.23017	-1.12109	2.17594
C	-3.12568	-0.16875	3.84593
H	-2.51302	0.73765	3.82659
H	-2.64361	-0.88748	4.51724
H	-4.10733	0.07468	4.27246
C	-4.14212	-2.02488	2.45384
H	-5.17107	-1.75837	2.72726
H	-3.76956	-2.75881	3.17711
H	-4.17154	-2.50979	1.47141
C	3.20238	-0.01563	0.02959
C	3.66988	0.03553	1.36275
C	4.66954	0.96373	1.67174
H	5.04484	1.01483	2.68861
C	5.18694	1.82154	0.70453
H	5.96127	2.53764	0.96658
C	4.70369	1.76050	-0.59795
H	5.10435	2.43626	-1.34721
C	3.70075	0.85442	-0.96796
C	3.15212	-0.92507	2.42175
H	2.16238	-1.26649	2.11675
C	2.98581	-0.27927	3.80532
H	3.94982	-0.04271	4.27360
H	2.45932	-0.97595	4.46657
H	2.39048	0.63526	3.73765
C	4.05626	-2.17022	2.51448
H	5.06983	-1.89691	2.83478
H	4.13929	-2.68478	1.55127
H	3.64460	-2.88117	3.23965
C	3.20207	0.85735	-2.41095
H	2.25756	0.30768	-2.44684
C	4.20709	0.16436	-3.35403
H	5.16678	0.69510	-3.34699
H	3.82998	0.16602	-4.38401
H	4.40455	-0.87175	-3.06678
C	2.92202	2.28313	-2.92848
H	3.85423	2.82499	-3.12895
H	2.33504	2.86125	-2.21278
H	2.36422	2.23378	-3.87050
N	2.12492	-0.91436	-0.28568
N	-0.07285	-2.21670	-0.97798
N	-2.24179	-0.91759	-0.23535
S	-0.00233	1.05148	2.01628
C	0.07289	2.58768	1.14548
C	-1.10930	3.24372	0.74929
H	-2.06964	2.79641	0.98825
C	-1.04228	4.43395	0.03209
H	-1.96099	4.92484	-0.27944
C	0.19939	4.99364	-0.29791
H	0.24543	5.92244	-0.86063
C	1.37521	4.35342	0.09670
H	2.34292	4.77633	-0.16129
C	1.31747	3.15275	0.80630
H	2.23006	2.63790	1.09026
O	-0.30085	0.67786	-1.20077
O	0.40810	1.68710	-1.47023
Cl	-0.07605	-2.38960	1.98595

[6]FeN4Py2PhBr
Charge: 2+
Energy: -3428220.8621865

Fe	0.15332	-0.38059	-0.16637
C	2.11000	-1.65991	-2.27024
C	2.96974	-2.61359	-2.80392
C	3.24786	-3.76017	-2.05830
C	2.65031	-3.91518	-0.80577
C	1.80328	-2.91692	-0.33396
C	1.16064	-2.97792	1.03220
C	-1.19633	-3.10730	0.38167
C	-2.00691	-2.40513	-0.68802
C	-3.20526	-2.95275	-1.13954
C	-3.88744	-2.32804	-2.18393
C	-3.35209	-1.16670	-2.74275
C	-2.16063	-0.66738	-2.23086
C	-0.52853	-1.65790	2.30496
C	0.54932	-0.67748	2.74124
C	0.79128	-0.40111	4.07645
C	1.70312	0.61462	4.38854
C	2.36829	1.26712	3.35904
C	2.12347	0.90669	2.02338
C	2.92506	1.47580	0.92561
C	3.08907	2.86343	0.80064
C	3.84939	3.38158	-0.24628
C	4.47296	2.52047	-1.15505
C	4.33713	1.13681	-1.01558
C	3.56163	0.61521	0.01711
C	-1.80991	-0.86953	2.09513
C	-2.98930	-1.15125	2.76505
C	-4.11325	-0.36665	2.47541
C	-3.98950	0.67418	1.56677
C	-2.75243	0.92509	0.94107
C	-2.58970	2.09568	0.05839
C	-3.51749	2.35406	-0.96401
C	-3.38057	3.48944	-1.76189
C	-2.33635	4.38846	-1.52525
C	-1.42406	4.14750	-0.49418
C	-1.54343	3.00110	0.29027
N	1.53982	-1.80544	-1.05753
N	-0.13877	-2.26028	0.99727
N	-1.49911	-1.27784	-1.22569

N	1.17972	-0.02686	1.73235
N	-1.68936	0.12686	1.18966
H	1.86573	-0.75008	-2.80365
H	3.40577	-2.45682	-3.78452
H	3.91278	-4.52552	-2.44654
H	2.83864	-4.79737	-0.20199
H	1.03322	-4.01355	1.36922
H	1.81523	-2.48320	1.75338
H	-1.85827	-3.51540	1.15390
H	-0.70390	-3.96351	-0.09073
H	-3.59337	-3.85828	-0.68328
H	-4.82105	-2.74146	-2.55289
H	-3.84716	-0.64794	-3.55631
H	-1.71725	0.24544	-2.60653
H	-0.67539	-2.43103	3.06921
H	0.27307	-0.95191	4.85452
H	1.90842	0.86786	5.42407
H	3.12026	2.01998	3.56712
H	2.60021	3.53257	1.50350
H	3.96056	4.45621	-0.35182
H	5.07442	2.92872	-1.96142
H	4.84328	0.46691	-1.70439
H	3.46520	-0.45814	0.14202
H	-3.03522	-1.95815	3.48919
H	-5.05954	-0.55570	2.97291
H	-4.82348	1.33490	1.35769
H	-4.33342	1.65808	-1.14101
H	-4.09281	3.67968	-2.55889
H	-2.24028	5.28021	-2.13695
H	-0.62091	4.85199	-0.30186
H	-0.83520	2.80711	1.09054
Br	0.59519	1.45727	-1.62662

^{6}FeN4Py2PhCl
Charge: 2+
Energy: -2101693.5512591

Fe	-0.00011	0.21291	-0.01368
C	-1.82799	2.19515	-1.54610
C	-2.58277	3.34513	-1.74628
C	-2.89318	4.14293	-0.64293
C	-2.43961	3.76235	0.62156
C	-1.69362	2.59296	0.74726
C	-1.23666	2.07177	2.09225
C	1.23591	2.07242	2.09207
C	1.69258	2.59364	0.74699
C	2.43819	3.76327	0.62118
C	2.89150	4.14396	-0.64336
C	2.58122	3.34604	-1.74666
C	1.82684	2.19582	-1.54637
C	0.00019	0.04968	2.85853
C	-1.20956	-0.81080	2.52588
C	-1.89080	-1.53499	3.49128
C	-2.87856	-2.43233	3.07072
C	-3.15969	-2.53732	1.71438
C	-2.47193	-1.73750	0.78693
C	-2.85177	-1.76418	-0.64323
C	-2.67975	-2.93055	-1.40094
C	-3.04636	-2.94413	-2.74655
C	-3.61171	-1.80743	-3.33130
C	-3.81664	-0.65551	-2.56718
C	-3.43439	-0.63099	-1.22684
C	1.21035	-0.81017	2.52575
C	1.89216	-1.53389	3.49110
C	2.88035	-2.43071	3.07046
C	3.16128	-2.53570	1.71408
C	2.47289	-1.73637	0.78666
C	2.85242	-1.76312	-0.64358
C	3.43435	-0.62977	-1.22754
C	3.81633	-0.65438	-2.56796
C	3.61180	-1.80654	-3.33180
C	3.04713	-2.94340	-2.74669
C	2.68082	-2.92974	-1.40101
N	-1.39981	1.82881	-0.32317
N	-0.00017	1.25361	1.98009
N	1.39891	1.82936	-0.32338
N	-1.48401	-0.90601	1.20316
N	1.48461	-0.90535	1.20299
H	-1.56009	1.52976	-2.35793
H	-2.91379	3.60763	-2.74517
H	-3.47635	5.05062	-0.76398
H	-2.66277	4.36240	1.49821
H	-1.09399	2.89573	2.80040
H	-2.03193	1.43988	2.49858
H	2.03152	1.44102	2.49849
H	1.09284	2.89642	2.80008
H	2.66125	4.36341	1.49778
H	3.47437	5.05183	-0.76451
H	2.91203	3.60863	-2.74560
H	1.55907	1.53032	-2.35815
H	0.00017	0.31813	3.92177
H	-1.64767	-1.41541	4.54202
H	-3.42688	-3.02597	3.79572
H	-3.93550	-3.20212	1.35139
H	-2.24098	-3.81353	-0.94448
H	-2.89792	-3.84320	-3.33646
H	-3.90802	-1.82624	-4.37561
H	-4.28812	0.21633	-3.01161
H	-3.61207	0.25202	-0.62173
H	1.64914	-1.41434	4.54188
H	3.42915	-3.02396	3.79542
H	3.93740	-3.20010	1.35102
H	3.61176	0.25344	-0.62264
H	4.28729	0.21761	-3.01267
H	3.90788	-1.82542	-4.37618
H	2.89901	-3.84267	-3.33639
H	2.24260	-3.81285	-0.94427
Cl	-0.00008	-0.72480	-1.99424

^{6}FeN4Py2PhF
Charge: 2+
Energy: -1875571.8051994

Fe	0.04350	-0.04469	-0.15824
C	2.02406	-0.02149	-2.47251
C	2.88783	-0.52558	-3.43743
C	3.19587	-1.88776	-3.41488
C	2.64365	-2.69847	-2.42085
C	1.79935	-2.12304	-1.47480
C	1.25477	-2.91091	-0.30127
C	-1.22170	-2.87880	-0.20043
C	-1.84950	-2.07311	-1.32094
C	-2.79537	-2.62341	-2.18197
C	-3.41531	-1.79674	-3.12181
C	-3.07320	-0.44376	-3.17721
C	-2.10800	0.03515	-2.29988
C	0.11548	-2.14920	1.79590
C	1.37926	-1.37940	2.13780
C	2.30039	-1.81854	3.07556
C	3.46967	-1.06918	3.25731
C	3.66411	0.07632	2.49653
C	2.68244	0.48675	1.57870
C	2.85695	1.71841	0.78074
C	1.91978	2.75662	0.86910
C	2.09580	3.92316	0.12842
C	3.20419	4.05552	-0.71198
C	4.14776	3.02649	-0.79748
C	3.98412	1.86464	-0.04413
C	-1.10648	-1.36988	2.25326
C	-1.89686	-1.77964	3.31543
C	-3.05032	-1.04120	3.60651
C	-3.37464	0.04623	2.80695
C	-2.53136	0.41934	1.74524
C	-2.89743	1.53911	0.85269
C	-4.16827	1.54469	0.25009
C	-4.52537	2.57595	-0.61629
C	-3.62748	3.61811	-0.87218
C	-2.37309	3.62772	-0.25747
C	-2.00954	2.59280	0.60248
N	1.49543	-0.81254	-1.51763
N	0.04751	-2.28115	0.29872
N	-1.51415	-0.77182	-1.39883
N	1.55552	-0.24809	1.41575
N	-1.39390	-0.27859	1.50471
H	1.72697	1.01931	-2.43194
H	3.29983	0.13505	-4.19229
H	3.85692	-2.31583	-4.16225
H	2.86924	-3.75951	-2.37690
H	1.04560	-3.94397	-0.59782
H	2.03891	-2.96187	0.46065
H	-1.93853	-2.92005	0.62560
H	-1.06069	-3.91354	-0.52016
H	-3.04704	-3.67733	-2.11425
H	-4.15636	-2.20590	-3.80168
H	-3.53805	0.22904	-3.88927
H	-1.78316	1.06879	-2.28617
H	0.13323	-3.13143	2.28224
H	2.12301	-2.73025	3.63653
H	4.21523	-1.38314	3.98136
H	4.55387	0.68463	2.61461
H	1.07371	2.65467	1.54183
H	1.37674	4.73207	0.21432
H	3.34277	4.96594	-1.28717
H	5.01643	3.13576	-1.43961
H	4.71915	1.06615	-0.10314
H	-1.63291	-2.66159	3.88972
H	-3.69002	-1.32607	4.43612
H	-4.26689	0.63285	2.99462
H	-4.86357	0.73273	0.44568
H	-5.50505	2.57259	-1.08425
H	-3.91206	4.42757	-1.53766
H	-1.68142	4.44428	-0.43950
H	-1.04150	2.60635	1.08831
F	0.07246	1.53652	-0.94749

^{6}FeN4Py2PhN$_3$
Charge: 2+

Energy: -1915961.0825936

Fe	0.06025	-0.41489	-0.23352
C	1.70261	-2.00471	-2.36100
C	2.32384	-3.09965	-2.95114
C	2.34457	-4.31076	-2.25576
C	1.74153	-4.38476	-0.99832
C	1.14398	-3.24369	-0.47001
C	0.51607	-3.20541	0.90512
C	-1.83049	-2.80910	0.30878
C	-2.46929	-1.94297	-0.76070
C	-3.75555	-2.21238	-1.22406
C	-4.28009	-1.43546	-2.25760
C	-3.50624	-0.40481	-2.79583
C	-2.23719	-0.18686	-2.27410
C	-0.82352	-1.57981	2.23650
C	0.45212	-0.87045	2.67165
C	0.78928	-0.73517	4.00911
C	1.89071	0.06287	4.33751
C	2.61870	0.66290	3.31862
C	2.25303	0.45803	1.97696
C	3.07685	1.01591	0.88487
C	3.48114	2.36038	0.91634
C	4.29785	2.86913	-0.09336
C	4.73245	2.03789	-1.13011
C	4.34265	0.69521	-1.16015
C	3.51604	0.18660	-0.16031
C	-1.89707	-0.51452	2.06591
C	-3.08761	-0.50822	2.77502
C	-3.99574	0.52904	2.52371
C	-3.65696	1.51872	1.61126
C	-2.41977	1.46429	0.94124
C	-1.99174	2.55397	0.04276
C	-2.86927	3.08175	-0.91734
C	-2.46320	4.14097	-1.72932
C	-1.19132	4.69816	-1.56929
C	-0.31964	4.18904	-0.60111
C	-0.71208	3.11447	0.19448
N	1.12896	-2.07516	-1.14549
N	-0.59986	-2.22558	0.91218
N	-1.73164	-0.94541	-1.28189
N	1.16090	-0.28841	1.67369
N	-1.57643	0.43119	1.15726
H	1.65349	-1.03875	-2.85000
H	2.77449	-3.00414	-3.93300
H	2.81726	-5.18731	-2.68800
H	1.73570	-5.31285	-0.43538
H	0.17889	-4.20012	1.22026
H	1.27049	-2.87911	1.62544
H	-2.56333	-3.04854	1.08779
H	-1.55547	-3.75951	-0.16029
H	-4.33430	-3.01952	-0.78532
H	-5.27914	-1.63094	-2.63497
H	-3.87785	0.22291	-3.59827
H	-1.59867	0.61425	-2.62623
H	-1.12987	-2.31285	2.99317
H	0.20095	-1.22674	4.77695
H	2.18234	0.19645	5.37465
H	3.49875	1.25697	3.53746
H	3.14578	3.00800	1.72203
H	4.59870	3.91181	-0.06986
H	5.37676	2.43422	-1.90858
H	4.69689	0.04323	-1.95332
H	3.22964	-0.85969	-0.16469
H	-3.30484	-1.28509	3.50085
H	-4.94188	0.57057	3.05457
H	-4.31459	2.36248	1.43433
H	-3.86074	2.65293	-1.03715
H	-3.14201	4.53997	-2.47681
H	-0.88324	5.53386	-2.19007
H	0.66170	4.63288	-0.46486
H	-0.04179	2.71671	0.95106
N	0.68155	0.91715	-1.34820
N	1.26395	1.79386	-1.93971
N	1.80678	2.63683	-2.49815

^{6}FeN4Py2PhNCS

Charge: 2+

Energy: -2121068.3165307

Fe	-0.04210	-0.44953	-0.20958
C	1.55108	-1.95895	-2.44064
C	2.02286	-3.04008	-3.17684
C	1.70434	-4.33074	-2.74950
C	0.92439	-4.49455	-1.60275
C	0.49389	-3.36396	-0.91406
C	-0.30133	-3.43854	0.36924
C	-2.42356	-2.44292	-0.35173
C	-2.74304	-1.27344	-1.26282
C	-3.98961	-1.16446	-1.87586
C	-4.21889	-0.11196	-2.76265
C	-3.19648	0.80743	-3.00711
C	-1.98372	0.64206	-2.34961
C	-1.46404	-1.82911	1.87071
C	-0.14398	-1.50725	2.55855
C	0.04002	-1.69822	3.91863
C	1.22007	-1.22162	4.50147
C	2.16922	-0.60122	3.69959
C	1.94551	-0.47202	2.31844
C	2.97442	0.11548	1.43693
C	3.55229	1.35494	1.75316
C	4.53322	1.89870	0.92437
C	4.95987	1.19991	-0.20902
C	4.40060	-0.04369	-0.51699
C	3.40766	-0.58203	0.29879
C	-2.27046	-0.53907	1.82605
C	-3.51703	-0.39465	2.41276
C	-4.15120	0.85104	2.30766
C	-3.49828	1.89092	1.66097
C	-2.22130	1.68290	1.10418
C	-1.45861	2.79279	0.50310
C	-2.07831	3.70875	-0.36303
C	-1.35171	4.77721	-0.88675
C	-0.01047	4.95266	-0.53213
C	0.60779	4.05210	0.34021
C	-0.10935	2.97251	0.85016
N	0.80507	-2.11830	-1.33135
N	-1.19488	-2.25652	0.46853
N	-1.76419	-0.38121	-1.50057
N	0.78402	-0.91021	1.77161
N	-1.64712	0.46138	1.16739
H	1.76679	-0.93565	-2.72260
H	2.62051	-2.87055	-4.06586
H	2.05205	-5.19749	-3.30307
H	0.65534	-5.48404	-1.24665
H	-0.86686	-4.37550	0.43754
H	0.39371	-3.42144	1.21260
H	-3.28322	-2.66881	0.28973
H	-2.27128	-3.32146	-0.98730
H	-4.76550	-1.89409	-1.66474
H	-5.18225	-0.01047	-3.25291
H	-3.33432	1.64059	-3.68747
H	-1.16301	1.33741	-2.47419
H	-2.00844	-2.60169	2.42784
H	-0.72257	-2.19068	4.51302
H	1.39644	-1.34845	5.56515
H	3.10634	-0.24691	4.11399
H	3.22347	1.89635	2.63630
H	4.97144	2.86192	1.16684
H	5.73361	1.61936	-0.84459
H	4.74804	-0.59685	-1.38462
H	2.98080	-1.55423	0.07516
H	-3.98255	-1.22269	2.93730
H	-5.13008	1.00710	2.75055
H	-3.93824	2.88080	1.61396
H	-3.12135	3.57417	-0.63716
H	-1.83214	5.47800	-1.56255
H	0.54923	5.79344	-0.93033
H	1.64729	4.18962	0.62174
H	0.36655	2.27056	1.52845
N	0.94776	0.88533	-1.05730
C	1.59845	1.64587	-1.72940
S	2.44528	2.64346	-2.61562

^{6}FeN4Py2PhOH

Charge: 2+

Energy: -1860488.5466077

Fe	-0.07701	0.39334	-0.29767
C	-2.33060	-0.53320	-2.14231
C	-3.63100	-0.78825	-2.55953
C	-4.68642	-0.20909	-1.85042
C	-4.40506	0.60937	-0.75616
C	-3.07532	0.82953	-0.40103
C	-2.71662	1.76740	0.73682
C	-0.66579	3.07122	1.11085
C	-0.27996	3.42987	-0.30692
C	-0.28997	4.73242	-0.79585
C	0.13890	4.96455	-2.10546
C	0.55653	3.88713	-2.88968
C	0.53211	2.61091	-2.33706
C	-1.02780	0.95393	2.37951
C	-1.54919	-0.46596	2.18131
C	-2.49107	-1.06629	3.00202
C	-2.86560	-2.38719	2.71806
C	-2.25620	-3.05728	1.66457
C	-1.28909	-2.39779	0.88554
C	-0.52824	-3.09028	-0.17409
C	0.87264	-2.97007	-0.20251
C	1.61446	-3.61941	-1.18825
C	0.96211	-4.39095	-2.15741
C	-0.42878	-4.52397	-2.12635
C	-1.17270	-3.88499	-1.13298
C	0.47458	0.84852	2.60849
C	1.02479	0.88680	3.87998
C	2.39079	0.61620	4.02135
C	3.14047	0.31658	2.89213
C	2.53261	0.31368	1.62431
C	3.31471	-0.01384	0.41346

C	3.25719	0.80440	-0.72431
C	3.99775	0.48152	-1.86037
C	4.79849	-0.66367	-1.87170
C	4.86832	-1.47987	-0.73760
C	4.13811	-1.15322	0.40487
N	-2.06790	0.26141	-1.08520
N	-1.28303	1.72125	1.13118
N	0.12604	2.39487	-1.07143
N	-0.98712	-1.10590	1.13440
N	1.21116	0.59006	1.49953
O	0.68421	-0.38720	-1.72911
H	-1.46023	-0.95800	-2.62782
H	-3.80937	-1.42723	-3.41745
H	-5.71534	-0.39110	-2.14538
H	-5.20477	1.07559	-0.18849
H	-2.94798	2.78675	0.41062
H	-3.35881	1.56872	1.60275
H	0.24007	3.04864	1.72267
H	-1.32958	3.82604	1.54892
H	-0.62473	5.54939	-0.16440
H	0.13996	5.97269	-2.50840
H	0.88895	4.02886	-3.91224
H	0.83458	1.72394	-2.88273
H	-1.51266	1.41813	3.24756
H	-2.92231	-0.52627	3.83865
H	-3.60482	-2.89016	3.33393
H	-2.48342	-4.09720	1.45713
H	1.37545	-2.37579	0.55543
H	2.69693	-3.52999	-1.19273
H	1.53792	-4.89932	-2.92472
H	-0.93349	-5.12986	-2.87250
H	-2.25468	-3.98502	-1.11385
H	0.40309	1.10837	4.74118
H	2.85715	0.64211	5.00134
H	4.20228	0.11028	2.96507
H	2.64502	1.69943	-0.70564
H	3.96054	1.12835	-2.73170
H	5.37834	-0.91238	-2.75529
H	5.49933	-2.36355	-0.73966
H	4.19020	-1.79128	1.28304
H	1.29609	-1.14362	-1.73203

^{4}FeN4Py2PhamideBrOtBu2
Charge: 0
Energy: -3633152.9475381

Fe	0.74241	-0.01451	0.24458
C	3.60709	-0.38377	0.87405
C	4.98451	-0.58632	0.85624
C	5.56550	-1.18053	-0.26155
C	4.72306	-1.57871	-1.30954
C	3.34537	-1.39166	-1.21115
C	2.45323	-1.93993	-2.26148
C	1.48009	-2.88730	-1.91857
C	0.66555	-3.44949	-2.89770
C	0.81023	-3.06566	-4.23294
C	1.78264	-2.12741	-4.58302
C	2.60695	-1.57312	-3.60358
C	2.95010	0.43508	1.97014
C	2.76157	1.81453	1.36659
C	3.71859	2.80916	1.53439
C	3.57633	4.00676	0.83617
C	2.43683	4.17490	0.03894
C	1.48664	3.15788	-0.05495
C	0.19189	3.42389	-0.72047
C	0.12741	4.07085	-1.96161
C	-1.10689	4.38884	-2.52777
C	-2.28907	4.08394	-1.85059
C	-2.23114	3.44663	-0.60841
C	-1.00111	3.10860	-0.05292
N	1.62750	-0.13744	2.33143
C	1.65550	-1.54990	2.74117
C	0.45914	-2.32406	2.21088
C	-0.14248	-3.35118	2.93045
C	-1.21009	-4.04999	2.35475
C	-1.62949	-3.69805	1.07235
C	-0.97610	-2.65604	0.41858
N	0.04048	-1.97763	0.97839
C	0.85287	0.70379	3.25705
C	-0.63312	0.40740	3.20286
C	-1.34648	0.18508	4.37438
C	-2.71903	-0.05584	4.26995
C	-3.32284	-0.08733	3.02457
C	-2.51929	0.13255	1.88165
N	-1.20171	0.39183	1.98163
N	-3.01734	0.08121	0.57519
C	-4.33617	-0.17479	0.20124
O	-5.23164	-0.31675	1.02539
C	-4.62477	-0.29995	-1.31012
C	-6.13875	-0.51699	-1.47906
C	-3.87121	-1.52566	-1.87474
C	-4.20845	0.98253	-2.06002
N	2.77845	-0.76615	-0.13824
N	1.67332	1.94912	0.55727
H	5.58649	-0.26540	1.70220
H	6.63610	-1.35381	-0.31052
H	5.12095	-2.07630	-2.18786
H	1.36953	-3.17324	-0.87928
H	-0.08730	-4.18212	-2.61781
H	0.16597	-3.49318	-4.99658
H	1.89362	-1.81851	-5.61894
H	3.35364	-0.83040	-3.87123
H	3.62598	0.50151	2.83712
H	4.56472	2.63521	2.19337
H	4.30461	4.80497	0.94084
H	2.24480	5.11830	-0.46101
H	1.04662	4.29627	-2.49552
H	-1.14501	4.86936	-3.50174
H	-3.25067	4.33090	-2.29251
H	-3.14609	3.19550	-0.07945
H	-0.95265	2.58804	0.89680
H	2.55811	-2.00436	2.32171
H	1.71883	-1.64971	3.83507
H	0.21058	-3.59252	3.92887
H	-1.70498	-4.84613	2.90313
H	-2.45585	-4.20688	0.58647
H	-1.25090	-2.32753	-0.57748
H	1.00887	1.74526	2.96798
H	1.21684	0.58855	4.29073
H	-0.84383	0.20042	5.33632
H	-3.31718	-0.22963	5.16030
H	-4.37659	-0.27893	2.90260
H	-6.37439	-0.60617	-2.54564
H	-6.47066	-1.42581	-0.96895
H	-6.70831	0.32001	-1.06422
H	-4.11146	-2.42996	-1.30107
H	-4.18021	-1.69413	-2.91296
H	-2.78995	-1.37355	-1.87903
H	-4.46997	0.88130	-3.11993
H	-3.13562	1.17633	-2.00715
H	-4.74325	1.85393	-1.66361
H	-2.31099	0.20588	-0.15641
Br	-0.49036	0.15425	-1.99069

^{4}FeN4Py2PhamideClOtBu2
Charge: 0
Energy: -2306624.5912740

Fe	-0.72713	-0.15448	-0.04907
C	-3.48454	-1.17838	-0.09391
C	-4.83849	-1.44142	0.08867
C	-5.49859	-0.87081	1.17495
C	-4.75573	-0.05908	2.04208
C	-3.39210	0.14305	1.82738
C	-2.60847	0.93077	2.80700
C	-1.41953	0.41498	3.33827
C	-0.71233	1.12151	4.30734
C	-1.17771	2.36047	4.75187
C	-2.35962	2.88631	4.22448
C	-3.07472	2.17320	3.26277
C	-2.77655	-1.59650	-1.36949
C	-2.71477	-0.32939	-2.20311
C	-3.70677	-0.02498	-3.12762
C	-3.69353	1.22549	-3.74486
C	-2.64348	2.10200	-3.44087
C	-1.65200	1.72619	-2.53515
C	-0.43958	2.55798	-2.37175
C	-0.51717	3.95365	-2.26058
C	0.64496	4.72271	-2.20084
C	1.89717	4.10850	-2.27288
C	1.98087	2.71874	-2.38864
C	0.82313	1.94800	-2.42242
N	-1.40366	-2.08186	-1.07855
C	-1.34403	-3.19163	-0.11702
C	-0.13800	-3.08697	0.80109
C	0.59487	-4.20251	1.19798
C	1.67441	-4.02989	2.06936
C	1.97671	-2.74615	2.51994
C	1.19435	-1.68342	2.07138
N	0.16452	-1.84767	1.22785
C	-0.61173	-2.33735	-2.29229
C	0.87942	-2.35816	-2.02196
C	1.66398	-3.41343	-2.47373
C	3.03674	-3.36460	-2.21664
C	3.57277	-2.29942	-1.51228
C	2.69834	-1.27782	-1.07434
N	1.38109	-1.30770	-1.34820
N	3.11559	-0.17975	-0.31612
C	4.41357	0.08837	0.10894
O	5.36712	-0.60950	-0.21714
C	4.60532	1.30499	1.04204
C	6.11327	1.45524	1.30834
C	3.87732	1.04316	2.38048
C	4.07190	2.59686	0.38826
N	-2.74278	-0.40971	0.75715
N	-1.71149	0.53158	-1.86919
H	-5.36315	-2.07339	-0.62281
H	-6.55218	-1.06115	1.35418

H	-5.21803	0.38682	2.91642
H	-1.05965	-0.54009	2.97743
H	0.21168	0.71063	4.70539
H	-0.61906	2.91779	5.49911
H	-2.72176	3.85547	4.55734
H	-3.98773	2.58767	2.84318
H	-3.37796	-2.35459	-1.89438
H	-4.48047	-0.75576	-3.34622
H	-4.45219	1.49775	-4.47194
H	-2.55080	3.05283	-3.95511
H	-1.49093	4.43226	-2.19698
H	0.57212	5.80187	-2.09458
H	2.80266	4.70788	-2.22863
H	2.94999	2.23082	-2.43394
H	0.88604	0.86689	-2.48049
H	-2.24292	-3.14414	0.50552
H	-1.35062	-4.16733	-0.62654
H	0.33387	-5.18616	0.81872
H	2.27089	-4.88286	2.38003
H	2.80976	-2.56099	3.19034
H	1.38593	-0.65701	2.36382
H	-0.82354	-1.53208	-2.99890
H	-0.91694	-3.28461	-2.76633
H	1.21535	-4.24447	-3.00896
H	3.68890	-4.16461	-2.55669
H	4.62467	-2.23117	-1.28554
H	6.28130	2.31461	1.96748
H	6.52465	0.56099	1.78509
H	6.66603	1.61543	0.37778
H	4.19562	0.08851	2.81858
H	4.12908	1.83893	3.09142
H	2.79243	1.04414	2.25846
H	4.27107	3.44586	1.05297
H	2.99557	2.56722	0.20903
H	4.58230	2.78974	-0.56302
H	2.35219	0.43454	-0.00634
Cl	0.59138	1.55932	0.93142

^{6}FeN4Py2PhamideFOtBu2
Charge: 0
Energy: -2080501.0658987

Fe	0.53818	0.26551	0.03814
C	3.40987	1.00838	0.46498
C	4.74408	1.08430	0.87521
C	5.17989	0.28767	1.92387
C	4.25181	-0.58275	2.53506
C	2.92964	-0.59875	2.10236
C	1.93200	-1.45845	2.78614
C	0.70022	-0.92590	3.19210
C	-0.22457	-1.71602	3.87110
C	0.06185	-3.05586	4.14241
C	1.28425	-3.59766	3.73732
C	2.21588	-2.80316	3.06867
C	2.94246	1.63516	-0.82910
C	2.91247	0.50703	-1.83061
C	3.99858	0.25648	-2.67241
C	4.02031	-0.91258	-3.42003
C	2.92430	-1.79130	-3.31950
C	1.85247	-1.47051	-2.48942
C	0.62684	-2.30255	-2.51633
C	0.69436	-3.70375	-2.52307
C	-0.46571	-4.46683	-2.65850
C	-1.70487	-3.83945	-2.80568
C	-1.77982	-2.44424	-2.79479
C	-0.62594	-1.68204	-2.63643
N	1.56543	2.19536	-0.65045
C	1.48894	3.20954	0.41880
C	0.15826	3.17317	1.12433
C	-0.56675	4.32543	1.43586
C	-1.78238	4.20506	2.10541
C	-2.24068	2.92767	2.44914
C	-1.45980	1.83110	2.09681
N	-0.29173	1.94018	1.44870
C	0.92137	2.63137	-1.90350
C	-0.58776	2.53911	-1.83334
C	-1.40057	3.53996	-2.35798
C	-2.78458	3.36855	-2.29061
C	-3.32111	2.23525	-1.69213
C	-2.43193	1.27919	-1.16258
N	-1.09107	1.42678	-1.25896
N	-2.83446	0.12832	-0.49107
C	-4.12057	-0.22977	-0.11979
O	-5.11411	0.41110	-0.44352
C	-4.22217	-1.50227	0.75699
C	-5.71007	-1.77029	1.03019
C	-3.47609	-1.27927	2.09232
C	-3.59350	-2.71242	0.03426
N	2.49645	0.18942	1.07883
N	1.84837	-0.34554	-1.72186
H	5.42371	1.75683	0.35780
H	6.20560	0.33930	2.27596
H	4.54292	-1.20927	3.37115
H	0.48528	0.11311	2.97215
H	-1.17277	-1.28737	4.18429
H	-0.66347	-3.67493	4.66382
H	1.51100	-4.64157	3.93774
H	3.16159	-3.22759	2.74248
H	3.65940	2.40404	-1.15205
H	4.81546	0.97183	-2.71882
H	4.84595	-1.13167	-4.09023
H	2.87199	-2.68501	-3.93161
H	1.65805	-4.19252	-2.40743
H	-0.40145	-5.55176	-2.64949
H	-2.60800	-4.43361	-2.91677
H	-2.73997	-1.94668	-2.89519
H	-0.67953	-0.59948	-2.61433
H	2.28399	2.96438	1.13560
H	1.69479	4.21673	0.02684
H	-0.18299	5.29896	1.14430
H	-2.36605	5.08803	2.34920
H	-3.18430	2.78206	2.96440
H	-1.77454	0.81864	2.31884
H	1.28516	1.97138	-2.69750
H	1.22330	3.65660	-2.16640
H	-0.95983	4.42636	-2.80352
H	-3.45019	4.12553	-2.69652
H	-4.38441	2.07333	-1.60399
H	-5.81341	-2.66848	1.64983
H	-6.17548	-0.92848	1.55131
H	-6.26126	-1.92348	0.09755
H	-3.84482	-0.38336	2.60803
H	-3.64759	-2.13824	2.75214
H	-2.39823	-1.19755	1.93296
H	-3.73335	-3.61151	0.64655
H	-2.52083	-2.58281	-0.12631
H	-4.07391	-2.88822	-0.93452
H	-2.04993	-0.45104	-0.14844
F	-0.66870	-1.08640	0.47392

^{4}FeN4Py2PhamideN$_3$OtBu2
Charge: 0
Energy: -2120887.3384010

Fe	-0.66724	-0.24183	-0.13842
C	-3.55214	-0.70677	0.00327
C	-4.88803	-0.77585	0.38783
C	-5.22030	-0.58751	1.72802
C	-4.17761	-0.35731	2.64449
C	-2.85815	-0.34026	2.20821
C	-1.74096	-0.21387	3.17939
C	-0.79874	-1.24803	3.28849
C	0.24585	-1.16096	4.20421
C	0.36444	-0.03364	5.02433
C	-0.57463	0.99306	4.92975
C	-1.62689	0.90234	4.01581
C	-3.13944	-0.69830	-1.45921
C	-2.92182	0.76598	-1.79279
C	-3.94565	1.53829	-2.33588
C	-3.75858	2.91220	-2.46061
C	-2.52291	3.45210	-2.07694
C	-1.51880	2.61940	-1.58272
C	-0.15726	3.16525	-1.36564
C	0.04289	4.37470	-0.68655
C	1.32119	4.92582	-0.58806
C	2.41073	4.28069	-1.17395
C	2.22019	3.07144	-1.85018
C	0.94723	2.51653	-1.93982
N	-1.87120	-1.45960	-1.63591
C	-1.93347	-2.85434	-1.17829
C	-0.63550	-3.30580	-0.52944
C	-0.11874	-4.58614	-0.70721
C	1.06303	-4.93932	-0.04546
C	1.68142	-3.99711	0.77408
C	1.09776	-2.73686	0.89689
N	-0.03177	-2.39595	0.25738
C	-1.22532	-1.31728	-2.94941
C	0.29208	-1.41984	-2.87317
C	1.01036	-2.10640	-3.84380
C	2.40573	-2.12650	-3.73784
C	3.03396	-1.49406	-2.67672
C	2.23078	-0.83417	-1.72099
N	0.88711	-0.79033	-1.84234
N	2.73513	-0.18928	-0.59351
C	4.03904	-0.24193	-0.11783
O	4.93205	-0.84832	-0.69921
C	4.29931	0.50334	1.21138
C	5.79486	0.36979	1.54206
C	3.46442	-0.13472	2.34572
C	3.93667	1.99690	1.06750
N	-2.53350	-0.48634	0.88823
N	-1.72900	1.28473	-1.39152
H	-5.65365	-0.96001	-0.36158
H	-6.25215	-0.63921	2.06084
H	-4.38188	-0.22996	3.70264
H	-0.89556	-2.11311	2.64338
H	0.96930	-1.96918	4.27809
H	1.18691	0.04281	5.73062

H	-0.47829	1.87986	5.54933
H	-2.33958	1.71602	3.92150
H	-3.95850	-1.09887	-2.07675
H	-4.87547	1.06443	-2.63831
H	-4.53527	3.54571	-2.87793
H	-2.31108	4.50706	-2.21447
H	-0.79964	4.86556	-0.20917
H	1.46559	5.85165	-0.03846
H	3.40618	4.70909	-1.09332
H	3.06501	2.55484	-2.29756
H	0.79250	1.57622	-2.45476
H	-2.72428	-2.92150	-0.42461
H	-2.20571	-3.53568	-1.99907
H	-0.62616	-5.29066	-1.35985
H	1.49249	-5.92807	-0.17801
H	2.60420	-4.22099	1.29960
H	1.53263	-1.96026	1.51450
H	-1.47890	-0.32919	-3.34093
H	-1.60940	-2.06076	-3.66540
H	0.49613	-2.61142	-4.65556
H	3.00359	-2.64740	-4.48076
H	4.10517	-1.50735	-2.54876
H	6.00979	0.89585	2.47924
H	6.08453	-0.67918	1.65415
H	6.41552	0.79892	0.74979
H	3.68648	-1.20582	2.43845
H	3.72281	0.34128	3.29905
H	2.39039	0.00128	2.19219
H	4.15410	2.51701	2.00760
H	2.88153	2.15268	0.83864
H	4.52892	2.46800	0.27480
H	2.03255	0.32428	-0.03561
N	0.57630	0.92253	0.97563
N	0.33226	1.93829	1.58662
N	0.13022	2.91100	2.17762
H	0.32216	-3.74486	4.54022
H	2.22521	-3.11632	3.08846
H	4.07091	1.67752	-1.48409
H	4.93935	-0.18873	-2.78365
H	4.46977	-2.33206	-4.01014
H	2.15738	-3.29041	-3.89834
H	0.46128	-4.27054	-2.28552
H	-1.88289	-5.01750	-2.52792
H	-3.67182	-3.37121	-3.04688
H	-3.09699	-0.95945	-3.29489
H	-0.74423	-0.22182	-3.04223
H	2.88176	2.73187	0.79075
H	2.52734	3.96065	-0.43171
H	0.98500	5.46721	0.69794
H	-1.15121	5.79639	1.97976
H	-2.42280	3.75188	2.72412
H	-1.50138	1.50011	2.14689
H	1.59003	1.64807	-2.95474
H	1.80708	3.34780	-2.52897
H	-0.25887	4.33406	-3.23275
H	-2.76539	4.41398	-3.05381
H	-3.94411	2.64924	-1.72783
H	-5.97861	-1.45474	1.99908
H	-5.93746	0.32234	1.91063
H	-6.40295	-0.61424	0.48956
H	-3.52629	0.28733	2.74681
H	-3.61586	-1.47965	2.84312
H	-2.30091	-0.73125	1.94700
H	-4.26213	-2.85122	0.78717
H	-2.99932	-2.11211	-0.18917
H	-4.68177	-2.03945	-0.73537
H	-1.99579	-0.12507	-0.19285
N	-0.44967	-1.28943	0.43627
C	-0.54496	-2.44976	0.68713
S	-0.70842	-4.02931	1.02223

[4]FeN4Py2PhamideNCSOtBu2
Charge: 0
Energy: -2325997.0507182

Fe	0.66749	0.39216	0.04996
C	3.60241	0.49957	0.26131
C	4.93001	0.30941	0.61896
C	5.22292	-0.41223	1.78000
C	4.15343	-0.88795	2.54893
C	2.83989	-0.62766	2.16127
C	1.70209	-1.02767	3.02465
C	0.78604	-0.05639	3.45735
C	-0.28116	-0.40724	4.27975
C	-0.44912	-1.73706	4.67882
C	0.46265	-2.70571	4.25931
C	1.53854	-2.35348	3.44304
C	3.21644	1.11056	-1.08125
C	2.93963	-0.08728	-1.98575
C	3.96090	-0.65835	-2.74323
C	3.69787	-1.84946	-3.41761
C	2.41501	-2.39232	-3.34732
C	1.42292	-1.73357	-2.60832
C	0.01679	-2.19638	-2.67110
C	-0.31131	-3.55148	-2.53972
C	-1.63578	-3.96997	-2.67091
C	-2.64024	-3.04366	-2.95150
C	-2.31903	-1.68942	-3.08848
C	-1.00004	-1.26955	-2.94666
N	2.00512	1.95023	-0.93071
C	2.14593	3.04423	0.04474
C	0.84284	3.32658	0.77002
C	0.40603	4.61579	1.04444
C	-0.78514	4.79801	1.76095
C	-1.49049	3.66744	2.17468
C	-0.98820	2.40913	1.85576
N	0.15294	2.23002	1.15982
C	1.37692	2.39396	-2.18626
C	-0.13422	2.52756	-2.06910
C	-0.80818	3.57259	-2.68760
C	-2.20232	3.61462	-2.58034
C	-2.87260	2.64012	-1.85448
C	-2.11348	1.62259	-1.24365
N	-0.76960	1.56611	-1.36979
N	-2.66368	0.60090	-0.47021
C	-3.96140	0.52814	0.02110
O	-4.81094	1.37218	-0.23911
C	-4.26302	-0.68390	0.92802
C	-5.73679	-0.60001	1.35725
C	-3.36301	-0.64122	2.18449
C	-4.03052	-1.99440	0.14535
N	2.55556	0.04166	1.00375
N	1.70337	-0.61384	-1.89979
H	5.72092	0.70646	-0.01174
H	6.24981	-0.58124	2.08819
H	4.32721	-1.43004	3.47283
H	0.91982	0.96911	3.13571
H	-0.98306	0.35531	4.60776
H	-1.29161	-2.01685	5.30536

[6]FeN4Py2PhamideOHOtBu2
Charge: 0
Energy: -2065410.6578657

Fe	-0.52015	-0.27589	0.04929
C	-3.36568	-1.16321	0.53264
C	-4.69343	-1.30490	0.94728
C	-5.19134	-0.46839	1.93546
C	-4.33362	0.51471	2.47392
C	-3.01419	0.59476	2.03935
C	-2.09456	1.59580	2.63525
C	-0.81573	1.21864	3.06760
C	0.04116	2.15203	3.64746
C	-0.36357	3.48036	3.79550
C	-1.63550	3.86848	3.36490
C	-2.49649	2.93196	2.79232
C	-2.85279	-1.84566	-0.71521
C	-2.88527	-0.78533	-1.78814
C	-3.98123	-0.64723	-2.64202
C	-4.07153	0.47223	-3.45863
C	-3.03056	1.42275	-3.40623
C	-1.94620	1.21342	-2.56061
C	-0.77710	2.12255	-2.61584
C	-0.93465	3.51688	-2.65181
C	0.17544	4.35187	-2.78993
C	1.45482	3.80369	-2.91045
C	1.61944	2.41607	-2.87281
C	0.51597	1.58283	-2.70956
N	-1.44627	-2.31013	-0.50165
C	-1.30834	-3.23859	0.63613
C	0.00694	-3.05343	1.35149
C	0.80075	-4.12185	1.77273
C	1.99589	-3.85837	2.43981
C	2.36422	-2.52892	2.66970
C	1.51864	-1.52235	2.21129
N	0.37104	-1.77174	1.56704
C	-0.78858	-2.79821	-1.72675
C	0.71668	-2.65200	-1.66908
C	1.55389	-3.66708	-2.12234
C	2.93235	-3.45262	-2.07179
C	3.43558	-2.26678	-1.55510
C	2.52210	-1.29683	-1.08951
N	1.18609	-1.48739	-1.17761
N	2.90191	-0.09178	-0.50030
C	4.18518	0.27507	-0.12619
O	5.17603	-0.40847	-0.36335
C	4.31223	1.62127	0.63116
C	5.80474	1.87033	0.90284
C	3.54653	1.55471	1.97200
C	3.74370	2.77438	-0.22051
N	-2.51396	-0.24170	1.08686
N	-1.87058	0.13331	-1.73242
H	-5.32009	-2.06054	0.48000
H	-6.21153	-0.56995	2.29276
H	-4.67561	1.18412	3.25585
H	-0.50643	0.18861	2.94067
H	1.03083	1.84357	3.97345
H	0.30805	4.21007	4.24031

H	-1.95526	4.90202	3.47000
H	-3.47982	3.23611	2.44359
H	-3.52131	-2.67566	-0.98774
H	-4.75502	-1.41068	-2.64464
H	-4.90583	0.60080	-4.14119
H	-3.03194	2.28504	-4.06436
H	-1.93011	3.94277	-2.55828
H	0.04050	5.43026	-2.80397
H	2.31918	4.45265	-3.02294
H	2.61063	1.98022	-2.95279
H	0.64130	0.50709	-2.65616
H	-2.12698	-3.00529	1.32951
H	-1.43289	-4.28382	0.31585
H	0.48812	-5.14148	1.56661
H	2.63364	-4.67449	2.76713
H	3.28999	-2.27530	3.17550
H	1.76002	-0.47340	2.33216
H	-1.17525	-2.20067	-2.55803
H	-1.05583	-3.84757	-1.92602
H	1.13642	-4.59490	-2.50100
H	3.61955	-4.21674	-2.42527
H	4.49411	-2.07454	-1.47853
H	5.92669	2.82173	1.43362
H	6.23471	1.07061	1.51270
H	6.37538	1.91363	-0.02957
H	3.88622	0.70357	2.57590
H	3.74275	2.46813	2.54706
H	2.46726	1.48371	1.80988
H	3.89594	3.72590	0.30332
H	2.67367	2.65889	-0.40138
H	4.25263	2.83919	-1.18939
H	2.09851	0.51305	-0.20883
O	0.68659	1.15388	0.41836
H	0.38750	2.04093	0.17123

$^{6}FeN_3PyamideSRBr$
Charge: 2+
Energy: -3689827.6566705

Fe	-0.36498	-0.77700	-0.02913
S	0.38415	1.56076	-0.92575
C	1.51381	2.36131	0.29904
C	1.66615	3.87839	0.08580
C	2.42771	4.39812	1.22439
N	3.00424	4.72170	2.17747
H	2.18951	4.09163	-0.85232
H	0.69210	4.37915	0.04710
H	2.47868	1.86458	0.16417
H	1.15837	2.15159	1.30781
C	-1.12574	2.53435	-0.84005
C	-1.40730	3.31675	-1.96553
C	-2.57184	4.08722	-2.01363
C	-3.45717	4.06484	-0.93814
C	-3.17755	3.27228	0.17800
C	-2.01919	2.49056	0.25184
C	-1.74072	1.74233	1.53574
N	-1.65247	0.23862	1.50616
C	-1.06191	-0.19267	2.81175
C	0.43851	-0.07407	2.74603
N	1.02203	-0.53837	1.59883
C	2.37576	-0.49131	1.49202
N	2.95900	-0.98380	0.33502
C	4.04510	-0.35590	-0.31672
O	4.38044	0.76504	0.02942
C	4.69930	-1.10875	-1.47811
C	6.21367	-0.81076	-1.42343
H	6.40312	0.26470	-1.42204
H	6.66984	-1.24181	-0.52561
H	6.70104	-1.25333	-2.29747
C	4.46860	-2.63040	-1.43052
H	5.05408	-3.10529	-2.22331
H	4.79385	-3.06096	-0.47696
H	3.42351	-2.91035	-1.60981
C	4.09832	-0.50973	-2.77489
H	4.28443	0.56760	-2.82546
H	4.56887	-0.98063	-3.64382
H	3.01818	-0.68685	-2.84062
H	2.52955	-1.78454	-0.11029
C	3.17296	0.05863	2.51381
C	2.56749	0.55344	3.65304
C	1.17051	0.48454	3.77553
H	0.66786	0.86292	4.65909
H	3.16812	0.98684	4.44631
H	4.24592	0.09170	2.38521
H	-1.46568	0.40753	3.63461
H	-1.33333	-1.23071	3.00574
C	-2.94880	-0.43469	1.18599
C	-2.75136	-1.93799	1.32723
N	-1.58218	-2.37849	0.81278
C	-1.30194	-3.69185	0.82355
C	-2.18909	-4.62399	1.35921
C	-3.39697	-4.17368	1.89182
C	-3.68591	-2.80348	1.87679
H	-4.61590	-2.42185	2.28568
H	-4.10802	-4.87592	2.31592
H	-1.93316	-5.67785	1.35202
H	-0.35556	-3.98430	0.38332
C	-3.26963	-0.18261	-0.28006
N	-2.21056	-0.34448	-1.09870
C	-2.37164	-0.22647	-2.42723
C	-3.61308	0.05835	-2.99016
C	-4.71285	0.22019	-2.14696
C	-4.53981	0.09416	-0.76512
H	-5.37344	0.21644	-0.08128
H	-5.69380	0.44039	-2.55657
H	-3.70928	0.14385	-4.06696
H	-1.48408	-0.37067	-3.03261
H	-3.75958	-0.08310	1.83477
H	-0.78717	2.07421	1.95196
H	-2.50930	2.00925	2.27250
H	-3.87132	3.27077	1.01483
H	-4.36096	4.66565	-0.95953
H	-2.77482	4.70364	-2.88364
H	-0.71091	3.33109	-2.79838
Br	0.54931	-2.14156	-1.80821

$^{6}FeN_3PyamideSRCl$
Charge: 2+
Energy: -2363300.4415889

Fe	-0.38908	-0.86793	-0.23145
S	0.55508	1.50633	-0.79867
C	1.73932	2.05260	0.51383
C	1.99338	3.57110	0.50209
C	2.79910	3.88898	1.68345
N	3.40661	4.05693	2.65713
H	2.52007	3.87229	-0.40980
H	1.05463	4.13463	0.54686
H	2.66833	1.51598	0.30653
H	1.37111	1.73202	1.48859
C	-0.87574	2.57195	-0.56792
C	-1.09596	3.51938	-1.57384
C	-2.19676	4.37705	-1.50405
C	-3.07994	4.27817	-0.43108
C	-2.86266	3.32187	0.56412
C	-1.76965	2.44918	0.51780
C	-1.55392	1.50908	1.68213
N	-1.59786	0.02306	1.44058
C	-1.05163	-0.63994	2.66659
C	0.45474	-0.65310	2.60478
N	0.99823	-0.95325	1.38638
C	2.35209	-1.00213	1.26256
N	2.87623	-1.28397	0.01336
C	4.03668	-0.66602	-0.51453
O	4.55815	0.25175	0.09428
C	4.49823	-1.14870	-1.89215
C	6.01004	-0.87224	-2.00851
H	6.23632	0.17852	-1.81525
H	6.57829	-1.47904	-1.29592
H	6.34824	-1.12545	-3.01788
C	4.22047	-2.64676	-2.12683
H	4.67232	-2.94799	-3.07667
H	4.65993	-3.26686	-1.33821
H	3.15176	-2.87970	-2.20423
C	3.72891	-0.28815	-2.92807
H	3.94516	0.77610	-2.78627
H	4.04620	-0.56771	-3.93780
H	2.64547	-0.44267	-2.86277
H	2.33109	-1.87175	-0.60585
C	3.19350	-0.74318	2.36181
C	2.63044	-0.42224	3.58243
C	1.23276	-0.36909	3.70946
H	0.76648	-0.11199	4.65443
H	3.26668	-0.21237	4.43632
H	4.26502	-0.78651	2.22875
H	-1.39947	-0.12665	3.56988
H	-1.41946	-1.66514	2.71707
C	-2.94450	-0.48399	1.03117
C	-2.87418	-2.00415	0.95932
N	-1.74010	-2.45916	0.38361
C	-1.56357	-3.77657	0.19698
C	-2.52714	-4.70287	0.59375
C	-3.69850	-4.23951	1.19280
C	-3.87881	-2.86285	1.37994
H	-4.77935	-2.47282	1.84323
H	-4.46621	-4.93729	1.51273
H	-2.35732	-5.76147	0.43033
H	-0.63952	-4.07232	-0.28687
C	-3.22454	-0.00881	-0.38870
N	-2.17228	-0.15291	-1.21881
C	-2.30091	0.13388	-2.52425
C	-3.50663	0.58774	-3.05309
C	-4.59962	0.74064	-2.19887
C	-4.45955	0.43210	-0.84171
H	-5.29130	0.53834	-0.15294
H	-5.55254	1.09205	-2.58227
H	-3.58223	0.80886	-4.11207
H	-1.41752	-0.01447	-3.13547

H	-3.73034	-0.15741	1.72209
H	-0.57437	1.69495	2.12775
H	-2.29510	1.73561	2.45932
H	-3.55365	3.26062	1.40099
H	-3.93337	4.94517	-0.36033
H	-2.35143	5.11976	-2.28028
H	-0.40076	3.59343	-2.40449
Cl	0.39047	-1.98138	-2.00479

$^{6}FeN_3$PyamideSRF
Charge: 2+
Energy: -2137177.8513909

Fe	-0.34889	-0.88275	-0.28461
S	0.58385	1.50901	-0.77357
C	1.79341	1.97531	0.54680
C	2.06124	3.48972	0.61260
C	2.88669	3.73852	1.79693
N	3.51030	3.84994	2.76852
H	2.57626	3.83604	-0.28988
H	1.12726	4.05608	0.70144
H	2.71216	1.44019	0.29332
H	1.43780	1.60473	1.50853
C	-0.84164	2.56825	-0.48023
C	-1.06172	3.56131	-1.44166
C	-2.16191	4.41569	-1.33382
C	-3.04553	4.26856	-0.26688
C	-2.82820	3.26843	0.68410
C	-1.73571	2.39759	0.59936
C	-1.52174	1.41095	1.72540
N	-1.56459	-0.06354	1.42444
C	-1.02083	-0.77346	2.62719
C	0.48763	-0.79731	2.55584
N	1.00773	-1.05313	1.32027
C	2.35648	-1.12601	1.15544
N	2.81608	-1.37176	-0.12253
C	3.97378	-0.78048	-0.68654
O	4.63156	0.01244	-0.03841
C	4.23857	-1.14241	-2.15143
C	5.66765	-0.69691	-2.50548
H	5.80789	0.37100	-2.32146
H	6.40868	-1.23923	-1.91037
H	5.86110	-0.89930	-3.56331
C	4.07692	-2.65755	-2.40086
H	4.36235	-2.88124	-3.43342
H	4.72397	-3.24397	-1.74039
H	3.04392	-3.00361	-2.27462
C	3.21289	-0.35195	-3.00617
H	3.30488	0.72663	-2.83271
H	3.41003	-0.53788	-4.06692
H	2.18223	-0.66011	-2.79859
H	2.16961	-1.82366	-0.76334
C	3.22640	-0.92415	2.24532
C	2.68864	-0.64363	3.48816
C	1.29341	-0.57398	3.65372
H	0.85501	-0.35202	4.62066
H	3.34592	-0.47709	4.33575
H	4.29403	-0.97696	2.08775
H	-1.36178	-0.29182	3.55018
H	-1.39567	-1.79791	2.64027
C	-2.90388	-0.55857	0.97263
C	-2.82244	-2.07554	0.83071
N	-1.68854	-2.48580	0.22433
C	-1.49227	-3.78359	-0.05010
C	-2.44174	-4.74472	0.29586
C	-3.61167	-4.33226	0.93490
C	-3.81137	-2.97160	1.20733
H	-4.71410	-2.62450	1.69955
H	-4.36670	-5.05878	1.21913
H	-2.26366	-5.78935	0.06519
H	-0.56559	-4.02725	-0.55874
C	-3.16480	-0.02821	-0.43542
N	-2.10560	-0.14900	-1.26200
C	-2.21691	0.17676	-2.55950
C	-3.41564	0.64902	-3.08826
C	-4.51499	0.78364	-2.23862
C	-4.39134	0.43486	-0.88911
H	-5.23037	0.52660	-0.20717
H	-5.46200	1.15234	-2.62051
H	-3.48117	0.90119	-4.14093
H	-1.32449	0.04875	-3.16391
H	-3.70522	-0.26690	1.66114
H	-0.54097	1.57873	2.17682
H	-2.26175	1.60869	2.51141
H	-3.51854	3.17078	1.51806
H	-3.89873	4.93200	-0.16602
H	-2.31557	5.19297	-2.07565
H	-0.36670	3.67257	-2.26832
F	0.47145	-1.81161	-1.57435

$^{6}FeN_3$PyamideSRN$_3$
Charge: 2+
Energy: -2177564.5155219

Fe	-0.35737	-0.83194	-0.04541
S	0.59938	1.46221	-0.89894
C	1.78820	2.14217	0.34439
C	2.04865	3.64947	0.17419
C	2.86036	4.08873	1.31185
N	3.47367	4.35709	2.25905
H	2.57096	3.85285	-0.76683
H	1.11097	4.21659	0.16317
H	2.71354	1.58107	0.19188
H	1.42383	1.92664	1.34915
C	-0.82721	2.55539	-0.79942
C	-1.03491	3.38437	-1.90766
C	-2.13759	4.24120	-1.95157
C	-3.03613	4.26143	-0.88712
C	-2.83013	3.42566	0.21321
C	-1.73544	2.55612	0.28137
C	-1.53110	1.76311	1.55278
N	-1.57637	0.25934	1.49556
C	-1.03794	-0.24233	2.80020
C	0.47034	-0.27657	2.74771
N	1.00944	-0.73599	1.58181
C	2.35954	-0.81629	1.46005
N	2.85230	-1.26603	0.24628
C	4.01047	-0.75761	-0.38376
O	4.63083	0.15874	0.12408
C	4.33847	-1.35809	-1.75647
C	5.83575	-1.13024	-2.03540
H	6.09661	-0.07327	-1.94941
H	6.45738	-1.69010	-1.32939
H	6.07516	-1.47132	-3.04730
C	4.01592	-2.86374	-1.83958
H	4.35319	-3.25076	-2.80584
H	4.52831	-3.42973	-1.05491
H	2.94171	-3.07920	-1.77377
C	3.48945	-0.56830	-2.78573
H	3.74527	0.49632	-2.76666
H	3.68907	-0.94716	-3.79333
H	2.41441	-0.66889	-2.59109
H	2.24139	-1.85671	-0.30691
C	3.21117	-0.42906	2.51111
C	2.65225	0.05310	3.68144
C	1.25598	0.13794	3.80617
H	0.79754	0.52031	4.71178
H	3.29380	0.36675	4.49881
H	4.28156	-0.49743	2.38070
H	-1.38413	0.38477	3.62940
H	-1.41246	-1.25028	2.98220
C	-2.92149	-0.29442	1.14727
C	-2.85493	-1.81287	1.26448
N	-1.72130	-2.33981	0.75501
C	-1.54714	-3.67016	0.74927
C	-2.51280	-4.53735	1.25796
C	-3.68650	-3.99732	1.78509
C	-3.86328	-2.60816	1.79068
H	-4.76314	-2.15937	2.19889
H	-4.45652	-4.64594	2.19126
H	-2.34316	-5.60838	1.23946
H	-0.61412	-4.02834	0.32706
C	-3.20048	0.00422	-0.32141
N	-2.14857	-0.23255	-1.13005
C	-2.27932	-0.07828	-2.45677
C	-3.48428	0.31190	-3.03508
C	-4.57870	0.55073	-2.20221
C	-4.43639	0.39299	-0.82023
H	-5.26685	0.57748	-0.14651
H	-5.53207	0.85763	-2.62103
H	-3.55796	0.42391	-4.11121
H	-1.39241	-0.26680	-3.05290
H	-3.71182	0.11330	1.78872
H	-0.55181	2.00005	1.97478
H	-2.27372	2.08815	2.29298
H	-3.53126	3.45912	1.04326
H	-3.89151	4.92953	-0.90406
H	-2.28173	4.89131	-2.80873
H	-0.32768	3.36621	-2.73123
N	0.37601	-1.93595	-1.37020
N	0.23602	-2.53186	-2.42299
N	0.12846	-3.09276	-3.41620

$^{6}FeN_3$PyamideSRNCS
Charge: 2+
Energy: -2382672.7491005

Fe	-0.36347	-0.73147	0.18783
S	0.54671	1.37580	-1.09261
C	1.68986	2.33426	0.00100
C	1.91064	3.78150	-0.47395
C	2.69001	4.47221	0.55636
N	3.27973	4.95172	1.43252
H	2.44321	3.80223	-1.43085
H	0.95766	4.30448	-0.61269
H	2.63394	1.78437	-0.01861
H	1.31067	2.31896	1.02325
C	-0.91299	2.41984	-1.23128

C	-1.12794	3.00010	-2.48644
C	-2.25256	3.79766	-2.71229
C	-3.16518	4.00825	-1.68097
C	-2.95194	3.41930	-0.43232
C	-1.83584	2.61310	-0.18036
C	-1.63084	2.09668	1.22644
N	-1.63595	0.61131	1.46891
C	-1.11063	0.39319	2.85394
C	0.39864	0.39617	2.83013
N	0.97282	-0.26057	1.78165
C	2.32635	-0.31709	1.69403
N	2.85747	-0.96956	0.59297
C	4.02496	-0.55977	-0.09171
O	4.59917	0.46134	0.24007
C	4.42642	-1.41662	-1.29797
C	5.91416	-1.15625	-1.59772
H	6.10689	-0.09175	-1.74764
H	6.54818	-1.50096	-0.77475
H	6.20400	-1.69769	-2.50351
C	4.20108	-2.92215	-1.05084
H	4.58068	-3.48701	-1.90773
H	4.73545	-3.26689	-0.15957
H	3.14312	-3.19015	-0.94337
C	3.56229	-0.92710	-2.48858
H	3.75327	0.13072	-2.69871
H	3.81713	-1.50148	-3.38510
H	2.49025	-1.05473	-2.29881
H	2.28036	-1.67905	0.15574
C	3.14574	0.28840	2.66491
C	2.55085	0.96535	3.71472
C	1.15083	1.02968	3.80081
H	0.66378	1.56370	4.60956
H	3.16741	1.44737	4.46674
H	4.22001	0.23115	2.56547
H	-1.49039	1.15967	3.53889
H	-1.46048	-0.57080	3.22508
C	-2.95998	-0.03784	1.21927
C	-2.85813	-1.50105	1.63578
N	-1.70334	-2.08668	1.25395
C	-1.49893	-3.38858	1.50404
C	-2.45344	-4.16616	2.15816
C	-3.64757	-3.56509	2.55759
C	-3.85699	-2.20599	2.29242
H	-4.77465	-1.71098	2.59351
H	-4.40930	-4.14313	3.07164
H	-2.25980	-5.21638	2.34722
H	-0.55303	-3.79738	1.16515
C	-3.21757	-0.04747	-0.28364
N	-2.14597	-0.41970	-1.01080
C	-2.25308	-0.55437	-2.34136
C	-3.45466	-0.32118	-3.00541
C	-4.56885	0.06256	-2.25716
C	-4.45130	0.19871	-0.87037
H	-5.29897	0.49743	-0.26227
H	-5.51971	0.25331	-2.74501
H	-3.51124	-0.44033	-4.08181
H	-1.35148	-0.85288	-2.86603
H	-3.77257	0.46657	1.75556
H	-0.66539	2.44132	1.60357
H	-2.39389	2.54131	1.87850
H	-3.66505	3.59984	0.36803
H	-4.03761	4.63427	-1.83990
H	-2.40264	4.25550	-3.68491
H	-0.40917	2.83588	-3.28339
N	0.40629	-2.07205	-0.88883
C	0.46762	-2.92843	-1.74361
S	0.56908	-4.03774	-2.86000

^{6}FeN$_3$PyamideSROH
Charge: 2+
Energy: -2122093.7000603

Fe	-0.35180	-0.90134	-0.32761
S	0.60450	1.51596	-0.74561
C	1.80119	1.95162	0.59630
C	2.07409	3.46313	0.69611
C	2.89332	3.68787	1.88957
N	3.51242	3.78210	2.86587
H	2.59514	3.82631	-0.19625
H	1.14125	4.03049	0.79035
H	2.72112	1.41926	0.34198
H	1.43650	1.56263	1.54746
C	-0.81616	2.57861	-0.44097
C	-1.02053	3.59891	-1.37711
C	-2.11603	4.45772	-1.25807
C	-3.01139	4.28889	-0.20416
C	-2.80947	3.26320	0.72244
C	-1.72194	2.38736	0.62496
C	-1.52199	1.37264	1.72833
N	-1.57717	-0.09386	1.39540
C	-1.04099	-0.83040	2.58470
C	0.46775	-0.86463	2.52128
N	0.99857	-1.09326	1.28554
C	2.34817	-1.16416	1.13472
N	2.82290	-1.36934	-0.14640
C	3.99666	-0.77686	-0.66714
O	4.65045	-0.00710	0.01308
C	4.29697	-1.09857	-2.13599
C	5.76513	-0.73347	-2.41744
H	5.96715	0.31190	-2.17312
H	6.44573	-1.35366	-1.82590
H	5.98557	-0.89614	-3.47696
C	4.05142	-2.58636	-2.46397
H	4.36451	-2.78223	-3.49426
H	4.63141	-3.24353	-1.80783
H	2.99425	-2.86988	-2.39122
C	3.36059	-0.20386	-2.98906
H	3.52522	0.85710	-2.76995
H	3.57543	-0.36408	-4.05080
H	2.30368	-0.43957	-2.81657
H	2.18110	-1.79503	-0.81299
C	3.20720	-1.00127	2.23949
C	2.65795	-0.75207	3.48401
C	1.26242	-0.67488	3.63428
H	0.81385	-0.47261	4.60088
H	3.30680	-0.61385	4.34308
H	4.27617	-1.05516	2.09273
H	-1.38091	-0.36417	3.51623
H	-1.42233	-1.85217	2.57955
C	-2.92190	-0.56511	0.94055
C	-2.86183	-2.08020	0.78154
N	-1.72854	-2.50656	0.18588
C	-1.54648	-3.81249	-0.05926
C	-2.50915	-4.75933	0.28820
C	-3.68406	-4.32527	0.90360
C	-3.86706	-2.95979	1.15740
H	-4.76794	-2.59497	1.64018
H	-4.45111	-5.03883	1.18841
H	-2.33666	-5.80966	0.08013
H	-0.61116	-4.07882	-0.54007
C	-3.18145	-0.00297	-0.45381
N	-2.12486	-0.10703	-1.28448
C	-2.23584	0.28440	-2.56352
C	-3.42752	0.79480	-3.07137
C	-4.52714	0.89951	-2.21760
C	-4.40456	0.49166	-0.88566
H	-5.24001	0.56700	-0.19727
H	-5.47010	1.29531	-2.58188
H	-3.48778	1.10122	-4.10989
H	-1.34241	0.18641	-3.17201
H	-3.71810	-0.27472	1.63622
H	-0.54101	1.52175	2.18534
H	-2.26215	1.56087	2.51689
H	-3.50795	3.14878	1.54750
H	-3.86094	4.95555	-0.09402
H	-2.25682	5.25565	-1.98031
H	-0.31570	3.72741	-2.19287
O	0.46589	-1.78228	-1.68804
H	0.18501	-2.19021	-2.52236

^{6}FeN4Py2PhF2Br
Charge: 2+
Energy: -3677419.2393942

Fe	-0.00024	0.41271	0.07513
C	-1.86705	2.06729	-1.77769
C	-2.65419	3.14809	-2.15459
C	-2.97177	4.11165	-1.19630
C	-2.49154	3.95778	0.10498
C	-1.71475	2.84416	0.41181
C	-1.23869	2.57426	1.82167
C	1.23852	2.57423	1.82163
C	1.71486	2.84384	0.41179
C	2.49201	3.95724	0.10506
C	2.97257	4.11092	-1.19612
C	2.65491	3.14740	-2.15443
C	1.86738	2.06684	-1.77764
C	-0.00010	0.71559	2.92578
C	-1.21476	-0.18062	2.75086
C	-1.90735	-0.70771	3.83099
C	-2.93479	-1.62009	3.57790
C	-3.24919	-1.92639	2.25879
C	-2.54102	-1.32229	1.21178
C	-2.96380	-1.55769	-0.18659
C	-2.74950	-2.78421	-0.82299
C	-3.16703	-3.03080	-2.12344
C	-3.84377	-2.01901	-2.80836
C	-4.10105	-0.78394	-2.20461
C	-3.66239	-0.58495	-0.90457
C	1.21461	-0.18058	2.75088
C	1.90730	-0.70750	3.83103
C	2.93486	-1.61975	3.57795
C	3.24921	-1.92612	2.25884
C	2.54086	-1.32223	1.21182
C	2.96361	-1.55779	-0.18654
C	3.66251	-0.58525	-0.90450
C	4.10132	-0.78444	-2.20446
C	3.84389	-2.01951	-2.80813

C	3.16684	-3.03110	-2.12324
C	2.74915	-2.78431	-0.82287
N	-1.40946	1.91934	-0.52006
N	-0.00009	1.74897	1.84929
N	1.40950	1.91906	-0.52011
N	-1.50490	-0.48883	1.46628
N	1.50466	-0.48886	1.46631
H	-1.59336	1.28649	-2.47649
H	-3.00548	3.22964	-3.17739
H	-3.58043	4.97201	-1.45680
H	-2.71976	4.68950	0.87364
H	-1.08864	3.51209	2.36762
H	-2.02991	2.02753	2.34277
H	2.02966	2.02764	2.34299
H	1.08840	3.51219	2.36734
H	2.72028	4.68894	0.87372
H	3.58155	4.97107	-1.45653
H	3.00642	3.22879	-3.17717
H	1.59360	1.28611	-2.47648
H	-0.00012	1.16964	3.92390
H	-1.64557	-0.42001	4.84404
H	-3.49069	-2.06655	4.39645
H	-4.05763	-2.60728	2.01797
F	-2.08319	-3.72945	-0.14024
H	-2.96391	-3.99468	-2.57571
H	-4.18531	-2.19832	-3.82260
H	-4.65480	-0.00136	-2.71089
F	-3.92066	0.59070	-0.28465
H	1.64555	-0.41974	4.84406
H	3.49088	-2.06608	4.39649
H	4.05771	-2.60693	2.01802
F	3.92094	0.59039	-0.28463
H	4.65529	-0.00200	-2.71072
H	4.18555	-2.19897	-3.82231
H	2.96359	-3.99498	-2.57544
F	2.08255	-3.72936	-0.14014
Br	-0.00004	-1.00062	-1.84880

^{6}FeN4Py2PhF2Cl
Charge: 2+
Energy: -2350891.4473615

Fe	0.14203	-0.53278	-0.23556
C	2.07791	-1.91477	-2.23626
C	2.98415	-2.86419	-2.69457
C	3.36057	-3.90175	-1.84069
C	2.81491	-3.95559	-0.55645
C	1.92075	-2.96635	-0.16287
C	1.34086	-2.90024	1.22902
C	-1.03622	-3.23162	0.71156
C	-1.94621	-2.68524	-0.36960
C	-3.16207	-3.29697	-0.66234
C	-3.93902	-2.79799	-1.70928
C	-3.47625	-1.70024	-2.43595
C	-2.25486	-1.13818	-2.08688
C	-0.37207	-1.52031	2.41072
C	0.67163	-0.43931	2.66262
C	0.97265	0.03026	3.93133
C	1.82756	1.13238	4.04437
C	2.38459	1.68360	2.89539
C	2.08511	1.12774	1.64598
C	2.76409	1.58421	0.41725
C	2.65927	2.89637	-0.05896
C	3.28592	3.31932	-1.22212
C	4.06769	2.40517	-1.93196
C	4.22059	1.08899	-1.48613
C	3.56832	0.71085	-0.32451
C	-1.68887	-0.80675	2.14878
C	-2.84346	-0.98913	2.89277
C	-3.97695	-0.24563	2.53666
C	-3.88677	0.67962	1.50405
C	-2.67006	0.84079	0.81981
C	-2.47655	1.91422	-0.17070
C	-3.34166	2.11427	-1.25267
C	-3.18484	3.15347	-2.15723
C	-2.12860	4.04913	-1.96407
C	-1.24061	3.89944	-0.89512
C	-1.43090	2.83735	-0.02748
N	1.55657	-1.96659	-0.99532
N	-0.00152	-2.26528	1.17257
N	-1.50822	-1.62257	-1.07393
N	1.20181	0.10755	1.54452
N	-1.61445	0.05787	1.11706
H	1.75138	-1.08826	-2.85448
H	3.37939	-2.78896	-3.70173
H	4.06261	-4.66182	-2.16937
H	3.08337	-4.75022	0.13244
H	1.29196	-3.89114	1.69545
H	1.99735	-2.28027	1.84376
H	-1.62613	-3.59582	1.56052
H	-0.51536	-4.10059	0.29635
H	-3.49525	-4.14964	-0.07867
H	-4.89290	-3.25759	-1.94898
H	-4.05205	-1.27369	-3.24932
H	-1.85426	-0.27188	-2.59776
H	-0.45553	-2.19170	3.27392
H	0.53889	-0.43825	4.80870
H	2.06951	1.53947	5.02116
H	3.07411	2.51812	2.94902
F	1.89555	3.76057	0.63319
H	3.16356	4.34503	-1.55072
H	4.57318	2.72509	-2.83724
H	4.84756	0.37440	-2.00715
F	3.71870	-0.55437	0.13705
H	-2.86454	-1.68872	3.72203
H	-4.90761	-0.37054	3.08143
H	-4.73056	1.30370	1.23376
F	-4.34490	1.22574	-1.42303
H	-3.88093	3.25594	-2.98190
H	-1.99653	4.87349	-2.65716
H	-0.41054	4.57580	-0.72793
F	-0.57582	2.66581	1.00279
Cl	0.39834	0.96506	-1.83898

^{6}FeN4Py2PhF2F
Charge: 2+
Energy: -2124768.6254933

Fe	0.14680	-0.43060	-0.20273
C	1.89718	-1.70311	-2.34079
C	2.71708	-2.65381	-2.93792
C	3.07582	-3.78539	-2.20218
C	2.60531	-3.93195	-0.89448
C	1.79591	-2.93661	-0.35817
C	1.29721	-2.94887	1.06994
C	-1.14041	-3.11491	0.73256
C	-1.99985	-2.52458	-0.37224
C	-3.23044	-3.08086	-0.71288
C	-3.95510	-2.52444	-1.76892
C	-3.42974	-1.43155	-2.46218
C	-2.19590	-0.92863	-2.06948
C	-0.23796	-1.51232	2.43433
C	0.88708	-0.50575	2.64480
C	1.34075	-0.12932	3.89977
C	2.26857	0.91528	3.98292
C	2.73652	1.51028	2.81500
C	2.27746	1.05086	1.57563
C	2.82440	1.56064	0.30034
C	2.68809	2.89675	-0.09478
C	3.18944	3.37128	-1.29887
C	3.87741	2.48745	-2.13322
C	4.06632	1.15101	-1.76821
C	3.53982	0.72089	-0.56120
C	-1.52506	-0.71246	2.28617
C	-2.60379	-0.80322	3.15150
C	-3.72565	-0.00642	2.88809
C	-3.70974	0.85548	1.79861
C	-2.57346	0.91391	0.97390
C	-2.48390	1.85834	-0.15490
C	-3.51865	2.00637	-1.09066
C	-3.45967	2.90926	-2.14103
C	-2.32659	3.71971	-2.26102
C	-1.26886	3.61630	-1.35404
C	-1.36943	2.69075	-0.33016
N	1.45176	-1.85208	-1.08065
N	-0.00775	-2.24023	1.15025
N	-1.50940	-1.46822	-1.04372
N	1.33761	0.08042	1.51296
N	-1.51556	0.11367	1.22044
H	1.57817	-0.79771	-2.84416
H	3.06085	-2.51039	-3.95647
H	3.71013	-4.54917	-2.64146
H	2.86770	-4.80146	-0.30021
H	1.22458	-3.96911	1.46374
H	2.02344	-2.41379	1.68731
H	-1.76336	-3.37332	1.59610
H	-0.72150	-4.05562	0.36069
H	-3.61595	-3.93240	-0.16048
H	-4.92006	-2.93857	-2.04445
H	-3.96656	-0.97127	-3.28389
H	-1.73086	-0.07054	-2.54060
H	-0.30551	-2.20041	3.28558
H	0.97031	-0.62492	4.79114
H	2.63236	1.24704	4.95043
H	3.47182	2.30611	2.84430
F	2.04065	3.73496	0.72982
H	3.05375	4.41542	-1.55720
H	4.28815	2.84847	-3.07051
H	4.63217	0.46105	-2.38380
F	3.73976	-0.55981	-0.16891
H	-2.57654	-1.47602	4.00241
H	-4.59497	-0.05304	3.53660
H	-4.55508	1.49670	1.58012
F	-4.59383	1.20034	-0.97212
H	-4.28963	2.97552	-2.83531
H	-2.26971	4.44050	-3.07013
H	-0.38277	4.23632	-1.42317
F	-0.35613	2.57745	0.55659

F	0.29006	0.72138	-1.53517

^{6}FeN4Py2PhF2N$_3$
Charge: 2+
Energy: -2165157.1852426

Fe	0.06613	-0.58491	-0.23639
C	1.87873	-1.95419	-2.34837
C	2.69256	-2.93793	-2.89756
C	2.94943	-4.08729	-2.14731
C	2.38251	-4.21223	-0.87760
C	1.58525	-3.18041	-0.39194
C	0.99322	-3.18921	0.99880
C	-1.40346	-3.20870	0.46042
C	-2.23159	-2.47682	-0.57888
C	-3.50495	-2.91980	-0.92907
C	-4.20515	-2.24734	-1.93196
C	-3.61293	-1.14914	-2.55847
C	-2.34110	-0.76423	-2.15431
C	-0.56742	-1.74791	2.30976
C	0.58366	-0.81249	2.66568
C	0.92093	-0.51501	3.97793
C	1.88178	0.47495	4.20679
C	2.49479	1.09236	3.12132
C	2.14500	0.70981	1.82085
C	2.86692	1.25064	0.64898
C	2.91637	2.62077	0.36176
C	3.61619	3.13321	-0.72249
C	4.31100	2.24889	-1.55062
C	4.30260	0.87340	-1.29988
C	3.58929	0.40906	-0.20590
C	-1.79998	-0.87413	2.12195
C	-2.96678	-0.99225	2.86173
C	-4.01326	-0.10391	2.58178
C	-3.82957	0.88484	1.62191
C	-2.60615	0.96457	0.93710
C	-2.30661	2.07145	0.00846
C	-3.15631	2.43098	-1.04366
C	-2.89287	3.49612	-1.89389
C	-1.74086	4.25573	-1.67237
C	-0.86258	3.94488	-0.62950
C	-1.16077	2.86216	0.18182
N	1.33718	-2.07436	-1.12326
N	-0.27121	-2.40817	1.00574
N	-1.66820	-1.41532	-1.18645
N	1.17333	-0.20663	1.61084
N	-1.63577	0.05915	1.16467
H	1.64160	-1.04266	-2.88419
H	3.10913	-2.80609	-3.89018
H	3.57665	-4.87838	-2.54650
H	2.56031	-5.09446	-0.27079
H	0.83471	-4.21080	1.36401
H	1.70464	-2.70816	1.67439
H	-2.04486	-3.57098	1.27211
H	-0.98009	-4.09592	-0.02186
H	-3.94189	-3.77533	-0.42319
H	-5.20126	-2.57327	-2.21499
H	-4.12794	-0.59172	-3.33243
H	-1.83801	0.09536	-2.58091
H	-0.73020	-2.48328	3.10734
H	0.43525	-1.02883	4.80111
H	2.15823	0.74663	5.22075
H	3.25988	1.84686	3.26309
F	2.23775	3.46088	1.16274
H	3.61404	4.20252	-0.90023
H	4.86876	2.63597	-2.39690
H	4.85911	0.17372	-1.91319
F	3.59673	-0.91565	0.07166
H	-3.06234	-1.75238	3.63029
H	-4.94976	-0.17129	3.12670
H	-4.60484	1.61165	1.40938
F	-4.25795	1.67738	-1.24537
H	-3.58553	3.72437	-2.69601
H	-1.52494	5.09946	-2.31950
H	0.03307	4.52275	-0.43166
F	-0.32033	2.54699	1.18927
N	0.43547	0.80770	-1.39567
N	0.81456	1.65880	-2.16402
N	1.16657	2.47889	-2.88685

^{6}FeN4Py2PhF2NCS
Charge: 2+
Energy: -2370264.9492997

Fe	0.06772	-0.58287	-0.22298
C	1.97930	-1.54380	-2.47307
C	2.81509	-2.41474	-3.16246
C	3.03626	-3.68805	-2.63437
C	2.41326	-4.04571	-1.43711
C	1.59746	-3.11668	-0.79928
C	0.94651	-3.38299	0.53835
C	-1.42466	-3.29255	-0.09599
C	-2.20488	-2.37713	-1.02045
C	-3.45782	-2.74195	-1.50754
C	-4.11201	-1.89235	-2.40112
C	-3.49488	-0.70029	-2.78471
C	-2.24546	-0.40200	-2.25624
C	-0.67511	-2.20549	2.02826
C	0.45572	-1.35525	2.59852
C	0.74101	-1.29834	3.95474
C	1.69328	-0.37202	4.39285
C	2.35263	0.42310	3.46013
C	2.05471	0.28037	2.10053
C	2.81628	1.00343	1.05966
C	2.84480	2.40049	0.97533
C	3.55511	3.07466	-0.00839
C	4.28400	2.33013	-0.93846
C	4.30112	0.93338	-0.88655
C	3.57334	0.30532	0.11151
C	-1.90372	-1.31036	1.95064
C	-3.10234	-1.56248	2.60016
C	-4.14348	-0.63938	2.43608
C	-3.92530	0.50728	1.68125
C	-2.67169	0.71310	1.08217
C	-2.33979	1.97182	0.38853
C	-3.15162	2.52863	-0.60674
C	-2.86375	3.73802	-1.22288
C	-1.72568	4.43911	-0.81369
C	-0.88469	3.93159	0.18080
C	-1.20653	2.71279	0.75438
N	1.38355	-1.88946	-1.31767
N	-0.32054	-2.61255	0.63721
N	-1.61787	-1.22412	-1.39357
N	1.08802	-0.57374	1.69550
N	-1.70411	-0.21778	1.18843
H	1.77073	-0.54461	-2.83551
H	3.27576	-2.10080	-4.09277
H	3.67906	-4.39549	-3.14906
H	2.56266	-5.02855	-1.00138
H	0.77708	-4.45424	0.69897
H	1.62702	-3.03932	1.32106
H	-2.10239	-3.79297	0.60521
H	-0.97793	-4.07935	-0.71271
H	-3.91448	-3.67452	-1.19038
H	-5.09196	-2.15569	-2.78700
H	-3.97407	-0.00718	-3.46660
H	-1.72672	0.51872	-2.49412
H	-0.86719	-3.07562	2.66804
H	0.22342	-1.94670	4.65420
H	1.92865	-0.28737	5.44918
H	3.11426	1.13205	3.76378
F	2.13523	3.10490	1.87409
H	3.53743	4.15831	-0.02958
H	4.85186	2.84414	-1.70696
H	4.88466	0.33880	-1.58022
F	3.59844	-1.04574	0.19526
H	-3.22625	-2.45007	3.21207
H	-5.10377	-0.80602	2.91420
H	-4.69735	1.25906	1.56670
F	-4.24015	1.82908	-0.99190
H	-3.52625	4.11767	-1.99236
H	-1.49135	5.39177	-1.27715
H	0.00256	4.45569	0.51691
F	-0.40289	2.20512	1.71189
N	0.47423	0.99316	-1.14494
C	0.75206	1.85848	-1.93809
S	1.10587	2.98420	-2.99102

^{6}FeN4Py2PhF2OH
Charge: 2+
Energy: -2109683.5185724

Fe	-0.00038	0.21927	-0.07981
C	-1.97807	1.48325	-2.01164
C	-2.86786	2.42583	-2.51134
C	-3.21557	3.50982	-1.70190
C	-2.66852	3.61266	-0.42162
C	-1.79276	2.62352	0.01931
C	-1.24029	2.61825	1.43293
C	1.23934	2.61893	1.43239
C	1.79230	2.62329	0.01893
C	2.66849	3.61202	-0.42208
C	3.21603	3.50849	-1.70209
C	2.86838	2.42423	-2.51121
C	1.97812	1.48213	-2.01147
C	0.00029	0.87739	2.74016
C	-1.23215	-0.00939	2.64716
C	-2.02115	-0.32785	3.74396
C	-3.14044	-1.13949	3.54062
C	-3.44225	-1.56310	2.24955
C	-2.60857	-1.19747	1.18595
C	-2.98948	-1.54562	-0.20727
C	-2.43419	-2.61091	-0.91551
C	-2.84581	-2.96592	-2.19113
C	-3.85833	-2.21456	-2.79420
C	-4.43089	-1.12195	-2.13773
C	-3.98564	-0.81348	-0.85996
C	1.23335	-0.00847	2.64670

C	2.02353	-0.32559	3.74303
C	3.14345	-1.13625	3.53922
C	3.44450	-1.56040	2.24817
C	2.60952	-1.19626	1.18506
C	2.98935	-1.54554	-0.20816
C	3.98644	-0.81526	-0.86155
C	4.43061	-1.12489	-2.13942
C	3.85606	-2.21685	-2.79521
C	2.84267	-2.96643	-2.19138
C	2.43214	-2.61026	-0.91573
N	-1.45877	1.58855	-0.77397
N	-0.00022	1.80745	1.56568
N	1.45835	1.58808	-0.77404
N	-1.50073	-0.45822	1.40260
N	1.50128	-0.45773	1.40215
O	-0.00078	-0.96723	-1.42912
H	-1.66007	0.61408	-2.57696
H	-3.27418	2.31282	-3.51036
H	-3.90273	4.26882	-2.06300
H	-2.92378	4.44423	0.22791
H	-1.07083	3.64423	1.77779
H	-2.00806	2.19575	2.08854
H	2.00723	2.19771	2.08868
H	1.06904	3.64514	1.77614
H	2.92371	4.44381	0.22718
H	3.90355	4.26715	-2.06324
H	3.27508	2.31068	-3.51001
H	1.66010	0.61280	-2.57655
H	0.00026	1.42058	3.69299
H	-1.77641	0.05774	4.72837
H	-3.77958	-1.41441	4.37389
H	-4.32219	-2.16345	2.04774
F	-1.41961	-3.29156	-0.33135
H	-2.38678	-3.81396	-2.68669
H	-4.20269	-2.48247	-3.78776
H	-5.21357	-0.52375	-2.59039
F	-4.49663	0.25656	-0.21546
H	1.77921	0.06032	4.72742
H	3.78356	-1.41007	4.37211
H	4.32477	-2.16014	2.04597
F	4.49943	0.25418	-0.21768
H	5.21402	-0.52807	-2.59265
H	4.19955	-2.48567	-3.78883
H	2.38216	-3.81400	-2.68637
F	1.41690	-3.28930	-0.33081
H	-0.00101	-1.93215	-1.30821

$^{6}FeN_3PyO2PhBr$
Charge: 1+
Energy: -3465187.7139371

Fe	0.12578	-0.21768	-0.13942
C	-3.76170	-2.54422	-1.18317
H	-4.54357	-2.29882	-0.46932
C	-4.07513	-2.71475	-2.52959
H	-5.10392	-2.61104	-2.86130
C	-3.06710	-3.01635	-3.44967
H	-3.31396	-3.15364	-4.49841
C	-1.74466	-3.14064	-3.02032
H	-0.95893	-3.37695	-3.73162
C	-1.42290	-2.95220	-1.67807
H	-0.39366	-3.02510	-1.34887
C	-2.42975	-2.64711	-0.75203
C	-2.11133	-2.49283	0.68263
C	-2.83141	-3.24270	1.63151
H	-3.62285	-3.89668	1.28390
C	-2.49081	-3.18342	2.97449
H	-3.02429	-3.78177	3.70684
C	-1.43346	-2.35838	3.36567
H	-1.12329	-2.28936	4.40313
C	-0.78916	-1.61059	2.39094
C	0.25455	-0.56446	2.76077
H	0.65060	-0.77865	3.76334
C	-0.49159	0.76360	2.77426
C	-1.07446	1.24156	3.94268
H	-0.91816	0.72668	4.88521
C	-1.87515	2.38169	3.86006
H	-2.36110	2.78119	4.74506
C	-2.01309	3.01338	2.63072
H	-2.58986	3.92613	2.53091
C	-1.34895	2.50538	1.50100
C	-1.38005	3.27129	0.23572
C	-0.17990	3.68486	-0.35537
H	0.76092	3.42915	0.11784
C	-0.19768	4.43417	-1.52955
H	0.73794	4.75647	-1.97808
C	-1.41562	4.77323	-2.12363
H	-1.43044	5.34985	-3.04385
C	-2.61602	4.37935	-1.52716
H	-3.56433	4.64154	-1.98642
C	-2.60040	3.64247	-0.34432
H	-3.53286	3.31921	0.10999
C	2.30395	0.55915	1.92207
H	3.18388	0.21346	2.47750
H	1.83609	1.34799	2.51704
C	2.72510	1.15206	0.59395
C	3.97351	1.74739	0.41255
H	4.69645	1.74863	1.22207
C	4.27521	2.31831	-0.82205
H	5.24295	2.78177	-0.98816
C	3.32393	2.27432	-1.84402
H	3.52397	2.69809	-2.82210
C	2.10387	1.65928	-1.59038
H	1.32030	1.58503	-2.33609
C	2.03446	-1.86836	1.66493
H	1.26183	-2.62881	1.53083
H	2.54275	-2.06488	2.61991
C	3.00884	-1.93471	0.52157
C	4.36505	-2.19356	0.71389
H	4.74500	-2.32764	1.72437
C	5.23642	-2.29100	-0.37517
H	6.28986	-2.49466	-0.21080
C	4.74238	-2.13440	-1.67552
H	5.41591	-2.21337	-2.52402
C	3.39141	-1.87855	-1.89093
H	2.98601	-1.74813	-2.88920
C	2.51150	-1.77025	-0.79745
N	-1.11391	-1.66384	1.08023
N	-0.62987	1.35987	1.57458
N	1.33201	-0.54822	1.74636
N	1.81339	1.12215	-0.39296
O	1.23022	-1.48212	-1.00093
Br	-1.40102	0.55524	-1.85488

$^{6}FeN_3PyO2PhCl$
Charge: 1+
Energy: -2138659.9685534

Fe	0.06330	-0.18380	-0.23815
C	-3.88014	-2.34154	-1.43325
H	-4.67655	-2.10682	-0.73192
C	-4.16266	-2.46647	-2.79152
H	-5.18150	-2.33782	-3.14466
C	-3.13657	-2.75559	-3.69553
H	-3.35923	-2.85817	-4.75363
C	-1.82723	-2.91255	-3.23768
H	-1.02743	-3.13957	-3.93622
C	-1.53613	-2.77077	-1.88265
H	-0.51666	-2.87376	-1.53139
C	-2.56106	-2.47949	-0.97201
C	-2.28058	-2.37386	0.47537
C	-3.05321	-3.12172	1.38424
H	-3.84826	-3.74869	0.99740
C	-2.76180	-3.09225	2.73964
H	-3.33701	-3.68871	3.44132
C	-1.70297	-2.29677	3.18516
H	-1.43485	-2.24739	4.23538
C	-1.00169	-1.55322	2.24739
C	0.04743	-0.53195	2.67034
H	0.38385	-0.75130	3.69338
C	-0.66692	0.81325	2.63707
C	-1.29344	1.32150	3.76940
H	-1.19083	0.81995	4.72640
C	-2.06836	2.47430	3.63079
H	-2.58606	2.89779	4.48617
C	-2.14322	3.08487	2.38514
H	-2.70307	4.00249	2.24256
C	-1.43865	2.54523	1.29548
C	-1.40864	3.27828	0.01021
C	-0.18196	3.68763	-0.52661
H	0.73449	3.45311	0.00256
C	-0.14327	4.40556	-1.71980
H	0.81210	4.72627	-2.12589
C	-1.33051	4.71579	-2.38743
H	-1.30093	5.26843	-3.32191
C	-2.55761	4.32439	-1.84638
H	-3.48215	4.56478	-2.36258
C	-2.59916	3.61957	-0.64448
H	-3.55179	3.30062	-0.23062
C	2.16509	0.53662	1.93424
H	3.00777	0.17175	2.53354
H	1.68799	1.33932	2.50309
C	2.66469	1.11380	0.62631
C	3.93553	1.67447	0.49797
H	4.62288	1.65920	1.33777
C	4.30504	2.23250	-0.72423
H	5.29142	2.66868	-0.84963
C	3.39789	2.21181	-1.78657
H	3.65199	2.62732	-2.75560
C	2.15162	1.63090	-1.58475
H	1.39680	1.57459	-2.36126
C	1.84475	-1.88431	1.66905
H	1.05939	-2.62414	1.49775
H	2.29989	-2.09240	2.64822
C	2.87173	-1.98070	0.57528
C	4.20943	-2.27458	0.83415
H	4.53607	-2.41459	1.86232
C	5.12999	-2.39930	-0.21090

H	6.16841	-2.62995	0.00531
C	4.70420	-2.23510	-1.53435
H	5.41597	-2.33519	-2.34871
C	3.37270	-1.94485	-1.81601
H	3.02008	-1.80798	-2.83327
C	2.44324	-1.80833	-0.76696
N	-1.27412	-1.58387	0.92415
N	-0.73921	1.39358	1.42415
N	1.17523	-0.54620	1.71297
N	1.79766	1.10572	-0.39965
O	1.18289	-1.48613	-1.03370
Cl	-1.22140	0.58723	-1.89015

$^{6}FeN_3PyO2PhF$
Charge: 1+
Energy: -1912535.3349336

Fe	0.09530	-0.10167	-0.27846
C	-3.82151	-2.33114	-1.48718
H	-4.54815	-2.40465	-0.68228
C	-4.25520	-2.16673	-2.80071
H	-5.31879	-2.12505	-3.01628
C	-3.32272	-2.05477	-3.83596
H	-3.66167	-1.93152	-4.86050
C	-1.95697	-2.10453	-3.55162
H	-1.22845	-2.02449	-4.35289
C	-1.51686	-2.25646	-2.23803
H	-0.45492	-2.29799	-2.02583
C	-2.44722	-2.36587	-1.19459
C	-2.01446	-2.54954	0.20804
C	-2.60876	-3.54995	1.00140
H	-3.35807	-4.19385	0.55561
C	-2.20831	-3.72557	2.31753
H	-2.64689	-4.50979	2.92718
C	-1.22719	-2.88165	2.84639
H	-0.89237	-2.97715	3.87401
C	-0.69085	-1.90344	2.02242
C	0.25747	-0.83361	2.55919
H	0.64112	-1.14045	3.54241
C	-0.60020	0.41879	2.69967
C	-1.19948	0.76368	3.90515
H	-0.96770	0.21385	4.81171
C	-2.11917	1.81516	3.90562
H	-2.61619	2.11168	4.82440
C	-2.38014	2.48179	2.71451
H	-3.07601	3.31251	2.67587
C	-1.70413	2.10776	1.54066
C	-1.92116	2.86348	0.28447
C	-0.85269	3.53268	-0.32372
H	0.13210	3.48063	0.12673
C	-1.05885	4.26868	-1.48815
H	-0.22722	4.79449	-1.94924
C	-2.33334	4.33510	-2.05698
H	-2.49341	4.90398	-2.96823
C	-3.40424	3.67794	-1.44706
H	-4.39641	3.72931	-1.88548
C	-3.20309	2.95418	-0.27178
H	-4.03377	2.43687	0.20089
C	2.22774	0.54024	1.91918
H	3.12427	0.20164	2.45237
H	1.68717	1.21504	2.58955
C	2.61427	1.31575	0.67605
C	3.83507	1.97731	0.54437
H	4.57870	1.90853	1.33178
C	4.08333	2.70293	-0.61942
H	5.03012	3.21844	-0.74892
C	3.10945	2.74859	-1.62108
H	3.27301	3.29518	-2.54345
C	1.91953	2.05951	-1.41991
H	1.11460	2.03604	-2.14701
C	2.14353	-1.84795	1.34181
H	1.42787	-2.63715	1.09835
H	2.66395	-2.13550	2.26719
C	3.11920	-1.68961	0.20945
C	4.49231	-1.86064	0.38293
H	4.87961	-2.09522	1.37220
C	5.37089	-1.74134	-0.69734
H	6.43734	-1.87874	-0.54851
C	4.86641	-1.45407	-1.97112
H	5.54484	-1.36435	-2.81479
C	3.49920	-1.28298	-2.16672
H	3.08656	-1.05431	-3.14422
C	2.60922	-1.39210	-1.08112
N	-1.05876	-1.74588	0.73158
N	-0.83525	1.07324	1.54613
N	1.34715	-0.60579	1.58750
N	1.68486	1.37162	-0.29067
O	1.31048	-1.17864	-1.26350
F	-0.93726	0.65583	-1.49716

$^{6}FeN_3PyO2PhN_3$
Charge: 1+
Energy: -1952924.2359476

Fe	0.18555	-0.11671	-0.21004
C	-3.68708	-2.67406	-1.12903
H	-4.38741	-2.68570	-0.29800
C	-4.16438	-2.67440	-2.43798
H	-5.23421	-2.69208	-2.62215
C	-3.26713	-2.63931	-3.50824
H	-3.63925	-2.63821	-4.52844
C	-1.89228	-2.60200	-3.26418
H	-1.19080	-2.58014	-4.09299
C	-1.40856	-2.59271	-1.95673
H	-0.34097	-2.55579	-1.77293
C	-2.30520	-2.62299	-0.87770
C	-1.82142	-2.65826	0.52057
C	-2.34712	-3.61661	1.40866
H	-3.08859	-4.31702	1.04197
C	-1.88620	-3.68549	2.71491
H	-2.27139	-4.43722	3.39719
C	-0.90763	-2.78072	3.13414
H	-0.51728	-2.79771	4.14639
C	-0.44379	-1.84643	2.21927
C	0.50836	-0.73018	2.63711
H	0.97541	-0.98549	3.59876
C	-0.36683	0.50673	2.79786
C	-0.90013	0.85855	4.03298
H	-0.60618	0.32412	4.93066
C	-1.83230	1.89677	4.07637
H	-2.27878	2.19853	5.01904
C	-2.16716	2.54794	2.89532
H	-2.86860	3.37480	2.89016
C	-1.55622	2.16704	1.68853
C	-1.84755	2.92225	0.44753
C	-0.80369	3.51550	-0.27510
H	0.21476	3.39829	0.07484
C	-1.07692	4.25793	-1.42143
H	-0.26225	4.72188	-1.97066
C	-2.39615	4.41325	-1.85755
H	-2.60909	4.98615	-2.75515
C	-3.44136	3.83542	-1.13414
H	-4.46639	3.94629	-1.47369
C	-3.17090	3.10086	0.02077
H	-3.98355	2.64035	0.57605
C	2.39559	0.65402	1.81082
H	3.31905	0.35340	2.32003
H	1.87434	1.35553	2.46833
C	2.71698	1.36732	0.51450
C	3.93742	2.00385	0.28858
H	4.72105	1.95617	1.03763
C	4.13515	2.67148	-0.91791
H	5.08068	3.16519	-1.12042
C	3.11045	2.68438	-1.86827
H	3.23159	3.18338	-2.82355
C	1.92538	2.02251	-1.57262
H	1.09102	1.97786	-2.26451
C	2.33122	-1.75673	1.33755
H	1.62180	-2.56728	1.15588
H	2.89922	-1.99675	2.24820
C	3.24878	-1.61376	0.15701
C	4.63454	-1.73351	0.27213
H	5.07345	-1.92430	1.24935
C	5.45781	-1.61607	-0.84964
H	6.53421	-1.71312	-0.74832
C	4.88332	-1.38331	-2.10457
H	5.51767	-1.29499	-2.98220
C	3.50269	-1.26463	-2.24082
H	3.03961	-1.08005	-3.20509
C	2.66809	-1.37405	-1.11377
N	-0.87820	-1.78173	0.94183
N	-0.67819	1.13925	1.65050
N	1.51829	-0.52047	1.57860
N	1.73451	1.39098	-0.40231
O	1.35129	-1.21364	-1.23693
N	-1.12285	0.44771	-1.42327
N	-2.18694	0.59580	-1.96440
N	-3.19782	0.73757	-2.49659

$^{5}FeN_3PyO2PhNCCH3$
Charge: 1+
Energy: -1933202.1000710

Fe	0.24777	-0.08955	-0.17567
C	-3.65059	-2.79750	-1.02382
H	-4.34271	-2.84620	-0.18709
C	-4.13758	-2.82099	-2.33044
H	-5.20667	-2.89868	-2.50703
C	-3.24845	-2.75959	-3.40869
H	-3.62560	-2.80321	-4.42720
C	-1.87456	-2.65757	-3.17198
H	-1.17748	-2.61495	-4.00411
C	-1.38336	-2.62236	-1.86623
H	-0.31620	-2.52946	-1.69007
C	-2.27081	-2.69413	-0.78218
C	-1.75868	-2.72105	0.60981
C	-2.21556	-3.70555	1.50380
H	-2.94677	-4.43090	1.16488

C	-1.69212	-3.76507	2.78883
H	-2.01953	-4.53326	3.48300
C	-0.72340	-2.83375	3.16703
H	-0.28041	-2.85196	4.15758
C	-0.33271	-1.87381	2.23988
C	0.62415	-0.74439	2.63233
H	1.12294	-1.01183	3.57587
C	-0.26499	0.47439	2.85756
C	-0.71137	0.81553	4.13183
H	-0.34114	0.28350	5.00234
C	-1.65028	1.84008	4.25319
H	-2.02476	2.13290	5.22950
C	-2.08846	2.48932	3.10413
H	-2.80106	3.30509	3.15795
C	-1.56696	2.11424	1.85597
C	-1.97542	2.84306	0.63012
C	-1.00502	3.39921	-0.21318
H	0.04168	3.27557	0.03492
C	-1.38454	4.09838	-1.35775
H	-0.62416	4.53630	-1.99850
C	-2.73816	4.24352	-1.67395
H	-3.03494	4.79373	-2.56260
C	-3.71191	3.69752	-0.83150
H	-4.76586	3.81875	-1.06623
C	-3.33321	3.00794	0.32147
H	-4.08954	2.58055	0.97459
C	2.46780	0.68164	1.77162
H	3.39796	0.39215	2.27686
H	1.94327	1.38125	2.42907
C	2.78109	1.39654	0.46927
C	4.04790	1.91163	0.19157
H	4.85912	1.76453	0.89663
C	4.25911	2.57111	-1.01640
H	5.24150	2.96319	-1.26115
C	3.19742	2.70208	-1.91469
H	3.32424	3.19620	-2.87199
C	1.96618	2.16293	-1.56139
H	1.10468	2.21688	-2.22032
C	2.40517	-1.71871	1.23025
H	1.68994	-2.52198	1.03815
H	3.00478	-1.99478	2.11096
C	3.28414	-1.52173	0.02742
C	4.67750	-1.58450	0.12080
H	5.13476	-1.78367	1.08856
C	5.48274	-1.39359	-1.00132
H	6.56378	-1.44722	-0.91691
C	4.87689	-1.14527	-2.23875
H	5.49298	-0.99805	-3.12225
C	3.49072	-1.08469	-2.35339
H	3.01109	-0.88891	-3.30792
C	2.66622	-1.27025	-1.22706
N	-0.83750	-1.80993	0.99106
N	-0.67442	1.10760	1.74243
N	1.59691	-0.49710	1.55060
N	1.75668	1.53291	-0.39449
N	-1.32823	0.53034	-1.47769
C	-2.21455	0.71886	-2.19564
C	-3.33516	0.92572	-3.10051
H	-3.49916	0.01159	-3.67858
H	-3.12657	1.76377	-3.77174
H	-4.23311	1.15462	-2.51968
O	1.34150	-1.17612	-1.33143

$^{6}FeN_3PyO2PhNCS$
Charge: 1+
Energy: -2158031.8542532

Fe	0.19854	-0.14085	-0.12854
C	-3.59933	-2.66224	-1.18445
H	-4.19376	-2.89809	-0.30559
C	-4.22928	-2.39095	-2.39751
H	-5.31277	-2.42300	-2.46186
C	-3.46746	-2.07344	-3.52472
H	-3.95838	-1.85949	-4.46926
C	-2.07469	-2.02433	-3.43412
H	-1.47974	-1.77809	-4.30829
C	-1.43964	-2.28142	-2.22045
H	-0.35918	-2.23295	-2.15203
C	-2.19971	-2.59735	-1.08454
C	-1.55020	-2.91117	0.20636
C	-1.91972	-4.07762	0.90345
H	-2.67147	-4.72746	0.47050
C	-1.29523	-4.40484	2.09763
H	-1.55855	-5.31576	2.62668
C	-0.31165	-3.54998	2.60248
H	0.20238	-3.76577	3.53335
C	-0.00916	-2.40234	1.88450
C	0.92710	-1.33645	2.44467
H	1.52327	-1.76238	3.26382
C	0.01140	-0.24323	2.98091
C	-0.38893	-0.22071	4.31199
H	0.03852	-0.91697	5.02641
C	-1.36563	0.70282	4.69020
H	-1.71397	0.74748	5.71768
C	-1.87092	1.57531	3.73398
H	-2.61137	2.32430	3.99203
C	-1.38476	1.52753	2.41651
C	-1.84616	2.52316	1.42255
C	-0.91976	3.36837	0.79953
H	0.13128	3.27915	1.04853
C	-1.34982	4.32390	-0.11897
H	-0.62640	4.98107	-0.59350
C	-2.70802	4.43783	-0.42500
H	-3.04243	5.17180	-1.15175
C	-3.63702	3.60508	0.20328
H	-4.69218	3.68730	-0.03825
C	-3.21062	2.65804	1.13362
H	-3.93076	2.00133	1.61429
C	2.61280	0.35444	1.76342
H	3.61311	0.02955	2.07382
H	2.14519	0.83572	2.62703
C	2.71308	1.37385	0.64829
C	3.84111	2.17305	0.46240
H	4.71083	2.04050	1.09776
C	3.83487	3.11894	-0.56048
H	4.70483	3.74601	-0.73009
C	2.70390	3.24009	-1.37219
H	2.66491	3.95702	-2.18504
C	1.62119	2.40398	-1.12885
H	0.71488	2.43563	-1.72345
C	2.63164	-1.88595	0.75439
H	1.95576	-2.69880	0.47864
H	3.33023	-2.26639	1.51378
C	3.37390	-1.41227	-0.46323
C	4.76598	-1.44262	-0.54702
H	5.34355	-1.80462	0.30095
C	5.42169	-1.02038	-1.70625
H	6.50541	-1.05100	-1.75999
C	4.67259	-0.56778	-2.79849
H	5.17738	-0.24185	-3.70352
C	3.28217	-0.53179	-2.73641
H	2.68303	-0.17999	-3.57036
C	2.61732	-0.94917	-1.56918
N	-0.60249	-2.08538	0.71251
N	-0.46825	0.60337	2.04984
N	1.78492	-0.80942	1.36129
N	1.62789	1.50172	-0.13354
O	1.29024	-0.87169	-1.49089
N	-1.25601	0.65290	-1.05763
C	-1.95744	1.10464	-1.91815
S	-2.88460	1.70307	-3.06946

$^{6}FeN_3PyO2PhOH$
Charge: 1+
Energy: -1897448.8730629

Fe	0.10751	-0.12696	-0.31571
C	-3.83810	-2.44754	-1.38378
H	-4.58303	-2.42973	-0.59234
C	-4.24191	-2.42341	-2.71696
H	-5.30019	-2.39796	-2.95995
C	-3.28558	-2.43465	-3.73659
H	-3.60074	-2.42324	-4.77607
C	-1.92705	-2.46328	-3.41704
H	-1.18000	-2.47508	-4.20498
C	-1.51696	-2.47291	-2.08520
H	-0.46019	-2.49087	-1.84571
C	-2.47076	-2.46185	-1.05767
C	-2.06991	-2.50781	0.36572
C	-2.69681	-3.42116	1.23588
H	-3.44763	-4.09275	0.83579
C	-2.32396	-3.48247	2.57013
H	-2.78765	-4.20011	3.24024
C	-1.33398	-2.61320	3.03623
H	-1.01422	-2.62343	4.07307
C	-0.76502	-1.72429	2.13564
C	0.20723	-0.64105	2.59588
H	0.58908	-0.89289	3.59564
C	-0.61634	0.63930	2.66509
C	-1.18383	1.07857	3.85731
H	-0.95780	0.57422	4.79139
C	-2.05842	2.16544	3.81178
H	-2.52650	2.53501	4.71917
C	-2.31255	2.77335	2.58693
H	-2.97427	3.62910	2.50996
C	-1.67379	2.29744	1.43141
C	-1.88932	2.97048	0.12632
C	-0.80722	3.53934	-0.55936
H	0.18496	3.47781	-0.12776
C	-1.00806	4.17219	-1.78442
H	-0.16505	4.61510	-2.30694
C	-2.28914	4.23446	-2.33975
H	-2.44337	4.71968	-3.29886
C	-3.37293	3.67517	-1.65823
H	-4.36965	3.72156	-2.08649
C	-3.17783	3.05477	-0.42205
H	-4.01849	2.61530	0.10828
C	2.20731	0.63959	1.87457

H	3.08516	0.31566	2.44656
H	1.67667	1.37675	2.48435
C	2.63640	1.30943	0.58559
C	3.88479	1.91027	0.42457
H	4.61643	1.86672	1.22483
C	4.17729	2.53688	-0.78521
H	5.14655	3.00167	-0.93837
C	3.21859	2.54559	-1.80233
H	3.41708	3.01176	-2.76133
C	1.99949	1.92052	-1.56900
H	1.20776	1.86387	-2.30879
C	2.07213	-1.77876	1.46279
H	1.34288	-2.56396	1.24994
H	2.56169	-2.01662	2.41866
C	3.07892	-1.70882	0.35022
C	4.44780	-1.86537	0.57386
H	4.80609	-2.03380	1.58745
C	5.35595	-1.81319	-0.48555
H	6.41808	-1.93869	-0.29976
C	4.88453	-1.60868	-1.78746
H	5.58519	-1.57077	-2.61701
C	3.52247	-1.45365	-2.03175
H	3.13808	-1.28894	-3.03342
C	2.60311	-1.49735	-0.96820
N	-1.11017	-1.67257	0.83061
N	-0.84567	1.23259	1.47926
N	1.29903	-0.50308	1.61121
N	1.71986	1.32976	-0.39545
O	1.30498	-1.30275	-1.19634
O	-0.94566	0.51646	-1.63992
H	-1.67723	1.13879	-1.50473

^{4}FetsalenpyBr
Charge: 0
Energy: -3520864.9692585

Fe	0.06863	-0.28430	-0.02244
S	1.54029	0.29849	-1.64681
S	-1.48380	-0.45219	-1.67292
N	1.35437	0.23994	1.45254
N	-1.25300	-0.52248	1.47337
C	3.16646	0.10694	-1.01303
C	4.19124	-0.00422	-1.97777
C	5.52572	-0.12524	-1.61704
C	5.90259	-0.13520	-0.26586
C	4.91892	-0.01640	0.69898
C	3.54974	0.09950	0.35919
C	2.64279	0.24559	1.47310
C	-3.08843	-0.66822	-1.00592
C	-4.13624	-0.73305	-1.95525
C	-5.45831	-0.91238	-1.58013
C	-5.80771	-1.03446	-0.22551
C	-4.80580	-0.97244	0.72390
C	-3.44517	-0.78834	0.36996
C	-2.52478	-0.73375	1.48234
C	0.61108	0.44354	2.69725
C	-0.52441	-0.57666	2.74914
N	-0.53439	2.17144	0.23134
C	0.43208	3.09698	0.16440
C	0.16856	4.46362	0.08266
C	-1.16121	4.88617	0.06216
C	-2.17139	3.92571	0.12458
C	-1.80942	2.58157	0.20719
H	-2.99408	-0.89152	2.45970
H	3.12954	0.37146	2.44678
H	-2.56005	1.79898	0.24359
H	3.91302	-0.00737	-3.02713
H	6.28111	-0.21908	-2.39285
H	6.94539	-0.23525	0.01862
H	5.19362	-0.02082	1.75159
H	-3.88131	-0.64475	-3.00696
H	-6.22763	-0.96090	-2.34643
H	-6.84204	-1.17809	0.07077
H	-5.05745	-1.06871	1.77795
H	0.19111	1.45520	2.67581
H	1.25949	0.34683	3.57755
H	-1.18825	-0.37381	3.59921
H	-0.10551	-1.58372	2.84077
H	1.44729	2.71209	0.16165
H	0.98818	5.17329	0.02796
H	-1.40532	5.94266	-0.00703
H	-3.22001	4.20559	0.10334
Br	0.78337	-2.77396	0.32278

^{4}FetsalenpyCl
Charge: 0
Energy: -2194335.0510606

Fe	0.12069	-0.54805	0.02772
S	1.61104	-0.04367	-1.61666
S	-1.44548	-0.71238	-1.62108
N	1.41292	0.04281	1.48470
N	-1.21963	-0.65161	1.52764
C	3.22843	-0.25020	-0.96520
C	4.25500	-0.42591	-1.91893
C	5.58451	-0.56546	-1.54693
C	5.95532	-0.53117	-0.19455
C	4.97046	-0.34858	0.75923
C	3.60628	-0.21080	0.40827
C	2.69973	0.00676	1.51215
C	-3.05771	-0.82251	-0.94683
C	-4.10848	-0.87550	-1.89417
C	-5.43745	-0.97586	-1.51442
C	-5.79218	-1.02537	-0.15655
C	-4.78804	-0.97201	0.79100
C	-3.42022	-0.86781	0.43236
C	-2.49831	-0.80940	1.54390
C	0.66853	0.30992	2.71548
C	-0.48643	-0.68731	2.79971
N	-0.41614	1.96552	0.16243
C	0.57990	2.85547	0.05944
C	0.36217	4.22403	-0.09507
C	-0.95274	4.68758	-0.15228
C	-1.99401	3.76431	-0.05199
C	-1.67644	2.41524	0.10323
H	-2.97397	-0.90786	2.52622
H	3.18767	0.15786	2.48202
H	-2.45311	1.66082	0.17172
H	3.98144	-0.46456	-2.96885
H	6.34042	-0.70913	-2.31462
H	6.99395	-0.64609	0.09945
H	5.24064	-0.31678	1.81261
H	-3.85018	-0.84203	-2.94823
H	-6.20829	-1.01851	-2.27957
H	-6.83214	-1.10667	0.14368
H	-5.04373	-1.01174	1.84775
H	0.26656	1.32717	2.65193
H	1.31022	0.23589	3.60315
H	-1.14105	-0.45194	3.64877
H	-0.08455	-1.69924	2.91217
H	1.58232	2.43937	0.08814
H	1.20511	4.90322	-0.17662
H	-1.16163	5.74641	-0.27819
H	-3.03280	4.07604	-0.09905
Cl	0.72094	-2.81739	0.45942

^{4}FetsalenpyF
Charge: 0
Energy: -1968207.0588783

Fe	0.12171	-0.82860	0.01724
S	1.63181	-0.26689	-1.61535
S	-1.47273	-0.79018	-1.64322
N	1.41907	-0.30341	1.50926
N	-1.25002	-0.91458	1.49372
C	3.25296	-0.36014	-0.95232
C	4.29812	-0.39300	-1.90544
C	5.63265	-0.43819	-1.53286
C	5.99681	-0.45066	-0.17726
C	4.99682	-0.40932	0.77608
C	3.62517	-0.36538	0.42462
C	2.70532	-0.28463	1.53759
C	-3.08660	-0.73898	-0.96787
C	-4.13551	-0.60452	-1.91081
C	-5.46739	-0.56677	-1.53167
C	-5.83015	-0.65859	-0.17763
C	-4.82947	-0.78768	0.76593
C	-3.45815	-0.82569	0.40762
C	-2.53621	-0.95141	1.51408
C	0.67086	-0.15252	2.75725
C	-0.50215	-1.13288	2.73397
N	-0.30492	1.77901	0.30028
C	0.74548	2.60419	0.19710
C	0.61796	3.98524	0.05071
C	-0.66361	4.53484	0.00245
C	-1.76238	3.68105	0.10341
C	-1.53232	2.31310	0.25044
H	-3.01753	-1.08569	2.49010
H	3.18748	-0.18193	2.51755
H	-2.35798	1.61243	0.31919
H	4.03240	-0.39270	-2.95820
H	6.39980	-0.46975	-2.30233
H	7.04076	-0.49148	0.11763
H	5.26009	-0.41393	1.83183
H	-3.87237	-0.53423	-2.96187
H	-6.23544	-0.46596	-2.29430
H	-6.87321	-0.63119	0.12180
H	-5.09027	-0.86253	1.81966
H	0.28222	0.87177	2.79479
H	1.30491	-0.32536	3.63716
H	-1.13620	-1.00514	3.62143
H	-0.11691	-2.15724	2.69845
H	1.72028	2.12650	0.21784
H	1.50346	4.60799	-0.03159
H	-0.80311	5.60585	-0.11712
H	-2.77888	4.06025	0.06326
F	0.48473	-2.59182	0.30983

^{4}FetsalenpyN$_3$
Charge: 0
Energy: -2008597.4843262

Fe	0.01576	-0.57791	-0.07194
S	1.47409	0.10265	-1.67737
S	-1.57484	-0.57099	-1.71419
N	1.32405	-0.20056	1.43152
N	-1.31130	-0.90725	1.40071
C	3.11439	0.08053	-1.04745
C	4.13469	0.22362	-2.01498
C	5.47755	0.22939	-1.66904
C	5.86963	0.09370	-0.32867
C	4.89120	-0.03763	0.63863
C	3.51303	-0.04403	0.31455
C	2.61454	-0.15076	1.44107
C	-3.18373	-0.68311	-1.03673
C	-4.24718	-0.56516	-1.96513
C	-5.57453	-0.64948	-1.57802
C	-5.91648	-0.85613	-0.23085
C	-4.90131	-0.97470	0.69800
C	-3.53355	-0.88925	0.33167
C	-2.59517	-1.02820	1.42025
C	0.60289	-0.18065	2.70600
C	-0.55887	-1.16866	2.63280
N	-0.50301	1.88203	0.39502
C	0.50737	2.76252	0.39492
C	0.31187	4.14274	0.41942
C	-0.99516	4.63113	0.43725
C	-2.05123	3.71951	0.43033
C	-1.75572	2.35665	0.40836
H	-3.05767	-1.26135	2.38608
H	3.10998	-0.15771	2.41787
H	-2.54520	1.61281	0.38912
H	3.84597	0.31776	-3.05745
H	6.22835	0.33314	-2.44807
H	6.92013	0.08814	-0.05527
H	5.17738	-0.14887	1.68199
H	-3.99883	-0.40736	-3.01025
H	-6.35537	-0.55528	-2.32829
H	-6.95601	-0.92440	0.07416
H	-5.14673	-1.13898	1.74518
H	0.20557	0.83176	2.84538
H	1.26208	-0.42167	3.55020
H	-1.19667	-1.08154	3.52210
H	-0.16834	-2.18926	2.56637
H	1.50354	2.33255	0.35900
H	1.16585	4.81294	0.41571
H	-1.18663	5.70061	0.45036
H	-3.08489	4.05115	0.43535
N	0.53329	-2.55886	0.07472
N	1.66374	-2.89620	0.33741
N	2.74098	-3.22596	0.61516

^{4}FetsalenpyNCS
Charge: 0
Energy: -2213706.9531132

Fe	0.00560	-0.20510	0.22457
S	-1.32520	0.88453	1.70641
S	1.61698	-0.24654	1.83508
N	-1.30971	0.11280	-1.29668
N	1.19324	-0.95755	-1.22053
C	-2.99192	0.60424	1.20923
C	-3.96345	0.75863	2.21989
C	-5.31729	0.58143	1.96544
C	-5.76248	0.24137	0.68093
C	-4.82959	0.09898	-0.33122
C	-3.44609	0.27485	-0.09944
C	-2.59838	0.12521	-1.26243
C	3.14775	-0.78459	1.17085
C	4.23959	-0.76233	2.07091
C	5.50941	-1.17468	1.69805
C	5.75849	-1.63168	0.39415
C	4.71199	-1.66145	-0.50774
C	3.40329	-1.24429	-0.15556
C	2.42861	-1.32688	-1.22031
C	-0.62341	-0.06102	-2.57666
C	0.38670	-1.19907	-2.42551
N	0.85408	1.99028	-0.56865
C	-0.00074	3.00827	-0.74235
C	0.41644	4.30411	-1.04185
C	1.78413	4.55475	-1.15941
C	2.67782	3.49965	-0.97300
C	2.16682	2.23632	-0.67850
H	2.81711	-1.75830	-2.14961
H	-3.13206	0.00798	-2.21016
H	2.82360	1.38913	-0.51366
H	-3.63093	1.00621	3.22330
H	-6.03156	0.69805	2.77628
H	-6.81838	0.08718	0.48219
H	-5.15606	-0.17340	-1.33174
H	4.06171	-0.41469	3.08402
H	6.31526	-1.14342	2.42671
H	6.75105	-1.95778	0.09970
H	4.88663	-2.01527	-1.52155
H	-0.09608	0.87055	-2.80880
H	-1.32883	-0.28548	-3.38644
H	1.01859	-1.27439	-3.31958
H	-0.15495	-2.14151	-2.29318
H	-1.05011	2.75983	-0.62034
H	-0.31637	5.09438	-1.17095
H	2.14639	5.55354	-1.38661
H	3.75064	3.64716	-1.04719
N	-0.85941	-2.11444	0.41850
C	-1.65146	-2.69554	-0.25290
S	-2.71842	-3.40752	-1.25369

^{2}FetsalenpyOH
Charge: 0
Energy: -1953118.6975929

Fe	0.11382	-0.38572	0.14092
S	1.65907	-0.41082	-1.57073
S	-1.42221	-1.05928	-1.43983
N	1.41833	0.29140	1.48090
N	-1.19310	-0.29077	1.63476
C	3.23571	-0.62391	-0.84526
C	4.27397	-1.04105	-1.71425
C	5.57494	-1.22328	-1.27574
C	5.91648	-0.99077	0.06737
C	4.92904	-0.56781	0.93571
C	3.58718	-0.37829	0.51748
C	2.69417	0.11446	1.53995
C	-3.02452	-1.08527	-0.74825
C	-4.08402	-1.38375	-1.64524
C	-5.40425	-1.44210	-1.23739
C	-5.75108	-1.20190	0.10481
C	-4.74506	-0.90926	1.00275
C	-3.38060	-0.83713	0.61471
C	-2.46080	-0.52689	1.68565
C	0.70920	0.80415	2.64787
C	-0.46699	-0.13590	2.89659
N	-0.31449	1.70762	-0.30140
C	0.69143	2.58476	-0.46281
C	0.47992	3.93742	-0.71653
C	-0.82936	4.40796	-0.81278
C	-1.87526	3.50089	-0.64880
C	-1.57437	2.16448	-0.39585
H	-2.92978	-0.49050	2.67594
H	3.18945	0.37725	2.48212
H	-2.35916	1.43051	-0.27307
H	4.02253	-1.23179	-2.75329
H	6.33430	-1.55455	-1.97980
H	6.93439	-1.13683	0.41558
H	5.17756	-0.37437	1.97748
H	-3.83071	-1.57385	-2.68397
H	-6.17761	-1.67839	-1.96412
H	-6.78616	-1.25002	0.42880
H	-4.99395	-0.72673	2.04643
H	0.33382	1.80814	2.41412
H	1.35794	0.86821	3.53166
H	-1.11491	0.23894	3.70015
H	-0.07974	-1.12349	3.17309
H	1.68882	2.16834	-0.39766
H	1.33075	4.59928	-0.84246
H	-1.02956	5.45632	-1.01563
H	-2.91247	3.81210	-0.72001
O	0.52769	-2.04957	0.70105
H	0.52437	-2.63025	-0.07849

^{4}FeN2S2Br
Charge: -2
Energy: -3412443.1030033

Fe	-0.00012	-0.68288	-0.30185
S	-1.65264	-2.01553	-1.09735
S	1.65180	-2.01420	-1.10083
N	-1.29337	0.77158	-0.33984
N	1.29319	0.77148	-0.33914
C	-3.06518	-0.91126	-0.62070
C	-2.62880	0.56945	-0.51180
C	-0.71376	2.03840	-0.14188
C	-1.40063	3.24893	0.04982
C	-0.69677	4.44148	0.24421
C	0.69703	4.44133	0.24469
C	1.40072	3.24861	0.05081
C	0.71365	2.03827	-0.14134
C	2.62867	0.56928	-0.51014
C	3.06475	-0.91136	-0.62197
C	-4.18327	-1.02847	-1.66732
C	-3.59927	-1.31567	0.76959
C	4.18255	-1.02663	-1.66915
C	3.59918	-1.31885	0.76725
O	-3.51348	1.44248	-0.53972
O	3.51356	1.44220	-0.53529
H	-2.48049	3.23115	0.03816
H	-1.24969	5.36893	0.39538

H	1.25007	5.36865	0.39620
H	2.48059	3.23046	0.04002
H	-5.00667	-0.35269	-1.40757
H	-4.55532	-2.06004	-1.70975
H	-3.81258	-0.75647	-2.66188
H	-4.41542	-0.64035	1.06554
H	-3.97892	-2.34520	0.74237
H	-2.79706	-1.26181	1.51166
H	5.00620	-0.35164	-1.40815
H	4.55431	-2.05822	-1.71389
H	3.81169	-0.75240	-2.66304
H	4.41560	-0.64436	1.06429
H	2.79730	-1.26629	1.50975
H	3.97857	-2.34842	0.73772
Br	0.00074	-1.10031	2.37094

^{4}FeN2S2Cl
Charge: -2
Energy: -2085911.0994973

Fe	-0.00002	-0.78704	0.00209
S	-1.65779	-2.17208	-0.72167
S	1.65769	-2.17217	-0.72159
N	-1.29448	0.66609	-0.17791
N	1.29449	0.66602	-0.17795
Cl	0.00002	-0.99877	2.46291
C	-3.06062	-1.03825	-0.28590
C	-2.62968	0.44775	-0.32337
C	-0.71400	1.94450	-0.10210
C	-1.40035	3.16869	-0.02766
C	-0.69678	4.37471	0.05151
C	0.69711	4.37465	0.05146
C	1.40057	3.16857	-0.02774
C	0.71410	1.94445	-0.10214
C	2.62967	0.44764	-0.32346
C	3.06056	-1.03837	-0.28587
C	-4.21972	-1.25274	-1.26993
C	-3.53197	-1.32141	1.15663
C	4.21972	-1.25301	-1.26980
C	3.53174	-1.32143	1.15671
O	-3.51718	1.31323	-0.42684
O	3.51716	1.31311	-0.42708
H	-2.48030	3.14935	-0.03820
H	-1.24977	5.31254	0.11250
H	1.25019	5.31244	0.11242
H	2.48052	3.14913	-0.03835
H	-5.03832	-0.56173	-1.03618
H	-4.58316	-2.28640	-1.20661
H	-3.89343	-1.06591	-2.29906
H	-4.33856	-0.62460	1.42945
H	-3.90706	-2.35007	1.23493
H	-2.69677	-1.20241	1.85320
H	5.03835	-0.56203	-1.03605
H	4.58310	-2.28668	-1.20637
H	3.89353	-1.06624	-2.29897
H	4.33825	-0.62456	1.42959
H	2.69643	-1.20241	1.85316
H	3.90684	-2.35007	1.23513

^{4}FeN2S2F
Charge: -2
Energy: -1859778.3144856

Fe	0.00002	-0.83279	0.06649
S	-1.69767	-2.18328	-0.72882
S	1.69771	-2.18301	-0.72935
N	-1.29878	0.64313	-0.09018
N	1.29872	0.64320	-0.09021
C	-3.02937	-1.08378	-0.03843
C	-2.63553	0.41087	-0.15016
C	-0.71568	1.91924	-0.06977
C	-1.40046	3.14720	-0.05183
C	-0.69704	4.35669	-0.02813
C	0.69677	4.35673	-0.02807
C	1.40026	3.14728	-0.05172
C	0.71555	1.91928	-0.06972
C	2.63550	0.41100	-0.14969
C	3.02940	-1.08370	-0.03862
C	-4.34610	-1.32624	-0.78651
C	-3.20971	-1.37909	1.46867
C	4.34607	-1.32576	-0.78694
C	3.20993	-1.37961	1.46833
O	-3.54147	1.26316	-0.21688
O	3.54145	1.26332	-0.21580
H	-2.48083	3.12534	-0.05999
H	-1.25045	5.29648	-0.01244
H	1.25013	5.29655	-0.01234
H	2.48064	3.12548	-0.05974
H	-5.12573	-0.65989	-0.39822
H	-4.66197	-2.37039	-0.66509
H	-4.22646	-1.12410	-1.85656
H	-3.94656	-0.68580	1.90386
H	-3.56726	-2.40801	1.60772
H	-2.24974	-1.27059	1.98268
H	5.12568	-0.65948	-0.39848
H	4.66206	-2.36993	-0.66594
H	4.22630	-1.12325	-1.85690
H	3.94682	-0.68647	1.90368
H	2.25002	-1.27129	1.98250
H	3.56750	-2.40857	1.60693
F	0.00017	-1.11663	1.91114

^{4}FeN2S2N$_3$
Charge: -2
Energy: -1900176.3900457

Fe	0.00001	-0.65171	-0.18721
S	-1.66854	-1.91096	-1.09652
S	1.66877	-1.91061	-1.09674
N	-1.29525	0.81991	-0.14339
N	1.29497	0.82020	-0.14358
C	-3.05475	-0.85907	-0.44927
C	-2.63011	0.62331	-0.31983
C	-0.71465	2.07744	0.09599
C	-1.40088	3.28147	0.33154
C	-0.69744	4.46648	0.57044
C	0.69647	4.46663	0.57037
C	1.40014	3.28177	0.33138
C	0.71414	2.07759	0.09591
C	2.62986	0.62388	-0.32014
C	3.05478	-0.85843	-0.44953
C	-4.26467	-0.96733	-1.38684
C	-3.44366	-1.32146	0.97181
C	4.26472	-0.96649	-1.38711
C	3.44379	-1.32070	0.97157
O	-3.51768	1.49489	-0.32066
O	3.51731	1.49558	-0.32044
H	-2.48094	3.26414	0.31620
H	-1.25054	5.38807	0.75392
H	1.24939	5.38834	0.75379
H	2.48020	3.26467	0.31592
H	-5.07302	-0.31903	-1.02859
H	-4.61832	-2.00531	-1.42917
H	-3.99658	-0.65365	-2.40164
H	-4.25363	-0.68843	1.36420
H	-3.78111	-2.36490	0.95293
H	-2.57742	-1.24890	1.63549
H	5.07296	-0.31803	-1.02889
H	4.61857	-2.00440	-1.42940
H	3.99657	-0.65289	-2.40191
H	4.25365	-0.68751	1.36393
H	2.57754	-1.24827	1.63524
H	3.78141	-2.36409	0.95273
N	0.00023	-1.19891	1.81793
N	0.00075	-2.29110	2.32022
N	0.00124	-3.32359	2.86395

^{4}FeN2S2NCS
Charge: -2
Energy: -2105291.2782304

Fe	0.00008	-0.51822	-0.56404
S	-1.65872	-1.57226	-1.70262
S	1.65837	-1.57052	-1.70506
N	-1.29300	0.89707	-0.20235
N	1.29338	0.89662	-0.20148
C	-3.05558	-0.67371	-0.87369
C	-2.62923	0.74293	-0.42181
C	-0.71342	2.07647	0.30092
C	-1.40074	3.20181	0.78636
C	-0.69663	4.30825	1.27107
C	0.69727	4.30790	1.27177
C	1.40132	3.20112	0.78776
C	0.71391	2.07613	0.30160
C	2.62970	0.74184	-0.41981
C	3.05549	-0.67422	-0.87412
C	-4.24292	-0.56519	-1.84013
C	-3.48077	-1.43164	0.40243
C	4.24304	-0.56432	-1.84019
C	3.48022	-1.43475	0.40058
O	-3.51346	1.59593	-0.23857
O	3.51444	1.59373	-0.23383
H	-2.48064	3.18851	0.76939
H	-1.24918	5.16930	1.64714
H	1.24987	5.16866	1.64841
H	2.48122	3.18722	0.77195
H	-5.05775	-0.00570	-1.36618
H	-4.59792	-1.56586	-2.11666
H	-3.95041	-0.03865	-2.75510
H	-4.28726	-0.88449	0.91184
H	-3.83819	-2.43605	0.14433
H	-2.63195	-1.53446	1.08356
H	5.05803	-0.00608	-1.36504
H	4.59768	-1.56462	-2.11859
H	3.95088	-0.03592	-2.75420
H	4.28681	-0.88883	0.91112
H	2.63128	-1.53855	1.08140
H	3.83735	-2.43879	0.14059

N	0.00061	-1.49069	1.33056
C	-0.00022	-2.09376	2.34620
S	-0.00125	-2.93554	3.76578

^{4}FeN2S2OH
Charge: -2
Energy: -1844683.1637925

Fe	0.00002	-0.84761	0.08742
S	-1.69550	-2.20460	-0.69164
S	1.69577	-2.20429	-0.69234
N	-1.29895	0.63326	-0.09995
N	1.29890	0.63333	-0.09992
C	-3.03944	-1.08792	-0.05634
C	-2.63658	0.40377	-0.17122
C	-0.71629	1.90980	-0.08389
C	-1.40057	3.13877	-0.06245
C	-0.69721	4.34803	-0.03537
C	0.69685	4.34809	-0.03558
C	1.40034	3.13891	-0.06279
C	0.71620	1.90985	-0.08395
C	2.63657	0.40391	-0.17105
C	3.03949	-1.08779	-0.05630
C	-4.33369	-1.33074	-0.84358
C	-3.26943	-1.36465	1.44708
C	4.33399	-1.33037	-0.84323
C	3.26918	-1.36488	1.44710
O	-3.53843	1.25973	-0.25093
O	3.53837	1.25994	-0.25040
H	-2.48094	3.11680	-0.07213
H	-1.25053	5.28781	-0.01723
H	1.25010	5.28792	-0.01759
H	2.48070	3.11703	-0.07268
H	-5.12172	-0.65643	-0.48704
H	-4.65900	-2.37186	-0.72130
H	-4.17885	-1.14133	-1.91157
H	-4.01508	-0.66155	1.85126
H	-3.63788	-2.38966	1.58646
H	-2.32086	-1.25845	1.98555
H	5.12189	-0.65612	-0.48632
H	4.65928	-2.37152	-0.72111
H	4.17946	-1.14071	-1.91122
H	4.01478	-0.66188	1.85154
H	2.32053	-1.25878	1.98542
H	3.63761	-2.38993	1.58628
O	0.00005	-1.04725	2.02345
H	-0.00025	-0.12542	2.33402

^{4}FeBNPAPh2OBrOTf
Charge: 0
Energy: -4109670.1822472

Fe	0.08226	-0.51813	-0.56896
C	-3.24107	0.10103	3.23279
H	-3.87514	0.86606	2.76796
H	-2.27351	0.10950	2.72223
H	-3.06601	0.39673	4.27393
C	-3.00911	-2.35104	3.82401
H	-2.80016	-2.09289	4.86885
H	-2.04789	-2.43810	3.30986
H	-3.49436	-3.33501	3.81050
C	-5.24691	-1.22346	3.96237
H	-5.77238	-2.18632	3.93315
H	-5.91644	-0.45715	3.55171
H	-5.06190	-0.97623	5.01377
C	-3.91752	-1.28336	3.18495
C	-4.26627	-1.66826	1.73053
H	-4.75935	-2.65286	1.73103
H	-4.99972	-0.94318	1.34558
C	-3.22060	-1.68601	-0.51156
C	-4.46310	-1.91169	-1.16584
C	-4.52283	-1.81515	-2.54168
C	-3.36914	-1.49316	-3.27028
H	-3.38992	-1.37607	-4.34837
C	-2.18801	-1.32310	-2.55973
C	-0.90238	-0.96100	-3.26065
H	-0.23876	-1.82849	-3.28205
H	-1.09934	-0.64039	-4.29223
C	1.16751	0.28810	-3.16662
H	1.05740	0.82384	-4.11868
H	1.55740	-0.71101	-3.37812
C	2.15642	0.98446	-2.27072
C	3.12438	1.81987	-2.80363
H	3.15153	2.02781	-3.86772
C	4.05690	2.37533	-1.91825
C	3.98073	2.09245	-0.57067
C	2.95207	1.23285	-0.09962
C	3.67706	1.47364	2.24420
H	3.67589	2.57004	2.16200
H	4.71346	1.13575	2.08253
C	3.24448	1.08703	3.67389
C	1.80126	1.55337	3.94532
H	1.70725	2.63672	3.79581
H	1.52083	1.33245	4.98207
H	1.07905	1.05454	3.29330
C	4.19978	1.80897	4.64401
H	5.24324	1.51973	4.46695
H	3.95428	1.55374	5.68118
H	4.12660	2.89913	4.54095
C	3.37292	-0.43443	3.88366
H	2.72967	-1.00618	3.20914
H	3.09137	-0.69937	4.90978
H	4.40700	-0.76234	3.72135
C	-0.97345	1.38097	-2.45411
H	-2.00207	1.10848	-2.68638
H	-0.63864	2.08297	-3.22259
C	-0.97786	1.99901	-1.02122
C	-2.38716	2.58842	-0.79130
C	-3.34262	1.83837	-0.09574
H	-3.05442	0.88713	0.33088
C	-4.64210	2.32263	0.06068
H	-5.37012	1.73115	0.61087
C	-5.00650	3.55567	-0.48364
H	-6.01872	3.93212	-0.36219
C	-4.05644	4.30636	-1.17956
H	-4.32545	5.27158	-1.60076
C	-2.75309	3.82844	-1.32850
H	-2.01657	4.43332	-1.84887
C	0.07522	3.07893	-0.72878
C	0.61421	3.92737	-1.69999
H	0.35329	3.80733	-2.74734
C	1.51061	4.94037	-1.34616
H	1.92758	5.58034	-2.11930
C	1.87511	5.12101	-0.01330
H	2.57384	5.90662	0.26150
C	1.33656	4.28017	0.96496
H	1.61440	4.40700	2.00798
C	0.44553	3.27074	0.61097
H	0.04427	2.60433	1.36558
N	-3.11687	-1.68351	0.83822
H	-2.18376	-1.55209	1.21754
N	-2.09587	-1.43352	-1.22396
N	-0.16401	0.11570	-2.53433
N	2.05751	0.68973	-0.96367
N	2.80605	0.94191	1.20985
H	2.18465	0.17125	1.42940
O	-0.80967	0.93316	-0.10258
O	0.90204	-2.09477	-1.23022
S	2.40097	-2.51070	-1.17029
C	2.13701	-4.33299	-0.89740
O	3.11205	-2.01116	0.00345
F	3.32456	-4.94696	-0.87012
F	1.40496	-4.83980	-1.89739
F	1.50618	-4.53921	0.25768
H	4.83802	3.03401	-2.28792
H	4.69581	2.51470	0.12276
H	-5.46697	-1.97728	-3.05459
H	-5.34611	-2.15596	-0.58882
O	3.00877	-2.37277	-2.49875
Br	0.19236	-1.33459	1.80096

^{6}FeBNPAPh2OClOTf
Charge: 0
Energy: -2783154.6742583

Fe	0.34688	-0.61456	-0.30251
C	-3.06466	-0.26507	3.08119
H	-3.86757	0.16576	2.47123
H	-2.11736	-0.07759	2.56647
H	-3.03607	0.27856	4.03283
C	-2.17831	-2.34822	4.21321
H	-2.14319	-1.82931	5.17836
H	-1.19506	-2.23885	3.74755
H	-2.34688	-3.41426	4.41029
C	-4.65113	-1.94303	4.07234
H	-4.86970	-3.00220	4.25786
H	-5.48111	-1.51972	3.49280
H	-4.62651	-1.43289	5.04179
C	-3.30680	-1.76567	3.34036
C	-3.41648	-2.54155	2.00760
H	-3.57683	-3.60807	2.22854
H	-4.30614	-2.18707	1.46572
C	-2.23718	-2.67570	-0.16770
C	-3.26713	-3.45916	-0.75607
C	-3.25540	-3.67755	-2.11727
C	-2.24038	-3.11527	-2.90443
H	-2.22661	-3.22949	-3.98256
C	-1.25273	-2.38324	-2.26453
C	-0.15712	-1.69916	-3.04055
H	0.77314	-2.25893	-2.92008
H	-0.41035	-1.65596	-4.10912
C	1.34867	0.20630	-3.03794
H	1.19707	0.59710	-4.05386
H	2.07119	-0.61266	-3.09193
C	1.93332	1.26493	-2.14442
C	2.62775	2.33703	-2.67537
H	2.72875	2.44665	-3.74925
C	3.17760	3.26685	-1.78442

C	3.00565	3.10166	-0.42734
C	2.27626	1.98245	0.05212
C	2.40629	2.76695	2.39091
H	2.03705	3.75040	2.06944
H	3.50142	2.84239	2.48642
C	1.80377	2.44309	3.77571
C	0.27200	2.30344	3.67916
H	-0.17851	3.21542	3.26737
H	-0.15611	2.13761	4.67492
H	-0.02350	1.46202	3.04623
C	2.14924	3.62375	4.70358
H	3.23408	3.77103	4.77588
H	1.76979	3.43827	5.71487
H	1.70208	4.55926	4.34414
C	2.42697	1.15570	4.34981
H	2.21901	0.27840	3.73108
H	2.02346	0.95421	5.34930
H	3.51549	1.25642	4.43910
C	-1.09777	0.55051	-2.63676
H	-1.94908	-0.09135	-2.86241
H	-0.96855	1.22033	-3.49246
C	-1.47594	1.33739	-1.32018
C	-3.01767	1.41942	-1.30448
C	-3.74138	0.52627	-0.50684
H	-3.19792	-0.15610	0.13290
C	-5.13680	0.53112	-0.52547
H	-5.68401	-0.16469	0.10651
C	-5.82760	1.42298	-1.34856
H	-6.91427	1.42786	-1.36323
C	-5.10982	2.31520	-2.14815
H	-5.63626	3.02009	-2.78654
C	-3.71367	2.31566	-2.12413
H	-3.16721	3.03144	-2.73140
C	-0.89689	2.75903	-1.18857
C	-0.55685	3.57468	-2.27140
H	-0.62721	3.20287	-3.28902
C	-0.10731	4.88359	-2.06881
H	0.16040	5.49578	-2.92609
C	0.00496	5.39656	-0.77821
H	0.35616	6.41285	-0.62095
C	-0.33671	4.58946	0.31107
H	-0.25443	4.97539	1.32419
C	-0.78302	3.28662	0.10731
H	-1.03321	2.65441	0.95068
N	-2.25385	-2.36998	1.14839
H	-1.43715	-1.89530	1.52040
N	-1.22359	-2.18252	-0.92956
N	0.08851	-0.34027	-2.49668
N	1.75860	1.07564	-0.81969
N	2.04583	1.79834	1.36912
H	1.74692	0.87398	1.65854
O	-1.04687	0.58639	-0.21822
O	1.78875	-1.92151	-0.85922
S	3.30664	-1.76148	-0.67755
C	3.72304	-3.50753	-0.19297
O	3.67662	-0.92365	0.46600
F	5.04488	-3.62354	-0.02149
F	3.33394	-4.35509	-1.15625
F	3.10410	-3.83151	0.94534
H	3.73428	4.12149	-2.15848
H	3.42887	3.80865	0.27352
H	-4.04045	-4.27123	-2.57737
H	-4.04597	-3.87887	-0.13225
O	3.96714	-1.52729	-1.96994
Cl	0.59365	-1.11042	1.97275

^{6}FeBNPAPh2OFOTf
Charge: 0
Energy: -2557038.1926391

Fe	0.04313	-0.09041	-0.26804
C	-2.07096	-2.85229	2.67267
H	-3.10379	-2.79723	2.30661
H	-1.53346	-1.97685	2.29621
H	-2.09895	-2.78085	3.76649
C	0.07394	-4.18291	2.71662
H	0.12023	-4.11789	3.81012
H	0.63833	-3.33444	2.31806
H	0.57904	-5.10818	2.41231
C	-2.14076	-5.36277	2.88232
H	-1.69579	-6.31993	2.58224
H	-3.19847	-5.37229	2.59052
H	-2.09682	-5.30239	3.97558
C	-1.39625	-4.17347	2.24913
C	-1.47495	-4.34881	0.71351
H	-0.98694	-5.29374	0.42808
H	-2.53123	-4.42578	0.41736
C	-1.11512	-2.87060	-1.25983
C	-1.75317	-3.72876	-2.19364
C	-1.96221	-3.27621	-3.48111
C	-1.55888	-1.98363	-3.85492
H	-1.73335	-1.60135	-4.85440
C	-0.94375	-1.19357	-2.89712
C	-0.50643	0.22793	-3.17853
H	0.57088	0.24814	-3.36301
H	-1.02182	0.61504	-4.06887
C	-0.06986	2.38830	-2.06393
H	-0.75391	3.17233	-2.41004
H	0.73758	2.29203	-2.79531
C	0.59142	2.81737	-0.76868
C	0.99496	4.13093	-0.59649
H	0.72963	4.88623	-1.32747
C	1.76842	4.43909	0.53022
C	2.10403	3.45287	1.43601
C	1.63406	2.13595	1.22229
C	3.07856	1.08871	2.93531
H	2.90787	1.66369	3.85796
H	3.91398	1.55753	2.39812
C	3.47274	-0.36077	3.30662
C	2.34193	-1.03764	4.10790
H	2.10029	-0.46547	5.01278
H	2.64975	-2.04382	4.41734
H	1.42873	-1.14453	3.51405
C	4.73677	-0.27358	4.18165
H	5.56698	0.18856	3.63361
H	5.05708	-1.27521	4.49072
H	4.55718	0.31565	5.09011
C	3.78316	-1.18224	2.03741
H	2.89264	-1.34310	1.42413
H	4.17303	-2.16798	2.32022
H	4.52690	-0.68169	1.41000
C	-2.22009	1.17055	-1.69616
H	-2.67222	0.24452	-2.04989
H	-2.68170	1.99307	-2.25450
C	-2.50739	1.24140	-0.16171
C	-3.93473	0.69518	0.05916
C	-4.09163	-0.69774	0.13971
H	-3.20786	-1.32529	0.10716
C	-5.35602	-1.26391	0.28813
H	-5.45686	-2.34456	0.35516
C	-6.48861	-0.44729	0.35712
H	-7.47547	-0.88683	0.47584
C	-6.34025	0.93728	0.28016
H	-7.21214	1.58348	0.34194
C	-5.07108	1.50581	0.13329
H	-4.97365	2.58552	0.09620
C	-2.32625	2.65583	0.41580
C	-2.74218	3.80872	-0.26431
H	-3.22440	3.73121	-1.23458
C	-2.54948	5.07650	0.28994
H	-2.87607	5.95734	-0.25688
C	-1.93412	5.21026	1.53447
H	-1.77300	6.19602	1.96254
C	-1.52685	4.06609	2.22462
H	-1.04109	4.15699	3.19235
C	-1.72617	2.80179	1.67276
H	-1.38830	1.91300	2.19288
N	-0.87027	-3.22569	0.01816
H	-0.30745	-2.57654	0.56622
N	-0.73178	-1.62192	-1.63612
N	-0.76675	1.08357	-1.99166
N	0.88336	1.85230	0.12446
N	1.88900	1.12863	2.09040
H	1.49269	0.22471	1.85137
O	-1.60833	0.36111	0.45687
O	1.81610	-0.51028	-1.27025
S	3.03277	0.30714	-1.68090
C	4.14903	-1.07989	-2.21305
O	3.73347	0.96117	-0.57018
F	5.30652	-0.58591	-2.66685
F	3.57090	-1.79533	-3.18753
F	4.39964	-1.88776	-1.17412
H	2.10468	5.45911	0.69464
H	2.69439	3.67403	2.31670
H	-2.44583	-3.92430	-4.20695
H	-2.04788	-4.72712	-1.89372
O	2.76852	1.10249	-2.89588
F	0.54702	-1.16715	1.18500

^{6}FeBNPAPh2ON$_3$OTf
Charge: 0
Energy: -2597420.3529213

Fe	0.43147	-0.42163	-0.32773
C	-3.13989	-1.02335	2.73720
H	-4.06920	-1.12077	2.16382
H	-2.40866	-0.52782	2.09035
H	-3.33732	-0.36091	3.58829
C	-1.37891	-2.21275	4.09678
H	-1.62047	-1.65206	5.00742
H	-0.60579	-1.64708	3.56933
H	-0.95661	-3.17917	4.39744
C	-3.74465	-3.05403	4.09536
H	-3.42107	-4.02925	4.48007
H	-4.66572	-3.20345	3.51823
H	-3.98930	-2.42008	4.95501
C	-2.64697	-2.39480	3.23917
C	-2.37523	-3.34369	2.04657

H	-2.07182	-4.32960	2.43048
H	-3.31507	-3.48586	1.49383
C	-1.25906	-3.15992	-0.17122
C	-1.92920	-4.28283	-0.72349
C	-1.85442	-4.50408	-2.08447
C	-1.13204	-3.62345	-2.90352
H	-1.09567	-3.74857	-3.97996
C	-0.46758	-2.56984	-2.29458
C	0.31261	-1.54705	-3.08887
H	1.37769	-1.77598	-3.00794
H	0.02126	-1.58113	-4.14827
C	1.13940	0.75302	-3.02136
H	0.85401	1.15155	-4.00511
H	2.07742	0.20304	-3.13379
C	1.40526	1.87798	-2.05343
C	1.78033	3.13304	-2.49724
H	1.85353	3.34074	-3.55881
C	2.04753	4.11588	-1.53514
C	1.91644	3.82551	-0.19320
C	1.51706	2.52196	0.19459
C	1.33367	3.12129	2.59180
H	0.69582	3.97729	2.32900
H	2.35061	3.50989	2.75991
C	0.81234	2.49379	3.90464
C	-0.60157	1.91341	3.70325
H	-1.29436	2.68369	3.34195
H	-0.99191	1.53009	4.65367
H	-0.60888	1.08797	2.98549
C	0.75731	3.61732	4.95658
H	1.74452	4.07130	5.10768
H	0.42037	3.22218	5.92174
H	0.06040	4.41013	4.65715
C	1.77405	1.39340	4.39381
H	1.87015	0.57488	3.67572
H	1.41248	0.96297	5.33503
H	2.77747	1.79867	4.56970
C	-1.29067	0.27441	-2.64473
H	-1.89127	-0.61018	-2.85627
H	-1.39746	0.94317	-3.50546
C	-1.89398	0.90090	-1.32704
C	-3.39678	0.53750	-1.35262
C	-3.80878	-0.65888	-0.75161
H	-3.07562	-1.25338	-0.22327
C	-5.14161	-1.06415	-0.81213
H	-5.44245	-1.99332	-0.33367
C	-6.08535	-0.28168	-1.48236
H	-7.12499	-0.59489	-1.52914
C	-5.68148	0.90938	-2.08732
H	-6.40689	1.53054	-2.60650
C	-4.34642	1.31710	-2.02224
H	-4.05191	2.25596	-2.48060
C	-1.73888	2.42493	-1.17166
C	-1.64106	3.32024	-2.24073
H	-1.60539	2.95779	-3.26365
C	-1.57949	4.69974	-2.01755
H	-1.49429	5.37557	-2.86456
C	-1.61938	5.20432	-0.71930
H	-1.56950	6.27596	-0.54592
C	-1.72178	4.31730	0.35652
H	-1.75409	4.69583	1.37542
C	-1.78143	2.94468	0.13148
H	-1.84583	2.25361	0.96310
N	-1.36908	-2.82173	1.13448
H	-0.82255	-2.01856	1.43474
N	-0.50073	-2.35807	-0.96388
N	0.11964	-0.19006	-2.51869
N	1.28558	1.56819	-0.74656
N	1.31929	2.18273	1.48538
H	1.21491	1.19251	1.68624
O	-1.28812	0.27789	-0.22717
O	2.24098	-1.27467	-0.88829
S	3.61376	-0.62029	-0.69687
C	4.66112	-2.15480	-0.59973
O	3.74490	0.05909	0.59716
F	5.94321	-1.81476	-0.42823
F	4.54552	-2.85134	-1.74128
F	4.27368	-2.92878	0.41741
H	2.34981	5.11284	-1.84343
H	2.11733	4.57495	0.56138
H	-2.37072	-5.35461	-2.52106
H	-2.48790	-4.94966	-0.07846
O	4.06678	0.07893	-1.90861
N	0.74227	-0.78278	1.58617
N	1.62021	-1.48612	2.06768
N	2.40788	-2.14026	2.58044

[6]FeBNPAPh2ONCSOTf
Charge: 0
Energy: -2802525.5082271

Fe	0.40836	-0.27083	-0.48286
C	-2.93932	-1.68681	2.63796
H	-3.87779	-1.80181	2.08336
H	-2.29406	-1.02378	2.05234
H	-3.16735	-1.18225	3.58431
C	-1.00372	-2.85476	3.75337
H	-1.26298	-2.46042	4.74296
H	-0.31548	-2.14019	3.29567
H	-0.46542	-3.79902	3.89576
C	-3.26197	-3.94778	3.69468
H	-2.82025	-4.92732	3.91623
H	-4.18928	-4.11088	3.13129
H	-3.52939	-3.47881	4.64821
C	-2.28078	-3.05202	2.91469
C	-1.96523	-3.78502	1.58771
H	-1.52613	-4.76855	1.81408
H	-2.91143	-3.96477	1.05852
C	-1.02464	-3.15930	-0.63134
C	-1.62047	-4.25727	-1.30658
C	-1.62852	-4.27145	-2.68691
C	-1.06065	-3.20875	-3.40527
H	-1.09563	-3.17132	-4.48834
C	-0.45391	-2.19120	-2.68560
C	0.16253	-0.99067	-3.36564
H	1.24652	-1.12003	-3.39598
H	-0.21342	-0.89794	-4.39428
C	0.79030	1.34346	-3.00508
H	0.40066	1.83962	-3.90486
H	1.76459	0.91074	-3.24610
C	1.01264	2.34551	-1.90226
C	1.20518	3.68719	-2.17611
H	1.16808	4.04974	-3.19717
C	1.43012	4.55108	-1.09631
C	1.44319	4.05928	0.19207
C	1.23667	2.67327	0.40442
C	1.17049	2.90785	2.86850
H	0.41440	3.69687	2.75453
H	2.13920	3.40353	3.04046
C	0.81853	2.05323	4.10717
C	-0.50851	1.30025	3.88826
H	-1.32602	1.99988	3.67392
H	-0.77668	0.73696	4.78993
H	-0.44771	0.58951	3.05887
C	0.66529	3.01890	5.29730
H	1.58394	3.59479	5.46462
H	0.44886	2.46204	6.21608
H	-0.15593	3.72802	5.13332
C	1.95404	1.05770	4.41099
H	2.13318	0.36084	3.58863
H	1.71010	0.45848	5.29582
H	2.89484	1.58541	4.60798
C	-1.55215	0.58400	-2.54920
H	-2.08894	-0.31095	-2.86342
H	-1.77850	1.36436	-3.28324
C	-2.10556	0.94065	-1.11459
C	-3.56436	0.42763	-1.10053
C	-3.80873	-0.88930	-0.69101
H	-2.98134	-1.47988	-0.32221
C	-5.09688	-1.42121	-0.73318
H	-5.26612	-2.44400	-0.40465
C	-6.16373	-0.64525	-1.19337
H	-7.16885	-1.05728	-1.22554
C	-5.92745	0.66652	-1.60680
H	-6.74962	1.28307	-1.96097
C	-4.63674	1.20026	-1.56000
H	-4.47308	2.22832	-1.86712
C	-2.08566	2.43188	-0.73216
C	-2.16435	3.48190	-1.65150
H	-2.17389	3.28255	-2.71878
C	-2.22730	4.81051	-1.21859
H	-2.27968	5.61050	-1.95252
C	-2.21677	5.10758	0.14278
H	-2.26473	6.13988	0.47889
C	-2.14201	4.06416	1.07028
H	-2.13363	4.27999	2.13598
C	-2.07770	2.74273	0.63649
H	-2.00586	1.93198	1.35107
N	-1.08557	-3.02345	0.71337
H	-0.56548	-2.25020	1.11302
N	-0.40374	-2.17780	-1.33800
N	-0.10208	0.24343	-2.58326
N	1.03386	1.84193	-0.65110
N	1.19817	2.13193	1.64114
H	1.29551	1.12451	1.70112
O	-1.35416	0.22954	-0.16687
O	2.22324	-0.80112	-1.32310
S	3.54825	-0.06938	-1.07932
C	4.71024	-1.51190	-1.24594
O	3.69044	0.42314	0.29535
F	5.96834	-1.10446	-1.04773
F	4.61057	-2.03066	-2.47981
F	4.41079	-2.46098	-0.35510
H	1.58766	5.61187	-1.26975
H	1.61872	4.71375	1.03587
H	-2.08990	-5.10158	-3.21464
H	-2.05838	-5.06772	-0.73742
O	3.88329	0.83572	-2.18886
N	0.96952	-0.91809	1.30776

C	1.80573	-1.59542	1.84849
S	2.85060	-2.50127	2.63790

^{6}FeBNPAPh2OOHOTf
Charge: 0
Energy: -2541952.3515761

Fe	-0.43669	-0.43839	-0.40411
C	0.12363	2.20324	3.24992
H	0.16976	3.25328	2.93487
H	0.32670	1.58797	2.36845
H	0.93051	2.03603	3.97326
C	-1.26123	0.40842	4.36490
H	-0.50516	0.25747	5.14481
H	-1.03719	-0.29142	3.55454
H	-2.23848	0.14681	4.79038
C	-1.48761	2.80183	5.09073
H	-2.45907	2.59937	5.55923
H	-1.46639	3.85797	4.79332
H	-0.71299	2.65447	5.85194
C	-1.23953	1.87397	3.88693
C	-2.37703	2.13476	2.86797
H	-3.34730	1.91693	3.34036
H	-2.37094	3.20189	2.61443
C	-2.51812	1.79790	0.40142
C	-3.32055	2.94328	0.14720
C	-3.52653	3.34302	-1.15759
C	-2.95383	2.62444	-2.21965
H	-3.08332	2.93286	-3.25098
C	-2.20926	1.49902	-1.90789
C	-1.54951	0.64489	-2.96755
H	-2.14351	-0.26358	-3.08728
H	-1.51589	1.17775	-3.92825
C	0.30756	-0.93121	-3.28989
H	0.73178	-0.62191	-4.25588
H	-0.55073	-1.58018	-3.48405
C	1.31902	-1.73258	-2.50206
C	2.35904	-2.40101	-3.12470
H	2.49160	-2.33616	-4.19899
C	3.24067	-3.13511	-2.31733
C	3.06807	-3.16867	-0.94922
C	1.98411	-2.45548	-0.37309
C	2.68443	-2.92347	1.95588
H	3.69579	-2.55561	1.72838
H	2.72159	-4.02367	1.91826
C	2.30202	-2.48163	3.38654
C	2.27569	-0.94398	3.48313
H	3.24701	-0.51529	3.20609
H	2.05177	-0.63243	4.51018
H	1.51205	-0.50782	2.83351
C	3.37735	-3.03721	4.33830
H	3.42520	-4.13226	4.29127
H	3.15318	-2.75694	5.37382
H	4.37119	-2.64233	4.09224
C	0.92663	-3.05517	3.78152
H	0.12233	-2.65721	3.15581
H	0.69306	-2.79358	4.82039
H	0.91705	-4.14878	3.69821
C	0.73687	1.39194	-2.44921
H	0.11603	2.28681	-2.49167
H	1.38911	1.41822	-3.32851
C	1.55157	1.49462	-1.09990
C	1.69596	3.00801	-0.82025
C	0.69600	3.64828	-0.07575
H	-0.10794	3.05233	0.33750
C	0.74516	5.02407	0.14437
H	-0.03688	5.50216	0.72942
C	1.79289	5.78412	-0.38243
H	1.83390	6.85637	-0.20964
C	2.78942	5.15364	-1.12870
H	3.61262	5.73315	-1.53885
C	2.74196	3.77381	-1.34590
H	3.53399	3.29343	-1.91212
C	2.94317	0.83472	-1.10392
C	3.72607	0.64295	-2.24585
H	3.34794	0.91194	-3.22743
C	5.00974	0.09442	-2.15182
H	5.59567	-0.05387	-3.05528
C	5.53172	-0.26502	-0.91100
H	6.52832	-0.69229	-0.83836
C	4.75952	-0.07005	0.23830
H	5.15396	-0.34268	1.21432
C	3.48173	0.47369	0.14118
H	2.87482	0.61394	1.02708
N	-2.21583	1.36590	1.64414
H	-1.72101	0.47041	1.70197
N	-2.00265	1.09271	-0.64036
N	-0.19352	0.22997	-2.52792
N	1.12460	-1.76628	-1.17013
N	1.76339	-2.41264	0.95668
H	0.90486	-1.94838	1.26450
O	0.79167	0.91649	-0.07568
O	-0.75261	-1.08746	1.33248
H	-1.39675	-1.83186	1.32257
O	-1.77141	-1.80931	-1.36197
S	-2.83399	-2.73550	-0.79706
C	-4.29345	-1.57937	-0.69666
O	-2.56826	-3.10554	0.60999
F	-5.42354	-2.26558	-0.51333
F	-4.40141	-0.86509	-1.83255
F	-4.13911	-0.72332	0.32695
H	4.07228	-3.67040	-2.76725
H	3.74719	-3.72398	-0.31500
H	-4.13403	4.22077	-1.36075
H	-3.77440	3.47981	0.97105
O	-3.22782	-3.78535	-1.73310

^{6}FeN$_3$PyO2PhBr
Charge: 1+
Energy: -3465187.7149536

Fe	0.12539	-0.21809	-0.13964
C	-3.76605	-2.53723	-1.18397
H	-4.54746	-2.29066	-0.47000
C	-4.07980	-2.70666	-2.53044
H	-5.10840	-2.60087	-2.86211
C	-3.07235	-3.00982	-3.45065
H	-3.31947	-3.14624	-4.49943
C	-1.75016	-3.13677	-3.02135
H	-0.96488	-3.37431	-3.73274
C	-1.42803	-2.94942	-1.67904
H	-0.39894	-3.02445	-1.34986
C	-2.43429	-2.64279	-0.75287
C	-2.11555	-2.48968	0.68185
C	-2.83681	-3.23879	1.63043
H	-3.62935	-3.89130	1.28255
C	-2.49605	-3.18062	2.97341
H	-3.03048	-3.77838	3.70556
C	-1.43737	-2.35745	3.36490
H	-1.12706	-2.28938	4.40238
C	-0.79191	-1.61027	2.39045
C	0.25343	-0.56593	2.76067
H	0.64898	-0.78098	3.76325
C	-0.49061	0.76331	2.77443
C	-1.07317	1.24164	3.94289
H	-0.91795	0.72614	4.88526
C	-1.87207	2.38302	3.86050
H	-2.35773	2.78287	4.74552
C	-2.00862	3.01552	2.63139
H	-2.58401	3.92916	2.53181
C	-1.34485	2.50704	1.50171
C	-1.37425	3.27348	0.23672
C	-0.17319	3.68524	-0.35381
H	0.76703	3.42786	0.11970
C	-0.18929	4.43499	-1.52774
H	0.74703	4.75586	-1.97581
C	-1.40645	4.77626	-2.12216
H	-1.41996	5.35319	-3.04219
C	-2.60772	4.38417	-1.52626
H	-3.55542	4.64808	-1.98578
C	-2.59377	3.64687	-0.34367
H	-3.52693	3.32498	0.11019
C	2.30471	0.55446	1.92232
H	3.18423	0.20713	2.47738
H	1.83833	1.34385	2.51774
C	2.72671	1.14719	0.59436
C	3.97604	1.74072	0.41325
H	4.69891	1.74057	1.22283
C	4.27873	2.31156	-0.82114
H	5.24716	2.77365	-0.98702
C	3.32745	2.26933	-1.84321
H	3.52822	2.69310	-2.82114
C	2.10644	1.65611	-1.58985
H	1.32282	1.58330	-2.33566
C	2.03112	-1.87260	1.66436
H	1.25718	-2.63160	1.52975
H	2.53893	-2.07043	2.61933
C	3.00557	-1.93997	0.52111
C	4.36144	-2.20052	0.71349
H	4.74103	-2.33586	1.72395
C	5.23296	-2.29796	-0.37545
H	6.28612	-2.50300	-0.21101
C	4.73940	-2.13952	-1.67576
H	5.41304	-2.21837	-2.52418
C	3.38877	-1.88197	-1.89125
H	2.98375	-1.75018	-2.88949
C	2.50868	-1.77386	-0.79789
N	-1.11681	-1.66246	1.07975
N	-0.62751	1.36039	1.57504
N	1.33095	-0.55121	1.74634
N	1.81503	1.11904	-0.39262
O	1.22773	-1.48437	-1.00127
Br	-1.40009	0.55790	-1.85486

^{6}FeN$_3$PyO2PhCl
Charge: 1+
Energy: -2138659.9681644

Fe	0.06322	-0.18361	-0.23811
C	-3.87963	-2.34206	-1.43360
H	-4.67607	-2.10783	-0.73214
C	-4.16216	-2.46665	-2.79191
H	-5.18103	-2.33816	-3.14499
C	-3.13599	-2.75517	-3.69604
H	-3.35866	-2.85745	-4.75417
C	-1.82659	-2.91191	-3.23828
H	-1.02675	-3.13846	-3.93693
C	-1.53549	-2.77050	-1.88321
H	-0.51598	-2.87320	-1.53200
C	-2.56050	-2.47980	-0.97247
C	-2.27996	-2.37456	0.47495
C	-3.05222	-3.12304	1.38361
H	-3.84704	-3.75021	0.99661
C	-2.76076	-3.09385	2.73901
H	-3.33569	-3.69076	3.44054
C	-1.70227	-2.29802	3.18474
H	-1.43416	-2.24881	4.23497
C	-1.00133	-1.55392	2.24716
C	0.04739	-0.53234	2.67030
H	0.38378	-0.75172	3.69334
C	-0.66740	0.81264	2.63714
C	-1.29428	1.32046	3.76947
H	-1.19169	0.81874	4.72637
C	-2.06957	2.47303	3.63095
H	-2.58752	2.89623	4.48632
C	-2.14441	3.08379	2.38538
H	-2.70446	4.00132	2.24290
C	-1.43948	2.54460	1.29573
C	-1.40949	3.27796	0.01064
C	-0.18282	3.68747	-0.52609
H	0.73361	3.45289	0.00307
C	-0.14412	4.40561	-1.71914
H	0.81124	4.72643	-2.12516
C	-1.33137	4.71588	-2.38675
H	-1.30180	5.26865	-3.32116
C	-2.55846	4.32433	-1.84579
H	-3.48300	4.56478	-2.36196
C	-2.60001	3.61931	-0.64401
H	-3.55265	3.30026	-0.23023
C	2.16475	0.53704	1.93445
H	3.00733	0.17254	2.53415
H	1.68717	1.33967	2.50296
C	2.66458	1.11421	0.62659
C	3.93544	1.67480	0.49829
H	4.62277	1.65946	1.33810
C	4.30499	2.23287	-0.72388
H	5.29141	2.66898	-0.84925
C	3.39784	2.21231	-1.78622
H	3.65199	2.62784	-2.75524
C	2.15155	1.63143	-1.58445
H	1.39677	1.57513	-2.36101
C	1.84522	-1.88395	1.66887
H	1.06011	-2.62398	1.49735
H	2.30037	-2.09209	2.64803
C	2.87223	-1.97991	0.57512
C	4.21002	-2.27349	0.83397
H	4.53670	-2.41350	1.86212
C	5.13057	-2.39794	-0.21111
H	6.16906	-2.62835	0.00503
C	4.70471	-2.23377	-1.53455
H	5.41651	-2.33370	-2.34891
C	3.37315	-1.94380	-1.81619
H	3.02049	-1.80693	-2.83344
C	2.44372	-1.80751	-0.76710
N	-1.27380	-1.58430	0.92393
N	-0.73966	1.39315	1.42431
N	1.17527	-0.54609	1.71301
N	1.79755	1.10620	-0.39940
O	1.18326	-1.48541	-1.03386
Cl	-1.22148	0.58725	-1.89000

$^{6}FeN_3PyO2PhF$
Charge: 1+
Energy: -1912535.3347956

Fe	0.09526	-0.10178	-0.27851
C	-3.82173	-2.33141	-1.48682
H	-4.54840	-2.40471	-0.68193
C	-4.25535	-2.16733	-2.80042
H	-5.31893	-2.12567	-3.01605
C	-3.32281	-2.05568	-3.83565
H	-3.66171	-1.93268	-4.86023
C	-1.95707	-2.10539	-3.55122
H	-1.22851	-2.02559	-4.35249
C	-1.51703	-2.25698	-2.23758
H	-0.45511	-2.29844	-2.02529
C	-2.44746	-2.36610	-1.19415
C	-2.01475	-2.54943	0.20855
C	-2.60904	-3.54967	1.00211
H	-3.35836	-4.19365	0.55646
C	-2.20859	-3.72501	2.31828
H	-2.64715	-4.50911	2.92810
C	-1.22746	-2.88097	2.84696
H	-0.89261	-2.97628	3.87458
C	-0.69113	-1.90293	2.02278
C	0.25726	-0.83305	2.55932
H	0.64085	-1.13973	3.54262
C	-0.60028	0.41948	2.69960
C	-1.19953	0.76466	3.90500
H	-0.96787	0.21493	4.81166
C	-2.11905	1.81630	3.90528
H	-2.61608	2.11302	4.82400
C	-2.37986	2.48281	2.71407
H	-3.07561	3.31362	2.67528
C	-1.70384	2.10851	1.54031
C	-1.92067	2.86404	0.28396
C	-0.85207	3.53305	-0.32420
H	0.13266	3.48105	0.12640
C	-1.05801	4.26887	-1.48879
H	-0.22627	4.79451	-1.94987
C	-2.33242	4.33528	-2.05781
H	-2.49233	4.90401	-2.96918
C	-3.40345	3.67829	-1.44793
H	-4.39557	3.72966	-1.88648
C	-3.20251	2.95472	-0.27249
H	-4.03330	2.43754	0.20015
C	2.22774	0.54038	1.91906
H	3.12431	0.20172	2.45216
H	1.68738	1.21532	2.58945
C	2.61426	1.31576	0.67583
C	3.83503	1.97740	0.54415
H	4.57860	1.90881	1.33163
C	4.08332	2.70284	-0.61974
H	5.03008	3.21843	-0.74924
C	3.10954	2.74826	-1.62150
H	3.27314	3.29470	-2.54395
C	1.91965	2.05912	-1.42032
H	1.11477	2.03548	-2.14746
C	2.14314	-1.84790	1.34216
H	1.42735	-2.63703	1.09882
H	2.66348	-2.13537	2.26761
C	3.11888	-1.68993	0.20982
C	4.49195	-1.86114	0.38337
H	4.87920	-2.09550	1.37271
C	5.37057	-1.74232	-0.69693
H	6.43699	-1.87987	-0.54805
C	4.86615	-1.45535	-1.97081
H	5.54462	-1.36600	-2.81449
C	3.49898	-1.28408	-2.16647
H	3.08636	-1.05565	-3.14404
C	2.60897	-1.39272	-1.08084
N	-1.05906	-1.74564	0.73191
N	-0.83514	1.07383	1.54596
N	1.34697	-0.60556	1.58761
N	1.68494	1.37140	-0.29098
O	1.31028	-1.17917	-1.26328
F	-0.93698	0.65551	-1.49760

$^{6}FeN_3PyO2PhN_3$
Charge: 1+
Energy: -1952924.2359727

Fe	0.18572	-0.11654	-0.21009
C	-3.68557	-2.67537	-1.12977
H	-4.38598	-2.68740	-0.29882
C	-4.16273	-2.67569	-2.43877
H	-5.23254	-2.69374	-2.62305
C	-3.26539	-2.64010	-3.50893
H	-3.63740	-2.63899	-4.52916
C	-1.89058	-2.60232	-3.26471
H	-1.18901	-2.58007	-4.09345
C	-1.40699	-2.59304	-1.95721
H	-0.33944	-2.55577	-1.77331
C	-2.30373	-2.62382	-0.87829
C	-1.82011	-2.65908	0.52004
C	-2.34551	-3.61776	1.40795
H	-3.08661	-4.31846	1.04108
C	-1.88476	-3.68656	2.71425
H	-2.26971	-4.43853	3.39641
C	-0.90666	-2.78140	3.13373
H	-0.51649	-2.79828	4.14606
C	-0.44308	-1.84682	2.21902
C	0.50848	-0.73015	2.63708
H	0.97550	-0.98528	3.59879
C	-0.36737	0.50629	2.79779
C	-0.90102	0.85768	4.03288
H	-0.60689	0.32331	4.93053
C	-1.83382	1.89533	4.07628
H	-2.28060	2.19673	5.01892
C	-2.16893	2.54640	2.89525
H	-2.87089	3.37282	2.89008
C	-1.55759	2.16602	1.68849
C	-1.84939	2.92121	0.44760
C	-0.80585	3.51477	-0.27525
H	0.21272	3.39768	0.07439
C	-1.07955	4.25736	-1.42135

H	-0.26514	4.72155	-1.97074
C	-2.39894	4.41253	-1.85704
H	-2.61225	4.98556	-2.75447
C	-3.44382	3.83436	-1.13346
H	-4.46897	3.94506	-1.47271
C	-3.17289	3.09962	0.02123
H	-3.98530	2.63885	0.57665
C	2.39518	0.65498	1.81107
H	3.31863	0.35479	2.32057
H	1.87346	1.35635	2.46834
C	2.71663	1.36815	0.51470
C	3.93709	2.00455	0.28864
H	4.72080	1.95681	1.03760
C	4.13476	2.67214	-0.91788
H	5.08032	3.16574	-1.12049
C	3.10996	2.68518	-1.86811
H	3.23103	3.18417	-2.82340
C	1.92483	2.02345	-1.57231
H	1.09040	1.97889	-2.26411
C	2.33202	-1.75575	1.33769
H	1.62299	-2.56662	1.15592
H	2.90003	-1.99551	2.24839
C	3.24963	-1.61224	0.15726
C	4.63544	-1.73115	0.27254
H	5.07434	-1.92179	1.24979
C	5.45878	-1.61309	-0.84911
H	6.53522	-1.70952	-0.74767
C	4.88431	-1.38054	-2.10408
H	5.51872	-1.29172	-2.98162
C	3.50362	-1.26266	-2.24048
H	3.04058	-1.07821	-3.20479
C	2.66894	-1.37271	-1.11357
N	-0.87732	-1.78221	0.94153
N	-0.67891	1.13878	1.65046
N	1.51844	-0.51989	1.57872
N	1.73404	1.39192	-0.40200
O	1.35208	-1.21293	-1.23689
N	-1.12274	0.44734	-1.42343
N	-2.18723	0.59527	-1.96378
N	-3.19844	0.73688	-2.49538

$^{6}FeN_3PyO2PhNCS$
Charge: 1+
Energy: -2158031.8553199

Fe	0.19851	-0.14080	-0.12859
C	-3.59969	-2.66222	-1.18405
H	-4.19410	-2.89784	-0.30512
C	-4.22970	-2.39115	-2.39714
H	-5.31319	-2.42316	-2.46142
C	-3.46792	-2.07391	-3.52444
H	-3.95887	-1.86017	-4.46902
C	-2.07514	-2.02484	-3.43393
H	-1.48022	-1.77884	-4.30818
C	-1.44004	-2.28171	-2.22024
H	-0.35957	-2.23335	-2.15191
C	-2.20007	-2.59738	-1.08422
C	-1.55052	-2.91105	0.20670
C	-1.92017	-4.07735	0.90397
H	-2.67201	-4.72715	0.47115
C	-1.29568	-4.40449	2.09818
H	-1.55911	-5.31529	2.62736
C	-0.31198	-3.54968	2.60288
H	0.20205	-3.76539	3.53376
C	-0.00940	-2.40216	1.88473
C	0.92697	-1.33631	2.44477
H	1.52310	-1.76225	3.26396
C	0.01148	-0.24291	2.98092
C	-0.38872	-0.22017	4.31204
H	0.03868	-0.91640	5.02651
C	-1.36521	0.70359	4.69023
H	-1.71345	0.74843	5.71773
C	-1.87044	1.57605	3.73394
H	-2.61072	2.32520	3.99198
C	-1.38442	1.52801	2.41643
C	-1.84576	2.52359	1.42240
C	-0.91930	3.36860	0.79918
H	0.13176	3.27928	1.04809
C	-1.34932	4.32413	-0.11933
H	-0.62585	4.98115	-0.59401
C	-2.70755	4.43829	-0.42517
H	-3.04192	5.17226	-1.15193
C	-3.63660	3.60576	0.20331
H	-4.69179	3.68816	-0.03805
C	-3.21024	2.65870	1.13366
H	-3.93042	2.00218	1.61452
C	2.61286	0.35424	1.76324
H	3.61316	0.02922	2.07353
H	2.14545	0.83566	2.62690
C	2.71320	1.37354	0.64803
C	3.84136	2.17255	0.46206
H	4.71106	2.03993	1.09743
C	3.83526	3.11832	-0.56093
H	4.70531	3.74527	-0.73059
C	2.70433	3.23953	-1.37267
H	2.66544	3.95638	-2.18560
C	1.62149	2.40362	-1.12924
H	0.71519	2.43539	-1.72384
C	2.63124	-1.88630	0.75442
H	1.95514	-2.69898	0.47870
H	3.32972	-2.26688	1.51385
C	3.37360	-1.41277	-0.46318
C	4.76568	-1.44317	-0.54690
H	5.34319	-1.80521	0.30110
C	5.42147	-1.02091	-1.70608
H	6.50519	-1.05159	-1.75976
C	4.67245	-0.56825	-2.79834
H	5.17729	-0.24227	-3.70332
C	3.28203	-0.53222	-2.73633
H	2.68294	-0.18038	-3.57030
C	2.61708	-0.94963	-1.56916
N	-0.60272	-2.08527	0.71272
N	-0.46810	0.60365	2.04978
N	1.78478	-0.80953	1.36129
N	1.62802	1.50149	-0.13380
O	1.29002	-0.87218	-1.49092
N	-1.25603	0.65287	-1.05781
C	-1.95735	1.10476	-1.91835
S	-2.88426	1.70337	-3.06977

$^{6}FeN_3PyO2PhOH$
Charge: 1+
Energy: -1897448.8658905

Fe	0.07705	-0.09901	-0.29055
C	-3.76116	-2.33616	-1.52442
H	-4.53513	-2.27420	-0.76406
C	-4.10353	-2.26283	-2.87447
H	-5.14529	-2.15457	-3.16128
C	-3.10871	-2.32572	-3.85341
H	-3.37670	-2.27383	-4.90465
C	-1.76921	-2.46488	-3.47738
H	-0.99302	-2.53262	-4.23440
C	-1.42066	-2.52861	-2.12761
H	-0.38025	-2.62151	-1.83726
C	-2.41639	-2.45293	-1.14156
C	-2.06978	-2.52759	0.29727
C	-2.73036	-3.44637	1.13172
H	-3.48226	-4.09890	0.70251
C	-2.38703	-3.53411	2.47428
H	-2.87487	-4.25632	3.12193
C	-1.39787	-2.68573	2.97733
H	-1.10192	-2.71873	4.02076
C	-0.80121	-1.78283	2.10724
C	0.16185	-0.70608	2.60298
H	0.51990	-0.96868	3.60893
C	-0.67452	0.56757	2.66467
C	-1.30364	0.96775	3.83812
H	-1.11044	0.44673	4.77042
C	-2.20062	2.03611	3.77333
H	-2.71976	2.37475	4.66495
C	-2.40716	2.66747	2.55267
H	-3.07998	3.51324	2.46395
C	-1.70135	2.23920	1.41564
C	-1.84840	2.96727	0.13392
C	-0.73193	3.56493	-0.46169
H	0.23537	3.48122	0.02024
C	-0.86843	4.27431	-1.65290
H	0.00083	4.74581	-2.10338
C	-2.12155	4.38617	-2.26021
H	-2.22825	4.93612	-3.19082
C	-3.24074	3.80191	-1.66203
H	-4.21709	3.89084	-2.12931
C	-3.10821	3.10446	-0.46188
H	-3.97600	2.64207	0.00087
C	2.17115	0.59004	1.93322
H	3.04767	0.26172	2.50525
H	1.63230	1.31323	2.55256
C	2.60712	1.28917	0.66119
C	3.85517	1.89756	0.52687
H	4.57913	1.83452	1.33277
C	4.15737	2.55886	-0.66168
H	5.12662	3.03042	-0.79253
C	3.20674	2.59687	-1.68551
H	3.40988	3.09503	-2.62725
C	1.98752	1.96315	-1.47995
H	1.19838	1.94132	-2.22392
C	2.04642	-1.81874	1.46924
H	1.32028	-2.60305	1.24245
H	2.54130	-2.07673	2.41742
C	3.04914	-1.72149	0.35386
C	4.41854	-1.88363	0.57093
H	4.77757	-2.07809	1.57957
C	5.32625	-1.80332	-0.48694
H	6.38854	-1.93321	-0.30517
C	4.85370	-1.56396	-1.78212
H	5.55315	-1.50303	-2.61132
C	3.49100	-1.40344	-2.02017

H	3.10735	-1.21190	-3.01750
C	2.57228	-1.47600	-0.95803
N	-1.11850	-1.70729	0.79807
N	-0.85966	1.18409	1.48186
N	1.27209	-0.55110	1.64312
N	1.69974	1.33436	-0.32843
O	-1.06292	0.53812	-1.54944
H	-1.23734	-0.01184	-2.33123
O	1.27172	-1.27889	-1.18227

^{6}FeMe3TACNBrS2SiMe2
Charge: 0
Energy: -3466414.4823297

Fe	-0.02008	-0.05650	0.00032
S	1.56422	0.40630	1.68904
S	1.56808	0.38859	-1.68974
Si	2.91442	0.37169	0.00133
N	-0.88794	2.16917	0.04947
N	-1.90257	-0.17447	1.41916
N	-1.84284	-0.11467	-1.48263
C	4.00258	1.91599	-0.01035
C	3.94552	-1.19914	0.01154
C	0.20153	3.15023	-0.13135
C	-1.43514	2.28072	1.41834
C	-1.91927	2.34305	-1.00602
C	-2.44011	1.17480	1.73324
C	-1.50346	-0.87358	2.66122
C	-2.85807	-0.99668	0.64344
C	-3.10580	-0.43444	-0.76017
C	-1.57953	-1.11021	-2.54687
C	-1.84667	1.24525	-2.06668
H	3.39677	2.82735	-0.03506
H	4.63295	1.94427	0.88667
H	4.65489	1.91312	-0.89206
H	4.58176	-1.25404	-0.88000
H	4.58332	-1.24051	0.90274
H	3.27297	-2.06271	0.01884
H	-0.17207	4.17851	-0.00253
H	0.98275	2.94618	0.60145
H	0.62951	3.02844	-1.12667
H	-0.58271	2.19877	2.09699
H	-1.90985	3.26354	1.57859
H	-2.91095	2.36884	-0.54823
H	-1.79471	3.31353	-1.50184
H	-3.36891	1.33261	1.17965
H	-2.71104	1.23765	2.79442
H	-0.98721	-1.79766	2.40036
H	-0.80684	-0.24254	3.21539
H	-2.38296	-1.09080	3.28704
H	-2.41545	-1.99009	0.55862
H	-3.82112	-1.08763	1.17331
H	-3.72903	0.46217	-0.70933
H	-3.68637	-1.17032	-1.32883
H	-0.58117	-0.94360	-2.95413
H	-1.59421	-2.10859	-2.11181
H	-2.33187	-1.03162	-3.34708
H	-0.91278	1.34833	-2.62412
H	-2.68252	1.36766	-2.77581
Br	0.16897	-2.63714	0.01565

^{6}FeMe3TACNClS2SiMe2
Charge: 0
Energy: -2139886.2569767

Fe	-0.01059	-0.31344	0.00489
S	1.59013	0.14868	1.69009
S	1.59357	0.09761	-1.69081
Si	2.93407	0.04265	0.00209
N	-0.82278	1.94047	0.03010
N	-1.89145	-0.36108	1.42340
N	-1.83063	-0.32955	-1.47734
C	4.09121	1.53573	-0.02280
C	3.88922	-1.57648	0.02864
C	0.29111	2.89199	-0.16030
C	-1.36715	2.08035	1.39759
C	-1.84913	2.13040	-1.02753
C	-2.39762	1.00144	1.72678
C	-1.49679	-1.06162	2.66528
C	-2.86196	-1.17157	0.65470
C	-3.09952	-0.61435	-0.75265
C	-1.57805	-1.35133	-2.51789
C	-1.80344	1.02121	-2.07854
H	3.52460	2.47193	-0.05333
H	4.72339	1.54358	0.87339
H	4.74141	1.49862	-0.90532
H	4.52226	-1.67408	-0.86151
H	4.52279	-1.64346	0.92127
H	3.17159	-2.40315	0.04321
H	-0.05597	3.93042	-0.03790
H	1.06908	2.67249	0.57148
H	0.71314	2.75198	-1.15564
H	-0.51637	1.98644	2.07671
H	-1.81871	3.07583	1.54671
H	-2.84010	2.18406	-0.57041
H	-1.70108	3.09340	-1.53147
H	-3.32425	1.17539	1.17420
H	-2.66357	1.08088	2.78823
H	-0.98953	-1.99009	2.40235
H	-0.79250	-0.43709	3.21698
H	-2.37663	-1.26967	3.29397
H	-2.43628	-2.17262	0.57653
H	-3.82629	-1.24124	1.18558
H	-3.70123	0.29707	-0.70687
H	-3.69847	-1.34012	-1.31568
H	-0.57685	-1.20621	-2.92637
H	-1.60499	-2.33842	-2.05821
H	-2.32792	-1.28275	-3.32140
H	-0.86732	1.09624	-2.63671
H	-2.63659	1.15610	-2.78872
Cl	0.05485	-2.67455	0.04360

^{6}FeMe3TACNFS2SiMe2
Charge: 0
Energy: -1913762.4282068

Fe	-0.03279	0.02072	-0.47823
S	1.61120	-1.68730	-0.17395
S	1.61871	1.69191	-0.03084
Si	2.95130	0.00005	-0.10734
N	-0.78180	-0.14441	1.81036
N	-1.90808	-1.38874	-0.53499
N	-1.83058	1.50570	-0.31283
C	4.05179	-0.06032	1.42925
C	4.01914	0.06070	-1.65913
C	0.36411	-0.01777	2.73370
C	-1.32727	-1.51770	1.88088
C	-1.79476	0.90405	2.10073
C	-2.38575	-1.78603	0.80842
C	-1.49693	-2.55529	-1.34174
C	-2.87008	-0.55573	-1.28694
C	-3.10311	0.80278	-0.62039
C	-1.55683	2.55491	-1.31578
C	-1.77016	2.03037	1.06353
H	3.45453	-0.07060	2.34637
H	4.67846	-0.96049	1.41587
H	4.70889	0.81759	1.45931
H	4.65964	0.95110	-1.65674
H	4.65698	-0.82906	-1.72732
H	3.37691	0.09659	-2.54488
H	0.05096	-0.18921	3.77619
H	1.12309	-0.74751	2.45084
H	0.79632	0.97792	2.62962
H	-0.47963	-2.18887	1.72088
H	-1.75124	-1.72868	2.87731
H	-2.78742	0.44933	2.14683
H	-1.61921	1.33808	3.09285
H	-3.31177	-1.25271	1.03904
H	-2.64215	-2.85307	0.82584
H	-0.97625	-2.19000	-2.22795
H	-0.79835	-3.16330	-0.76489
H	-2.36759	-3.16588	-1.62885
H	-2.42192	-0.39492	-2.26737
H	-3.83542	-1.07437	-1.41187
H	-3.68245	0.68520	0.29868
H	-3.72138	1.41651	-1.28784
H	-0.58612	3.00668	-1.10720
H	-1.49241	2.07893	-2.29433
H	-2.34034	3.32846	-1.30672
H	-0.82647	2.57436	1.15065
H	-2.59426	2.73520	1.26636
F	-0.28368	0.08575	-2.28336

^{6}FeMe3TACNN$_3$S2SiMe2
Charge: 0
Energy: -1954148.9489519

Fe	0.07815	0.25854	0.02647
S	-1.50603	-0.37589	1.69281
S	-1.52923	-0.18771	-1.67647
Si	-2.84371	-0.51464	0.00448
N	1.10676	-1.90959	-0.02426
N	1.95888	0.43734	1.43258
N	1.87873	0.48097	-1.46975
C	-3.65237	-2.22144	-0.09629
C	-4.18535	0.80267	0.08832
C	0.08076	-2.94923	-0.23755
C	1.66975	-2.03683	1.33691
C	2.13545	-1.97221	-1.09438
C	2.59660	-0.87536	1.69666
C	1.49018	1.06448	2.68512
C	2.82792	1.36536	0.67787
C	3.11642	0.86709	-0.74207
C	1.50278	1.51779	-2.45253
C	1.97094	-0.84413	-2.11468
H	-2.91163	-3.02111	-0.18829
H	-4.25332	-2.40927	0.80193

H	-4.31519	-2.26862	-0.96917
H	-4.83041	0.74562	-0.79722
H	-4.80677	0.65716	0.98062
H	-3.74259	1.80183	0.13073
H	0.52116	-3.95730	-0.17470
H	-0.69229	-2.83703	0.52252
H	-0.37906	-2.80057	-1.21518
H	0.81634	-2.03853	2.01989
H	2.21152	-2.99017	1.45861
H	3.13164	-1.94139	-0.64639
H	2.07600	-2.93154	-1.62321
H	3.53381	-0.94387	1.13862
H	2.87263	-0.96013	2.75533
H	0.88432	1.93594	2.43384
H	0.85647	0.35747	3.22307
H	2.33858	1.35870	3.32271
H	2.28838	2.31202	0.62071
H	3.78140	1.53536	1.20564
H	3.80249	0.01682	-0.71761
H	3.64332	1.65987	-1.28751
H	0.53206	1.27005	-2.88471
H	1.39985	2.46989	-1.93138
H	2.25793	1.59886	-3.24996
H	1.03535	-0.99160	-2.66003
H	2.80137	-0.88152	-2.83998
N	-0.00136	2.23552	0.13107
N	-0.99765	2.92232	0.06985
N	-1.92075	3.61122	0.01400

^{6}FeMe3TACNNCSS2SiMe2
Charge: 0
Energy: -2159257.0323172

Fe	0.11485	0.02072	0.01754
S	-1.14745	-1.09115	1.69089
S	-1.20037	-0.97817	-1.68825
Si	-2.41366	-1.55734	0.00291
N	1.81270	-1.62616	-0.00700
N	1.78021	0.87791	1.43304
N	1.71797	0.87206	-1.46832
C	-2.78541	-3.40831	-0.05612
C	-4.00014	-0.54885	0.06130
C	1.21928	-2.96436	-0.21524
C	2.38051	-1.54062	1.35764
C	2.81036	-1.33414	-1.07177
C	2.83669	-0.12467	1.71344
C	1.11022	1.31256	2.67651
C	2.27271	2.04774	0.67414
C	2.73474	1.67278	-0.73683
C	1.00609	1.70675	-2.45896
C	2.27741	-0.33784	-2.10358
H	-1.86192	-3.99421	-0.10401
H	-3.34268	-3.71446	0.83751
H	-3.38954	-3.64668	-0.93994
H	-4.61653	-0.74761	-0.82392
H	-4.58346	-0.79805	0.95614
H	-3.76737	0.52062	0.08643
H	1.98371	-3.75123	-0.11726
H	0.43193	-3.11765	0.52324
H	0.76611	-3.00141	-1.20603
H	1.58193	-1.84319	2.03944
H	3.22336	-2.24089	1.48171
H	3.72938	-0.95778	-0.61619
H	3.09110	-2.25849	-1.59087
H	3.74295	0.13713	1.16164
H	3.11509	-0.10100	2.77447
H	0.23443	1.90796	2.41595
H	0.76693	0.43379	3.22428
H	1.79475	1.89807	3.30970
H	1.43397	2.74199	0.60210
H	3.09683	2.54950	1.20808
H	3.67439	1.11629	-0.69676
H	2.95692	2.59528	-1.28730
H	0.17625	1.13792	-2.88061
H	0.58650	2.57472	-1.95035
H	1.68622	2.03165	-3.26144
H	1.46253	-0.80394	-2.66275
H	3.08017	-0.08365	-2.81604
N	-0.72069	1.82660	0.09397
C	-1.64647	2.57881	0.05525
S	-2.88191	3.61103	0.00358

^{6}FeMe3TACNOHS2SiMe2
Charge: 0
Energy: -1898672.2052389

Fe	-0.05375	0.06886	-0.49655
S	1.62713	-1.66199	-0.35159
S	1.62956	1.69491	0.08152
Si	2.95533	0.00627	-0.07752
N	-0.78452	-0.33062	1.79155
N	-1.92359	-1.32976	-0.66568
N	-1.85058	1.52875	-0.14553
C	4.01314	-0.18328	1.47918
C	4.09793	0.19817	-1.56977
C	0.37220	-0.28910	2.70637
C	-1.32104	-1.70542	1.72128
C	-1.79739	0.67685	2.19418
C	-2.38864	-1.86155	0.63620
C	-1.52317	-2.41350	-1.58548
C	-2.89515	-0.42653	-1.31844
C	-3.12413	0.85854	-0.51618
C	-1.59449	2.68899	-1.02206
C	-1.77642	1.90327	1.27902
H	3.39386	-0.26102	2.37797
H	4.63522	-1.08422	1.41077
H	4.67441	0.68439	1.59508
H	4.73139	1.08721	-1.46273
H	4.74516	-0.68103	-1.67637
H	3.51064	0.30307	-2.48817
H	0.07431	-0.55406	3.73404
H	1.12565	-0.99094	2.34853
H	0.80489	0.71202	2.68754
H	-0.47204	-2.35090	1.48130
H	-1.73504	-2.02616	2.69275
H	-2.78939	0.21832	2.19655
H	-1.61930	1.00688	3.22553
H	-3.31209	-1.35462	0.92837
H	-2.64646	-2.92453	0.54578
H	-1.02263	-1.96278	-2.44334
H	-0.80937	-3.06579	-1.07947
H	-2.39667	-3.00197	-1.90852
H	-2.46330	-0.16831	-2.28628
H	-3.86187	-0.93254	-1.48149
H	-3.69969	0.64921	0.38894
H	-3.74567	1.53516	-1.11624
H	-0.61928	3.11323	-0.77845
H	-1.55027	2.33282	-2.05141
H	-2.37594	3.45617	-0.90332
H	-0.82808	2.43000	1.41345
H	-2.59428	2.58796	1.56141
O	-0.28388	0.32034	-2.34011
H	0.56643	0.51772	-2.76304

^{6}FeBrMe3TACNOSiPh22O
Charge: 0
Energy: -3821678.0351163

Fe	-1.52197	-0.17845	-0.41945
O	-0.15498	-1.45590	-0.46728
O	-0.62004	1.43202	-0.12650
N	-2.91277	-1.79001	-1.35269
N	-3.47679	0.99944	-0.93803
N	-1.33963	0.22344	-2.71207
Si	1.39636	-1.34896	0.07758
Si	0.83851	1.62407	0.61466
O	1.70069	0.20151	0.59907
C	-4.29518	-1.27892	-1.55211
H	-5.02614	-2.03557	-1.24295
H	-4.46848	-1.11205	-2.61845
C	-4.55834	0.00773	-0.75678
H	-5.53699	0.42442	-1.04762
H	-4.58687	-0.22937	0.30804
C	-3.41450	1.53446	-2.32347
H	-3.80967	2.55768	-2.35266
H	-4.06817	0.94298	-2.96909
C	-1.98696	1.53987	-2.86745
H	-1.99211	1.86344	-3.92172
H	-1.38297	2.24201	-2.28979
C	-1.98811	-0.86298	-3.48564
H	-1.36596	-1.14168	-4.34530
H	-2.93253	-0.50454	-3.90195
C	-2.21114	-2.10262	-2.61978
H	-2.75952	-2.86498	-3.19731
H	-1.24011	-2.51086	-2.33185
C	-2.89529	-2.98308	-0.47635
H	-3.43169	-2.75784	0.44464
H	-1.85885	-3.20381	-0.21695
H	-3.35717	-3.84516	-0.98247
C	-3.58629	2.11051	0.03373
H	-4.51970	2.67393	-0.11928
H	-2.72106	2.76208	-0.09218
H	-3.55024	1.70725	1.04530
C	0.09793	0.30800	-3.03108
H	0.25237	0.61943	-4.07581
H	0.55836	-0.66447	-2.86649
H	0.56985	1.02978	-2.36503
C	1.66647	-2.57659	1.45979
C	0.59658	-2.96322	2.28785
H	-0.39293	-2.55286	2.11055
C	0.79447	-3.85494	3.34395
H	-0.04326	-4.13639	3.97748
C	2.06514	-4.38262	3.58645
H	2.21957	-5.07803	4.40810
C	3.13783	-4.01607	2.76973
H	4.12770	-4.42714	2.95305
C	2.93718	-3.12178	1.71644
H	3.77836	-2.85110	1.08175

C	2.59469	-1.68216	-1.33068
C	2.78269	-2.98723	-1.82101
H	2.28466	-3.82224	-1.33162
C	3.61219	-3.23668	-2.91655
H	3.74653	-4.25375	-3.27718
C	4.27400	-2.17842	-3.54503
H	4.92154	-2.36985	-4.39729
C	4.10614	-0.87532	-3.06988
H	4.62393	-0.04848	-3.55035
C	3.27621	-0.63314	-1.97318
H	3.15281	0.38403	-1.61245
C	1.81039	2.86119	-0.41137
C	1.15319	3.83262	-1.18665
H	0.06585	3.86991	-1.18144
C	1.86892	4.74656	-1.96392
H	1.34096	5.49066	-2.55587
C	3.26492	4.70127	-1.98233
H	3.82553	5.40820	-2.58892
C	3.93889	3.74475	-1.21812
H	5.02541	3.70621	-1.22995
C	3.21675	2.83823	-0.43943
H	3.75002	2.09331	0.14679
C	0.66599	2.16827	2.38996
C	0.52400	1.21620	3.41573
H	0.54070	0.15701	3.17610
C	0.35404	1.61496	4.74177
H	0.24195	0.86560	5.52122
C	0.32528	2.97383	5.06636
H	0.19334	3.28409	6.10023
C	0.47089	3.93349	4.06180
H	0.45670	4.99172	4.31182
C	0.64139	3.53026	2.73586
H	0.76806	4.28571	1.96234
Br	-2.39600	-0.60488	1.98498

^{6}FeClMe3TACNOSiPh22O
Charge: 0
Energy: -2495150.0337088

Fe	-1.64897	-0.28301	0.02992
O	-0.25898	-1.52433	-0.17506
O	-0.77766	1.37368	-0.08910
N	-3.11864	-2.03090	-0.39467
N	-3.71610	0.77437	-0.20884
N	-1.95635	-0.17638	-2.28097
Si	1.35476	-1.31773	0.07604
Si	0.77212	1.68325	0.36988
O	1.67558	0.28611	0.38157
C	-4.53384	-1.57950	-0.35758
H	-5.14994	-2.30730	0.18436
H	-4.93068	-1.54942	-1.37571
C	-4.68462	-0.20973	0.31881
H	-5.72193	0.14558	0.20133
H	-4.47219	-0.31205	1.38411
C	-3.96807	1.13156	-1.62843
H	-4.40600	2.13553	-1.69558
H	-4.71407	0.45082	-2.04588
C	-2.68458	1.09445	-2.45798
H	-2.92211	1.27818	-3.51915
H	-2.00910	1.87811	-2.10999
C	-2.69422	-1.36756	-2.76698
H	-2.24623	-1.73956	-3.69692
H	-3.71955	-1.08611	-3.01900
C	-2.67889	-2.49214	-1.73077
H	-3.29935	-3.33189	-2.08515
H	-1.65232	-2.84197	-1.60427
C	-2.85612	-3.08550	0.60932
H	-3.19735	-2.74066	1.58468
H	-1.77831	-3.24415	0.66748
H	-3.36922	-4.02098	0.33657
C	-3.66310	1.99167	0.63026
H	-4.63406	2.51089	0.63026
H	-2.88086	2.64348	0.24029
H	-3.38265	1.71266	1.64559
C	-0.61681	-0.10058	-2.89494
H	-0.68976	0.07546	-3.97941
H	-0.08492	-1.03175	-2.70756
H	-0.05875	0.71237	-2.43115
C	1.89366	-2.37757	1.51736
C	1.00387	-2.61039	2.58324
H	0.00577	-2.18228	2.55033
C	1.39246	-3.37366	3.68573
H	0.69417	-3.53815	4.50298
C	2.67542	-3.92512	3.73904
H	2.97778	-4.52130	4.59677
C	3.56922	-3.70962	2.68739
H	4.56756	-4.13908	2.72406
C	3.17903	-2.94209	1.58767
H	3.88139	-2.78694	0.77146
C	2.30272	-1.76907	-1.48131
C	2.46329	-3.11277	-1.86578
H	2.10165	-3.90562	-1.21351
C	3.09387	-3.45245	-3.06481
H	3.21143	-4.49768	-3.34093
C	3.57778	-2.44770	-3.90694
H	4.06986	-2.70926	-4.84063
C	3.43259	-1.10699	-3.54171
H	3.81253	-0.32064	-4.18972
C	2.80327	-0.77430	-2.34027
H	2.69692	0.27147	-2.06642
C	1.51943	2.80847	-0.93479
C	0.70666	3.64829	-1.71603
H	-0.36902	3.64689	-1.55322
C	1.25351	4.47905	-2.69715
H	0.60699	5.12177	-3.29027
C	2.63277	4.48072	-2.91780
H	3.06187	5.12310	-3.68283
C	3.45973	3.65398	-2.15230
H	4.53369	3.65164	-2.32192
C	2.90640	2.83041	-1.16991
H	3.55723	2.18435	-0.58504
C	0.86280	2.43243	2.07644
C	0.86320	1.60518	3.21445
H	0.83784	0.52576	3.09713
C	0.88764	2.15390	4.49684
H	0.88525	1.49959	5.36502
C	0.91441	3.54112	4.66478
H	0.93484	3.96841	5.66459
C	0.91979	4.37809	3.54654
H	0.94795	5.45780	3.67332
C	0.89563	3.82472	2.26448
H	0.91248	4.48531	1.39947
Cl	-2.00349	-0.42286	2.37556

^{6}FeFMe3TACNOSiPh22O
Charge: 0
Energy: -2269027.2979663

Fe	1.68593	0.02774	0.03830
O	0.49452	1.44428	-0.30341
O	0.56443	-1.48733	-0.05191
N	3.39957	1.51691	-0.38323
N	3.55673	-1.32591	-0.02364
N	2.08159	-0.23952	-2.23870
Si	-1.11050	1.51472	0.03774
Si	-1.02884	-1.53666	0.32980
O	-1.71975	-0.02508	0.21582
C	4.72247	0.86652	-0.22803
H	5.41453	1.52907	0.30774
H	5.16479	0.70262	-1.21394
C	4.60951	-0.45642	0.53876
H	5.58866	-0.96318	0.55558
H	4.30325	-0.24432	1.56430
C	3.83559	-1.80289	-1.39842
H	4.10766	-2.86632	-1.38740
H	4.70542	-1.27390	-1.79640
C	2.62241	-1.61183	-2.31590
H	2.89284	-1.88269	-3.35010
H	1.81708	-2.26863	-1.98085
C	3.00873	0.80639	-2.73663
H	2.66817	1.18721	-3.70775
H	3.99291	0.36536	-2.91458
C	3.11121	1.97916	-1.75495
H	3.87004	2.69632	-2.10979
H	2.14429	2.48395	-1.70520
C	3.20513	2.59541	0.60681
H	3.34718	2.17606	1.60283
H	2.17367	2.94309	0.53926
H	3.90626	3.42645	0.43318
C	3.23760	-2.44104	0.89064
H	4.11480	-3.08705	1.05145
H	2.41227	-3.01317	0.46728
H	2.89449	-2.01929	1.83583
C	0.76968	-0.15074	-2.91120
H	0.86144	-0.36789	-3.98676
H	0.36277	0.84971	-2.76468
H	0.08840	-0.86521	-2.44951
C	-1.32221	2.48846	1.61954
C	-0.34182	2.36042	2.62408
H	0.51710	1.71355	2.46011
C	-0.46804	3.04702	3.83278
H	0.29260	2.93299	4.60190
C	-1.56820	3.87969	4.05709
H	-1.66359	4.41599	4.99836
C	-2.54629	4.02019	3.07028
H	-3.40385	4.66682	3.24086
C	-2.42229	3.32722	1.86352
H	-3.18933	3.44564	1.10097
C	-2.03788	2.26875	-1.40759
C	-2.06416	3.65810	-1.62418
H	-1.60220	4.32410	-0.89782
C	-2.68616	4.20327	-2.74963
H	-2.70019	5.28084	-2.89539
C	-3.29335	3.36281	-3.68626
H	-3.77892	3.78465	-4.56299
C	-3.27935	1.97954	-3.48961
H	-3.75572	1.32190	-4.21306
C	-2.65974	1.44067	-2.36005

H	-2.66130	0.36382	-2.21047
C	-1.92163	-2.58730	-0.94249
C	-1.25961	-3.65079	-1.58099
H	-0.22611	-3.86793	-1.31826
C	-1.90112	-4.42636	-2.54888
H	-1.37130	-5.24392	-3.03239
C	-3.22565	-4.14932	-2.89773
H	-3.72775	-4.75044	-3.65186
C	-3.90190	-3.09615	-2.27687
H	-4.93136	-2.87530	-2.54853
C	-3.25361	-2.32383	-1.31000
H	-3.78138	-1.49601	-0.84230
C	-1.22061	-2.17638	2.07555
C	-0.30913	-1.74864	3.06164
H	0.49785	-1.07042	2.79368
C	-0.43270	-2.18707	4.38092
H	0.27411	-1.84435	5.13330
C	-1.46112	-3.06454	4.73715
H	-1.55493	-3.40602	5.76542
C	-2.36747	-3.50317	3.76958
H	-3.16695	-4.18816	4.04216
C	-2.24502	-3.06083	2.45005
H	-2.95368	-3.41228	1.70248
F	2.06602	0.19879	1.85369

$^{6}FeN_3Me3TACNOSiPh22O$
Charge: 0
Energy: -2309409.8609088

Fe	-1.58638	-0.08796	-0.51189
O	-0.08570	0.75030	-1.30973
O	-1.00004	-0.37490	1.26747
N	-2.86023	0.73854	-2.27579
N	-3.79270	-0.50112	0.14423
N	-2.37937	2.01235	0.26748
Si	1.47792	0.82742	-0.81643
Si	0.57014	-0.65142	1.65421
O	1.60913	0.29852	0.75975
C	-4.28500	0.33938	-2.15289
H	-4.67216	0.00467	-3.12350
H	-4.88308	1.21133	-1.87652
C	-4.47825	-0.78978	-1.13127
H	-5.55590	-0.96874	-0.97981
H	-4.02502	-1.70297	-1.52145
C	-4.37254	0.65105	0.87816
H	-4.94523	0.30005	1.74625
H	-5.09091	1.16480	0.23428
C	-3.29109	1.62087	1.35823
H	-3.76644	2.50073	1.82441
H	-2.66806	1.12235	2.10378
C	-3.03062	2.76527	-0.82917
H	-2.74312	3.82389	-0.79209
H	-4.11526	2.74538	-0.69704
C	-2.64030	2.19870	-2.19615
H	-3.18994	2.72996	-2.99104
H	-1.56902	2.34959	-2.34669
C	-2.24671	0.19214	-3.50294
H	-2.40987	-0.88584	-3.52724
H	-1.17144	0.37282	-3.46019
H	-2.67714	0.65770	-4.40342
C	-3.72626	-1.69632	1.00828
H	-4.73376	-2.04162	1.28861
H	-3.14824	-1.44408	1.89799
H	-3.18963	-2.48328	0.47719
C	-1.22065	2.75218	0.79755
H	-1.53869	3.67072	1.31591
H	-0.55398	3.01023	-0.02389
H	-0.67785	2.10863	1.48908
C	2.52737	-0.25320	-1.92243
C	1.91930	-1.21965	-2.73924
H	0.83681	-1.26155	-2.79036
C	2.68150	-2.13586	-3.46548
H	2.18615	-2.89284	-4.06723
C	4.07535	-2.08835	-3.39558
H	4.67386	-2.80296	-3.95548
C	4.70191	-1.12090	-2.60359
H	5.78735	-1.07884	-2.55286
C	3.93248	-0.21345	-1.87368
H	4.43092	0.53193	-1.25655
C	2.10976	2.59375	-0.79042
C	2.39089	3.27995	-1.98521
H	2.29303	2.76314	-2.93838
C	2.80972	4.61197	-1.97260
H	3.02423	5.12451	-2.90735
C	2.95987	5.28351	-0.75627
H	3.28820	6.32000	-0.74330
C	2.69546	4.61689	0.44286
H	2.82054	5.13354	1.39157
C	2.27635	3.28479	0.42333
H	2.07806	2.76711	1.35878
C	0.82657	-0.11402	3.43052
C	-0.21432	-0.21675	4.36982
H	-1.17514	-0.62212	4.05870
C	-0.04041	0.20215	5.69031
H	-0.85755	0.11425	6.40264
C	1.18455	0.73911	6.09491
H	1.32276	1.06795	7.12203
C	2.22995	0.85558	5.17525
H	3.18264	1.27808	5.48560
C	2.04997	0.43258	3.85667
H	2.86348	0.53711	3.14274
C	0.97605	-2.43591	1.27104
C	2.17702	-2.79607	0.63615
H	2.90398	-2.02865	0.38641
C	2.43549	-4.12281	0.28621
H	3.36052	-4.37556	-0.22543
C	1.49716	-5.11529	0.57187
H	1.69179	-6.14699	0.29011
C	0.29664	-4.77797	1.20314
H	-0.44143	-5.54800	1.41502
C	0.04000	-3.45029	1.54375
H	-0.90946	-3.19208	2.00841
N	-1.62203	-1.88721	-1.30771
N	-0.92360	-2.79219	-1.69686
N	-0.29827	-3.67640	-2.09511

$^{6}FeNCSMe3TACNOSiPh22O$
Charge: 0
Energy: -2514521.2739837

Fe	1.05403	-0.59803	-1.00136
O	0.10071	1.01312	-1.16288
O	0.00948	-1.59700	0.19836
N	2.23445	0.03389	-2.90152
N	2.29801	-2.49010	-1.53062
N	-0.15734	-1.56880	-2.71333
Si	-0.97524	1.68190	-0.11103
Si	-0.86299	-0.96359	1.44374
O	-1.31703	0.60001	1.10680
C	3.25350	-0.97995	-3.27246
H	4.19108	-0.49004	-3.56300
H	2.91513	-1.52845	-4.15518
C	3.54106	-1.94802	-2.11711
H	4.20621	-2.75426	-2.46776
H	4.05077	-1.40805	-1.31741
C	1.54495	-3.37040	-2.45847
H	1.65158	-4.42074	-2.15869
H	1.97965	-3.29802	-3.45854
C	0.05690	-3.01389	-2.49196
H	-0.45285	-3.61765	-3.26080
H	-0.38715	-3.23654	-1.51981
C	0.31438	-1.08589	-4.03564
H	-0.54040	-0.87677	-4.69069
H	0.88623	-1.87540	-4.52928
C	1.15324	0.18673	-3.89898
H	1.55521	0.47426	-4.88456
H	0.51560	0.99293	-3.53024
C	2.85144	1.34502	-2.60793
H	3.65405	1.20910	-1.88306
H	2.09487	1.99166	-2.16104
H	3.25475	1.80398	-3.52378
C	2.55602	-3.17161	-0.24444
H	3.21969	-4.03892	-0.38275
H	1.60103	-3.48367	0.17870
H	3.00508	-2.46151	0.45032
C	-1.57411	-1.21184	-2.49569
H	-2.22689	-1.74060	-3.20711
H	-1.69270	-0.13568	-2.61304
H	-1.85146	-1.47704	-1.47571
C	-0.22197	3.23387	0.60443
C	1.17329	3.30489	0.77283
H	1.79267	2.47732	0.44362
C	1.77331	4.41718	1.36458
H	2.85170	4.43831	1.49844
C	0.98360	5.49021	1.78610
H	1.44648	6.35968	2.24659
C	-0.40264	5.44484	1.61560
H	-1.01830	6.28048	1.93981
C	-0.99843	4.32442	1.03193
H	-2.07866	4.30084	0.90378
C	-2.60122	2.03035	-0.97845
C	-2.74066	3.12642	-1.84882
H	-1.91686	3.82814	-1.96603
C	-3.92561	3.34211	-2.55594
H	-4.01497	4.19828	-3.22033
C	-4.99806	2.45915	-2.40447
H	-5.92212	2.62538	-2.95288
C	-4.88191	1.36702	-1.54070
H	-5.71654	0.68170	-1.41312
C	-3.69560	1.15825	-0.83421
H	-3.61805	0.30990	-0.15924
C	-2.43650	-1.97153	1.59099
C	-2.46639	-3.32064	1.19614
H	-1.56009	-3.78124	0.80814
C	-3.63831	-4.07543	1.28645
H	-3.64095	-5.11820	0.97757
C	-4.80936	-3.48718	1.77038
H	-5.72421	-4.07060	1.83883

C	-4.80257	-2.14632	2.16424
H	-5.71322	-1.68461	2.53794
C	-3.62625	-1.39913	2.07658
H	-3.63197	-0.35361	2.37595
C	0.16267	-0.94589	3.00120
C	1.04652	0.12160	3.24322
H	1.06690	0.97267	2.56828
C	1.90914	0.10481	4.33937
H	2.59753	0.93063	4.49442
C	1.89297	-0.97833	5.22242
H	2.56500	-0.99325	6.07708
C	1.01122	-2.04062	5.00781
H	0.99055	-2.88005	5.69893
C	0.15577	-2.02288	3.90387
H	-0.52918	-2.85444	3.74670
N	2.59360	-0.02718	0.15703
C	3.43769	0.49855	0.81229
S	4.58501	1.23235	1.67727

^{6}FeOHMe3TACNOSiPh22O
Charge: 0
Energy: -2253935.7202243

Fe	-1.59612	-0.47668	0.28243
O	-0.04534	-1.50977	-0.14817
O	-1.05406	1.27236	-0.26556
N	-2.75205	-2.46898	0.39038
N	-3.83043	0.19462	0.32059
N	-2.36076	-0.81667	-1.93629
Si	1.51757	-1.04204	-0.21159
Si	0.48894	1.78811	-0.08900
O	1.61087	0.61261	-0.45343
C	-4.18708	-2.24471	0.68961
H	-4.53529	-2.95838	1.44735
H	-4.78001	-2.44386	-0.20683
C	-4.44088	-0.82159	1.20053
H	-5.52529	-0.65727	1.31913
H	-3.95358	-0.70546	2.17051
C	-4.41958	0.25841	-1.03650
H	-5.04237	1.15638	-1.14358
H	-5.09150	-0.59148	-1.18101
C	-3.33271	0.27659	-2.11578
H	-3.80222	0.24679	-3.11404
H	-2.75992	1.20273	-2.02641
C	-2.93475	-2.17433	-2.08106
H	-2.61384	-2.62843	-3.02763
H	-4.02462	-2.10826	-2.13534
C	-2.50462	-3.08854	-0.92809
H	-3.01365	-4.06304	-1.01565
H	-1.42598	-3.24551	-0.98787
C	-2.08122	-3.22311	1.46927
H	-2.22821	-2.68904	2.40818
H	-1.01062	-3.23879	1.26125
H	-2.47595	-4.24897	1.54012
C	-3.81369	1.52007	0.96397
H	-4.83500	1.88829	1.15178
H	-3.27219	2.21212	0.31786
H	-3.26232	1.43508	1.90079
C	-1.19391	-0.63234	-2.81802
H	-1.49162	-0.63583	-3.87891
H	-0.47598	-1.43017	-2.63092
H	-0.71632	0.31571	-2.56987
C	2.35387	-1.48155	1.40519
C	1.57753	-1.55025	2.57798
H	0.50184	-1.39878	2.51814
C	2.17610	-1.77916	3.81820
H	1.56368	-1.81768	4.71612
C	3.56020	-1.95039	3.90860
H	4.02641	-2.12766	4.87507
C	4.34480	-1.89474	2.75373
H	5.42163	-2.03212	2.81942
C	3.74323	-1.66236	1.51443
H	4.36302	-1.62429	0.62055
C	2.40549	-1.79396	-1.68194
C	2.87334	-3.11971	-1.65740
H	2.77986	-3.70556	-0.74476
C	3.47180	-3.69622	-2.77989
H	3.83074	-4.72195	-2.73943
C	3.61341	-2.95155	-3.95375
H	4.08004	-3.39744	-4.82888
C	3.16107	-1.63017	-3.99716
H	3.27811	-1.04486	-4.90630
C	2.56609	-1.05874	-2.87038
H	2.22819	-0.02567	-2.90353
C	0.80567	3.17989	-1.29923
C	-0.23922	4.02878	-1.70372
H	-1.23933	3.86845	-1.30610
C	-0.01775	5.06299	-2.61519
H	-0.83865	5.70952	-2.91688
C	1.26014	5.26336	-3.14373
H	1.43572	6.06693	-3.85490
C	2.31067	4.42577	-2.75990
H	3.30458	4.57500	-3.17503
C	2.08289	3.39435	-1.84668
H	2.90111	2.73690	-1.56262
C	0.73787	2.22415	1.72292
C	1.92602	1.90502	2.40247
H	2.74291	1.43754	1.86065
C	2.05823	2.13571	3.77344
H	2.97864	1.85878	4.28081
C	1.00137	2.69692	4.49330
H	1.10034	2.87106	5.56194
C	-0.18870	3.02663	3.83770
H	-1.01567	3.46057	4.39501
C	-0.31596	2.78883	2.46734
H	-1.25263	3.02726	1.96822
O	-1.62397	-0.36659	2.16797
H	-1.10154	0.38409	2.49795

^{6}FeBNPAPh2OBrOH
Charge: 0
Energy: -3553744.6596375

Fe	-0.32011	-1.15062	-0.65425
C	0.28854	4.53447	-1.09977
H	-0.44162	3.77181	-0.80921
H	0.59396	4.32941	-2.13329
H	-0.21768	5.50687	-1.08389
C	2.48883	5.63923	-0.57346
H	2.01747	6.62720	-0.51479
H	2.83037	5.49233	-1.60562
H	3.37333	5.65205	0.07655
C	1.02710	4.79332	1.29091
H	0.36143	3.99682	1.63835
H	0.48066	5.74226	1.35393
H	1.87461	4.85067	1.98545
C	1.49983	4.53877	-0.15038
C	2.24107	3.17938	-0.24947
H	2.62030	3.06076	-1.27086
H	3.11957	3.18296	0.40567
C	1.26151	1.36294	1.20379
C	1.97568	1.70630	2.38121
H	2.72851	2.48340	2.35675
C	1.67865	1.04472	3.55585
H	2.22291	1.28813	4.46460
C	0.65861	0.08416	3.57952
H	0.36366	-0.40886	4.49947
C	0.01382	-0.20452	2.38429
C	-1.22822	-1.06979	2.39452
H	-1.21158	-1.73819	3.26527
H	-2.07181	-0.38852	2.52950
C	-0.98248	-3.23969	1.31079
H	-1.22655	-3.76755	0.38590
H	-1.46631	-3.73988	2.16265
C	0.51850	-3.23487	1.47749
C	1.14112	-4.01248	2.44215
H	0.55496	-4.64138	3.10312
C	2.53697	-3.94370	2.53638
H	3.06615	-4.53000	3.28291
C	3.24432	-3.12158	1.68331
H	4.32195	-3.05556	1.75259
C	2.53956	-2.35767	0.71210
C	4.64378	-1.45686	-0.20269
H	5.06666	-2.46572	-0.33070
H	5.01135	-1.07456	0.76162
C	5.18892	-0.55470	-1.32854
C	6.72317	-0.53611	-1.18366
H	7.17106	0.08336	-1.96887
H	7.14615	-1.54459	-1.27243
H	7.02972	-0.12224	-0.21466
C	4.64688	0.87706	-1.17766
H	3.56301	0.91155	-1.30569
H	5.09258	1.53471	-1.93337
H	4.88768	1.28576	-0.18782
C	4.81956	-1.12741	-2.71039
H	3.73842	-1.15207	-2.87421
H	5.20842	-2.14688	-2.82552
H	5.25604	-0.50930	-3.50375
C	-2.84371	-1.76296	0.64425
H	-3.57408	-1.89498	1.45340
H	-2.95900	-2.57834	-0.07093
C	-3.05436	-0.43130	-0.15094
C	-3.29200	0.78063	0.77870
C	-2.44143	1.88834	0.70058
H	-1.62782	1.86121	-0.01277
C	-2.63057	2.99122	1.53587
H	-1.96244	3.84453	1.45568
C	-3.67072	3.00114	2.46636
H	-3.81539	3.85744	3.11986
C	-4.53185	1.90325	2.54468
H	-5.35299	1.90298	3.25710
C	-4.34759	0.80657	1.70182
H	-5.03974	-0.02899	1.75918
C	-4.26856	-0.57740	-1.08789
C	-5.41825	-1.29735	-0.73700
H	-5.48047	-1.80775	0.22003
C	-6.50336	-1.38034	-1.61330
H	-7.38460	-1.94793	-1.32498

C	-6.45429	-0.74231	-2.85298
H	-7.29743	-0.80711	-3.53570
C	-5.31005	-0.02453	-3.21058
H	-5.25844	0.47179	-4.17637
C	-4.22644	0.05606	-2.33641
H	-3.32820	0.59764	-2.61194
N	1.41628	2.01940	0.02800
H	0.94480	1.60070	-0.76799
N	0.34738	0.35859	1.20836
N	-1.46075	-1.85062	1.16053
N	1.18703	-2.42020	0.63415
N	3.19005	-1.53911	-0.15035
H	2.63757	-1.12120	-0.89415
O	-1.90876	-0.21697	-0.91918
O	-0.67893	-2.74543	-1.53998
H	-1.28719	-2.57264	-2.27813
Br	1.03969	-0.02644	-2.54914

^{6}FeBNPAPh2OClCl
Charge: 0
Energy: -2468431.0874273

Fe	-0.21859	-1.07048	-0.56993
Cl	-0.65357	-3.12440	-1.61540
Cl	1.07196	-0.17606	-2.32623
C	0.42887	4.37995	-1.68423
H	-0.28090	3.61489	-1.35163
H	0.80526	4.08190	-2.67067
H	-0.12312	5.31955	-1.80388
C	2.54199	5.64790	-1.16628
H	2.02340	6.61006	-1.24921
H	2.95397	5.40413	-2.15343
H	3.38232	5.78014	-0.47254
C	1.00814	4.94097	0.69798
H	0.35034	4.15984	1.09226
H	0.42480	5.86669	0.62231
H	1.80713	5.10959	1.43071
C	1.57918	4.55199	-0.67626
C	2.38510	3.22914	-0.57876
H	2.82855	3.01657	-1.55802
H	3.22327	3.35163	0.11653
C	1.37796	1.56482	1.02488
C	2.04216	2.05395	2.18076
H	2.79715	2.82371	2.08921
C	1.70206	1.54168	3.41531
H	2.21082	1.89788	4.30714
C	0.68402	0.58415	3.51675
H	0.35310	0.20647	4.47801
C	0.08299	0.15040	2.34366
C	-1.16369	-0.69994	2.42299
H	-1.17941	-1.25246	3.37115
H	-2.00401	-0.00285	2.44634
C	-0.88238	-2.98142	1.64248
H	-1.16620	-3.66139	0.83590
H	-1.32908	-3.33663	2.58246
C	0.62400	-2.95900	1.74419
C	1.28498	-3.65345	2.74526
H	0.72457	-4.20751	3.49018
C	2.68479	-3.60705	2.76003
H	3.24315	-4.13142	3.53084
C	3.35845	-2.88727	1.79506
H	4.43927	-2.83826	1.80000
C	2.61698	-2.20184	0.79358
C	4.68236	-1.47432	-0.34220
H	5.05724	-2.50866	-0.38771
H	5.14047	-1.00470	0.54151
C	5.16195	-0.72625	-1.60339
C	6.70214	-0.77583	-1.59565
H	7.10315	-0.26267	-2.47696
H	7.06936	-1.80943	-1.61555
H	7.11490	-0.28471	-0.70532
C	4.70083	0.74158	-1.56555
H	3.61215	0.82035	-1.59701
H	5.10090	1.28777	-2.42807
H	5.05319	1.24195	-0.65436
C	4.63969	-1.41931	-2.87694
H	3.54826	-1.39523	-2.94593
H	4.96134	-2.46755	-2.91010
H	5.03541	-0.91776	-3.76790
C	-2.75861	-1.62488	0.77072
H	-3.48759	-1.68025	1.58969
H	-2.86152	-2.50700	0.13797
C	-2.98030	-0.37874	-0.14950
C	-3.26075	0.91576	0.64663
C	-2.42228	2.02493	0.48706
H	-1.58378	1.94527	-0.19323
C	-2.65324	3.19961	1.20595
H	-1.99415	4.05202	1.06462
C	-3.72312	3.28172	2.09832
H	-3.90073	4.19457	2.66067
C	-4.57092	2.18211	2.25651
H	-5.41441	2.23676	2.94001
C	-4.34491	1.01215	1.53074
H	-5.02618	0.17423	1.64769
C	-4.15756	-0.63886	-1.10541
C	-5.30792	-1.33242	-0.70840
H	-5.38828	-1.74340	0.29416
C	-6.36892	-1.51867	-1.59759
H	-7.25178	-2.06407	-1.27392
C	-6.29234	-1.01345	-2.89574
H	-7.11604	-1.16030	-3.58932
C	-5.14509	-0.32582	-3.29875
H	-5.07031	0.06229	-4.31126
C	-4.08565	-0.14031	-2.41127
H	-3.18388	0.37400	-2.72380
N	1.59564	2.06865	-0.21313
H	1.16432	1.55160	-0.97464
N	0.45710	0.56823	1.11855
N	-1.37332	-1.63458	1.29362
N	1.25905	-2.23842	0.79483
N	3.23511	-1.48693	-0.17603
H	2.64941	-1.11609	-0.91945
O	-1.81073	-0.21171	-0.89647

^{6}FeBNPAPh2OClOH
Charge: 0
Energy: -2227218.7154508

Fe	0.05994	-0.98595	-0.76447
Cl	1.56719	0.18597	-2.20878
C	0.12009	3.60832	-2.02071
H	-0.37933	2.67405	-1.74287
H	0.95603	3.34576	-2.67969
H	-0.59043	4.21237	-2.59741
C	1.25006	5.71451	-1.22188
H	0.51773	6.35207	-1.73076
H	2.08207	5.54180	-1.91584
H	1.63813	6.27391	-0.36039
C	-0.59243	4.68246	0.13715
H	-1.04053	3.75820	0.50844
H	-1.36660	5.23993	-0.40410
H	-0.29068	5.28398	1.00451
C	0.60293	4.38809	-0.78431
C	1.68795	3.56796	-0.03202
H	2.58923	3.53616	-0.65539
H	1.97352	4.08265	0.89263
C	0.66350	1.70277	1.32722
C	0.40416	2.48277	2.48103
H	0.74911	3.50710	2.53224
C	-0.33178	1.93202	3.51117
H	-0.56176	2.52698	4.39089
C	-0.79983	0.62075	3.40399
H	-1.42227	0.17626	4.17221
C	-0.47859	-0.09623	2.25690
C	-0.91543	-1.54481	2.18355
H	-0.17441	-2.13043	2.73832
H	-1.86897	-1.65714	2.71232
C	-0.40885	-3.46969	0.78682
H	-0.56073	-3.85430	-0.22418
H	-0.87722	-4.14783	1.51522
C	1.07574	-3.35340	1.04443
C	1.72995	-4.24870	1.87978
H	1.18175	-5.05141	2.36079
C	3.10254	-4.06400	2.09132
H	3.65175	-4.73438	2.74716
C	3.75823	-3.01842	1.47426
H	4.81558	-2.85780	1.63931
C	3.02623	-2.14890	0.61770
C	5.05795	-0.86199	0.05607
H	5.61685	-1.78189	-0.17617
H	5.31160	-0.58664	1.09144
C	5.55335	0.25288	-0.88935
C	7.05963	0.43386	-0.61829
H	7.47382	1.20731	-1.27491
H	7.61422	-0.49429	-0.80499
H	7.24654	0.73952	0.41876
C	4.82412	1.57682	-0.59793
H	3.75614	1.50446	-0.81336
H	5.23601	2.38031	-1.22018
H	4.93731	1.86848	0.45351
C	5.34992	-0.15653	-2.36076
H	4.29288	-0.28656	-2.60952
H	5.87319	-1.09580	-2.57983
H	5.75297	0.61530	-3.02703
C	-2.37635	-2.10891	0.23255
H	-3.12160	-2.51887	0.92637
H	-2.32467	-2.76277	-0.63716
C	-2.75450	-0.69031	-0.30213
C	-3.25117	0.26388	0.79688
C	-2.92645	1.62261	0.70168
H	-2.30737	1.94394	-0.12765
C	-3.37070	2.53300	1.65902
H	-3.10278	3.58202	1.56837
C	-4.14956	2.10185	2.73543
H	-4.48975	2.81048	3.48604
C	-4.49491	0.75377	2.83286
H	-5.11183	0.40494	3.65736
C	-4.05489	-0.15455	1.86636

H	-4.35658	-1.19449	1.95095
C	-3.82094	-0.89251	-1.40199
C	-5.18360	-0.64178	-1.21808
H	-5.54424	-0.25278	-0.27173
C	-6.09340	-0.87275	-2.25518
H	-7.14947	-0.66788	-2.09721
C	-5.64920	-1.35428	-3.48579
H	-6.35634	-1.53008	-4.29261
C	-4.28653	-1.60644	-3.67515
H	-3.92920	-1.97944	-4.63185
C	-3.37768	-1.37719	-2.64416
H	-2.31833	-1.57497	-2.78359
N	1.34662	2.18608	0.25694
H	1.39523	1.55782	-0.54074
N	0.25109	0.40757	1.24537
N	-1.01902	-2.12408	0.82773
N	1.69146	-2.32245	0.42799
N	3.62901	-1.12566	-0.03126
H	3.06021	-0.61626	-0.70329
O	-1.59921	-0.16064	-0.89963
O	-0.18934	-2.43979	-1.92188
H	0.63911	-2.68503	-2.36475

^{6}FeBNPAPh2OFOH
Charge: 0
Energy: -2001100.1346932

Fe	-0.20202	-0.95212	0.54196
C	-1.41454	3.42651	2.12669
H	-0.97963	2.42609	2.03762
H	-2.46706	3.30367	2.41297
H	-0.90444	3.94964	2.94443
C	-1.98716	5.59305	0.98147
H	-1.52400	6.16761	1.79228
H	-3.05084	5.47256	1.22330
H	-1.91488	6.19176	0.06410
C	0.18847	4.43983	0.46834
H	0.69247	3.48389	0.30493
H	0.70639	4.96126	1.28224
H	0.30279	5.04078	-0.44282
C	-1.29390	4.22909	0.81700
C	-2.01337	3.46849	-0.33010
H	-3.07387	3.36648	-0.06651
H	-1.98316	4.06649	-1.24679
C	-0.56953	1.78786	-1.52149
C	-0.08448	2.67184	-2.51786
H	-0.42472	3.69869	-2.55149
C	0.85208	2.21170	-3.42320
H	1.24860	2.88468	-4.17871
C	1.30300	0.89096	-3.35192
H	2.06255	0.51311	-4.02631
C	0.78365	0.08395	-2.34666
C	1.17986	-1.37675	-2.29705
H	0.48373	-1.91652	-2.94911
H	2.18191	-1.50143	-2.72560
C	0.49926	-3.35214	-1.05045
H	0.58343	-3.80705	-0.06031
H	1.00731	-3.98889	-1.78956
C	-0.97592	-3.22674	-1.36417
C	-1.63134	-4.12109	-2.19830
H	-1.08284	-4.91061	-2.70038
C	-3.01668	-3.96694	-2.36015
H	-3.56695	-4.63810	-3.01446
C	-3.68634	-2.95943	-1.69413
H	-4.75321	-2.82061	-1.81986
C	-2.95064	-2.08446	-0.84938
C	-4.96323	-0.97836	0.08624
H	-5.39374	-1.98100	0.22710
H	-5.45413	-0.53880	-0.79646
C	-5.30134	-0.12535	1.33143
C	-6.83408	-0.12567	1.47842
H	-7.13539	0.47159	2.34652
H	-7.22088	-1.14228	1.62180
H	-7.32111	0.30166	0.59267
C	-4.80540	1.32292	1.15342
H	-3.71412	1.37074	1.15078
H	-5.15648	1.94727	1.98392
H	-5.17774	1.76140	0.21900
C	-4.65608	-0.73638	2.59167
H	-3.56307	-0.69486	2.54672
H	-4.95672	-1.78349	2.72053
H	-4.97392	-0.18232	3.48309
C	2.38120	-2.01042	-0.20045
H	3.22236	-2.35659	-0.81559
H	2.24225	-2.72250	0.61307
C	2.65322	-0.62831	0.47913
C	3.26891	0.42422	-0.46405
C	2.91819	1.76476	-0.26242
H	2.20778	1.99088	0.52307
C	3.44691	2.77388	-1.06331
H	3.14452	3.80430	-0.89533
C	4.34856	2.46220	-2.08422
H	4.75912	3.24702	-2.71420
C	4.71799	1.13246	-2.28690
H	5.42073	0.87461	-3.07553
C	4.18338	0.12278	-1.48197
H	4.48386	-0.90401	-1.66919
C	3.62100	-0.90455	1.65268
C	4.94578	-1.30895	1.44227
H	5.34282	-1.36842	0.43368
C	5.77559	-1.61883	2.52070
H	6.80115	-1.92994	2.33789
C	5.29472	-1.52280	3.82861
H	5.94207	-1.76035	4.66873
C	3.97864	-1.11191	4.04619
H	3.59540	-1.02475	5.05993
C	3.14724	-0.80775	2.96591
H	2.12703	-0.47550	3.12322
N	-1.50555	2.13722	-0.59991
H	-1.64212	1.43681	0.13090
N	-0.12651	0.50286	-1.45417
N	1.11322	-2.01047	-0.96285
N	-1.60432	-2.22038	-0.72860
N	-3.53265	-1.09636	-0.13582
H	-2.90102	-0.56354	0.46450
O	1.43786	-0.15396	0.97750
O	-0.14497	-2.40851	1.71815
H	0.51951	-2.24699	2.40799
F	-1.56258	0.17251	1.26696

^{6}FeBNPAPh2ON$_3$OH
Charge: 0
Energy: -2041479.0302821

Fe	0.36245	0.30787	0.11460
C	-3.76619	-0.74053	-3.23883
H	-2.67718	-0.71745	-3.12542
H	-4.14536	0.26810	-3.03648
H	-3.99316	-0.98015	-4.28443
C	-5.93879	-1.75799	-2.47575
H	-6.21236	-2.00811	-3.50736
H	-6.35289	-0.76659	-2.25226
H	-6.42751	-2.48565	-1.81475
C	-3.86708	-3.17702	-2.63105
H	-2.78349	-3.22894	-2.48243
H	-4.07411	-3.42916	-3.67789
H	-4.33457	-3.94742	-2.00489
C	-4.40999	-1.77684	-2.29931
C	-4.10576	-1.40864	-0.82138
H	-4.55346	-0.43017	-0.60730
H	-4.59309	-2.12464	-0.15034
C	-1.90312	-2.27511	0.03329
C	-2.37420	-3.55889	0.42220
H	-3.41054	-3.82980	0.26910
C	-1.49036	-4.45466	0.98892
H	-1.84159	-5.43776	1.29150
C	-0.14749	-4.09542	1.18045
H	0.56526	-4.77239	1.63851
C	0.24171	-2.82906	0.76946
C	1.65072	-2.31990	0.95265
H	2.24437	-3.01108	1.56962
H	2.12963	-2.23764	-0.02347
C	1.06140	-0.99498	2.92105
H	1.58178	-0.23535	3.51490
H	1.24568	-1.96240	3.40690
C	-0.41700	-0.64990	2.96807
C	-1.25660	-1.13217	3.96210
H	-0.90348	-1.86223	4.68243
C	-2.56821	-0.63460	4.00047
H	-3.26249	-0.99467	4.75532
C	-2.97813	0.33775	3.10514
H	-3.97292	0.76212	3.16154
C	-2.05886	0.78775	2.12426
C	-3.50638	2.60047	1.24643
H	-3.50018	3.26538	2.12697
H	-4.38808	1.95296	1.33819
C	-3.65711	3.44902	-0.03687
C	-4.90161	4.33809	0.13925
H	-5.07467	4.93615	-0.76266
H	-4.78307	5.03005	0.98234
H	-5.80152	3.73557	0.31839
C	-3.85243	2.52081	-1.24813
H	-3.02896	1.80805	-1.33200
H	-3.89992	3.09680	-2.17888
H	-4.78730	1.95208	-1.15503
C	-2.41986	4.34435	-0.24889
H	-1.51251	3.76740	-0.45382
H	-2.23443	4.97165	0.63226
H	-2.57838	5.00570	-1.10810
C	2.90131	-0.24275	1.44931
H	3.71791	-0.80116	1.92769
H	2.75789	0.69711	1.98577
C	3.21337	0.09962	-0.05851
C	4.17583	-0.92634	-0.70078
C	3.84755	-1.48850	-1.94046
H	2.91315	-1.19707	-2.40708
C	4.69945	-2.41054	-2.55239
H	4.42518	-2.83777	-3.51375

C	5.89586	-2.78249	-1.93724
H	6.55864	-3.50078	-2.41264
C	6.23692	-2.21804	-0.70595
H	7.16916	-2.49280	-0.21873
C	5.38499	-1.29631	-0.09635
H	5.67956	-0.85677	0.85245
C	3.85872	1.49969	-0.14131
C	4.82877	1.93582	0.76998
H	5.15426	1.28597	1.57821
C	5.38549	3.21193	0.66357
H	6.13344	3.53411	1.38375
C	4.97947	4.07233	-0.35815
H	5.40926	5.06720	-0.43894
C	4.01506	3.64367	-1.27273
H	3.68832	4.30406	-2.07193
C	3.46085	2.36669	-1.16671
H	2.70644	2.03022	-1.86969
N	-2.69980	-1.30662	-0.48198
H	-2.19728	-0.49626	-0.84876
N	-0.59818	-1.94324	0.20285
N	1.62047	-0.97008	1.55467
N	-0.82519	0.23074	2.04411
N	-2.31550	1.76869	1.22132
H	-1.45953	2.17514	0.82851
O	2.01145	0.10077	-0.76334
O	0.44234	2.14452	0.56076
H	1.03488	2.63313	-0.03534
N	-0.76202	0.51539	-1.55690
N	-0.60964	1.52938	-2.20654
N	-0.48084	2.48638	-2.83804

^{6}FeBNPAPh2ONCSOH
Charge: 0
Energy: -2246584.0903507

Fe	-0.25288	-1.00336	0.01063
C	1.69934	3.19156	-2.48079
H	0.85125	2.60545	-2.11274
H	2.29440	2.53720	-3.12909
H	1.30070	4.00371	-3.10016
C	3.68478	4.61984	-1.88472
H	3.28939	5.45543	-2.47386
H	4.33834	4.03013	-2.53955
H	4.30175	5.04052	-1.07994
C	1.63854	4.62474	-0.42011
H	0.80204	4.04522	-0.01520
H	1.21801	5.46059	-0.99260
H	2.19800	5.04512	0.42476
C	2.53768	3.76109	-1.32218
C	3.18344	2.60107	-0.51375
H	3.84301	2.03555	-1.18169
H	3.82258	3.01228	0.27501
C	1.59926	1.77098	1.24524
C	2.08490	2.58732	2.30185
H	2.99931	3.15252	2.17472
C	1.38396	2.63880	3.48797
H	1.75187	3.24884	4.30883
C	0.19802	1.90588	3.62655
H	-0.38915	1.94131	4.53783
C	-0.22096	1.14078	2.54624
C	-1.57443	0.47768	2.58490
H	-1.92241	0.38494	3.62458
H	-2.26681	1.14715	2.07412
C	-1.15940	-1.90071	2.81912
H	-1.44744	-2.86261	2.38143
H	-1.62216	-1.82672	3.81481
C	0.35072	-1.89107	2.91697
C	1.04677	-2.07100	4.10220
H	0.52288	-2.14299	5.04895
C	2.44637	-2.15709	4.02384
H	3.03360	-2.27892	4.93014
C	3.08467	-2.12364	2.79680
H	4.15881	-2.24124	2.72378
C	2.30002	-1.96975	1.62516
C	4.16592	-2.35924	0.04547
H	4.38764	-3.39174	0.36556
H	4.83395	-1.69468	0.60882
C	4.47976	-2.21169	-1.46056
C	5.93361	-2.67130	-1.67472
H	6.21733	-2.56100	-2.72744
H	6.06539	-3.72559	-1.40094
H	6.63332	-2.07446	-1.07565
C	4.33534	-0.73937	-1.88322
H	3.32211	-0.37949	-1.69502
H	4.54295	-0.62218	-2.95249
H	5.03562	-0.10394	-1.32561
C	3.53862	-3.09515	-2.30393
H	2.49347	-2.77438	-2.24090
H	3.59359	-4.14429	-1.98681
H	3.82163	-3.04376	-3.36097
C	-2.98507	-1.09982	1.35363
H	-3.76946	-0.76765	2.04719
H	-3.08046	-2.17858	1.21305
C	-3.11400	-0.45452	-0.06338
C	-3.29541	1.08060	-0.00176
C	-2.31595	1.91995	-0.54698
H	-1.45598	1.47737	-1.03542
C	-2.43744	3.30812	-0.44709
H	-1.66288	3.94306	-0.87003
C	-3.54106	3.87597	0.19080
H	-3.63321	4.95580	0.27198
C	-4.53478	3.04439	0.71611
H	-5.40650	3.47556	1.20189
C	-4.41544	1.65832	0.61348
H	-5.20132	1.02214	1.01183
C	-4.30493	-1.06291	-0.82306
C	-5.47836	-1.49021	-0.18927
H	-5.57709	-1.43109	0.89114
C	-6.54369	-2.00498	-0.93375
H	-7.44513	-2.33574	-0.42401
C	-6.44896	-2.09677	-2.32208
H	-7.27636	-2.49747	-2.90174
C	-5.28040	-1.67220	-2.96100
H	-5.19467	-1.74209	-4.04233
C	-4.21799	-1.16028	-2.21808
H	-3.30413	-0.83785	-2.70543
N	2.24629	1.65006	0.05810
H	1.76173	1.04660	-0.60764
N	0.45815	1.04524	1.38819
N	-1.63982	-0.83852	1.91477
N	0.96403	-1.77566	1.73001
N	2.78958	-2.01128	0.36011
H	2.07332	-2.27487	-0.32181
O	-1.93648	-0.75942	-0.73818
O	0.16341	-2.73241	-0.62294
H	-0.25121	-2.86067	-1.49337
N	0.69193	-0.09875	-1.56948
C	0.79854	-0.23954	-2.75222
S	0.99092	-0.40396	-4.34122

^{6}FeBNPAPh2OOHBr
Charge: 0
Energy: -3553757.0576684

Fe	0.17534	-0.76296	-0.19622
O	1.49157	0.12765	-1.26709
H	1.46194	-0.19409	-2.18209
C	1.01667	3.32124	-2.73293
H	0.49606	2.40394	-2.43827
H	2.02695	3.04218	-3.05923
H	0.49063	3.74832	-3.59480
C	1.80507	5.60930	-2.03881
H	1.27721	6.07784	-2.87762
H	2.82573	5.38191	-2.37146
H	1.87020	6.34889	-1.23024
C	-0.35628	4.69360	-1.13269
H	-0.87837	3.81250	-0.75008
H	-0.93543	5.09115	-1.97469
H	-0.35029	5.45334	-0.34082
C	1.07191	4.33776	-1.57693
C	1.87221	3.73499	-0.39080
H	2.90341	3.56019	-0.72276
H	1.93291	4.46247	0.42520
C	0.52189	2.27537	1.14800
C	0.10526	3.32200	2.01076
H	0.43947	4.33577	1.83481
C	-0.75973	3.03904	3.04733
H	-1.10159	3.83837	3.69923
C	-1.21217	1.73093	3.24082
H	-1.92023	1.48496	4.02353
C	-0.76108	0.75132	2.36684
C	-1.16840	-0.68388	2.62535
H	-0.47672	-1.07489	3.37967
H	-2.16935	-0.70149	3.07142
C	-0.48092	-2.87372	1.85252
H	-0.57131	-3.56320	1.00831
H	-0.97289	-3.32227	2.72793
C	0.98962	-2.64370	2.11553
C	1.66515	-3.31341	3.12384
H	1.13714	-3.99486	3.78181
C	3.04066	-3.07294	3.25830
H	3.60597	-3.56101	4.04782
C	3.68033	-2.21163	2.39056
H	4.73918	-2.00921	2.49119
C	2.93023	-1.57725	1.36124
C	4.93541	-0.60564	0.28827
H	5.42990	-1.58021	0.41253
H	5.32874	0.05658	1.07601
C	5.33505	-0.03977	-1.09353
C	6.87167	0.06460	-1.11490
H	7.21521	0.45323	-2.08036
H	7.34102	-0.91531	-0.96326
H	7.23697	0.74150	-0.33235
C	4.72990	1.36089	-1.31029
H	3.64034	1.31872	-1.38430
H	5.11009	1.79656	-2.24232
H	4.99535	2.03757	-0.48819
C	4.86960	-0.99223	-2.21197

H	3.78127	-1.10665	-2.22289
H	5.30736	-1.98984	-2.08613
H	5.17900	-0.60920	-3.19168
C	-2.39888	-1.78854	0.74515
H	-3.22018	-2.01159	1.43871
H	-2.25651	-2.65196	0.09387
C	-2.70780	-0.58620	-0.19964
C	-3.26400	0.65023	0.52782
C	-2.89661	1.91927	0.06377
H	-2.20124	1.97902	-0.76521
C	-3.39410	3.07307	0.66601
H	-3.08581	4.04704	0.29580
C	-4.27546	2.98081	1.74592
H	-4.66042	3.88030	2.21913
C	-4.66066	1.72263	2.20914
H	-5.35212	1.63484	3.04350
C	-4.16039	0.56775	1.60223
H	-4.48379	-0.40030	1.97384
C	-3.70523	-1.09069	-1.26750
C	-5.09343	-0.97243	-1.13444
H	-5.51984	-0.45414	-0.28236
C	-5.94788	-1.49882	-2.10705
H	-7.02349	-1.39296	-1.98888
C	-5.42551	-2.14726	-3.22617
H	-6.09059	-2.55369	-3.98395
C	-4.04035	-2.26660	-3.36555
H	-3.61940	-2.76940	-4.23250
C	-3.18617	-1.74361	-2.39537
H	-2.11156	-1.84227	-2.49822
N	1.36674	2.47001	0.10717
H	1.48794	1.66169	-0.51275
N	0.08798	0.99633	1.35156
N	-1.11587	-1.59827	1.46165
N	1.58555	-1.77354	1.27614
N	3.49983	-0.77124	0.44145
H	2.87337	-0.41823	-0.29208
O	-1.49482	-0.25305	-0.82501
Br	0.37405	-2.97812	-1.57506

^{6}FeBNPAPh2OOHCl
Charge: 0
Energy: -2227228.1477590

Fe	-0.18342	-0.89472	0.42555
C	-0.95940	3.49027	2.39401
H	-0.43110	2.55099	2.19901
H	-1.95269	3.23963	2.78851
H	-0.41341	4.03114	3.17588
C	-1.81231	5.66101	1.44474
H	-1.26247	6.24144	2.19481
H	-2.81549	5.46452	1.84367
H	-1.92135	6.28880	0.55084
C	0.33220	4.66700	0.58372
H	0.85508	3.75220	0.29267
H	0.93434	5.17297	1.34788
H	0.28463	5.32291	-0.29485
C	-1.07298	4.35085	1.12161
C	-1.90265	3.59065	0.05170
H	-2.92157	3.45646	0.43610
H	-1.99524	4.20254	-0.85169
C	-0.57783	1.94683	-1.31376
C	-0.19031	2.87220	-2.31716
H	-0.53187	3.89771	-2.27105
C	0.65716	2.46024	-3.32485
H	0.97722	3.16795	-4.08482
C	1.12054	1.14218	-3.35039
H	1.81753	0.79959	-4.10635
C	0.69566	0.28459	-2.34438
C	1.11930	-1.16727	-2.41370
H	0.42633	-1.66509	-3.10098
H	2.11641	-1.23216	-2.86419
C	0.46641	-3.23900	-1.34014
H	0.57011	-3.80097	-0.40818
H	0.95703	-3.80048	-2.14869
C	-1.00880	-3.06191	-1.62122
C	-1.68333	-3.86528	-2.52820
H	-1.15295	-4.62406	-3.09309
C	-3.06107	-3.65405	-2.68647
H	-3.62582	-4.24691	-3.40118
C	-3.70429	-2.68897	-1.93825
H	-4.76513	-2.50940	-2.05967
C	-2.95402	-1.91846	-1.00656
C	-4.95842	-0.81698	-0.06703
H	-5.45203	-1.80000	-0.05274
H	-5.35402	-0.27273	-0.93951
C	-5.35788	-0.06282	1.22157
C	-6.89462	0.04102	1.23021
H	-7.23786	0.56213	2.13123
H	-7.36248	-0.95125	1.21949
H	-7.26185	0.59958	0.36009
C	-4.75405	1.35476	1.23838
H	-3.66443	1.32328	1.31574
H	-5.13348	1.91704	2.10034
H	-5.02052	1.90875	0.32947
C	-4.88941	-0.84702	2.46265
H	-3.80012	-0.94966	2.49003
H	-5.32057	-1.85535	2.47673
H	-5.20316	-0.33298	3.37895
C	2.38259	-1.99121	-0.41622
H	3.19835	-2.30246	-1.08195
H	2.25548	-2.75676	0.34988
C	2.69188	-0.66477	0.34676
C	3.23700	0.45604	-0.55491
C	2.86568	1.77708	-0.27666
H	2.17628	1.95232	0.54074
C	3.35131	2.83380	-1.04414
H	3.03964	3.84965	-0.81673
C	4.22492	2.59010	-2.10664
H	4.60025	3.41315	-2.70912
C	4.61592	1.28004	-2.38436
H	5.30300	1.07576	-3.20179
C	4.12806	0.22310	-1.61142
H	4.45848	-0.78666	-1.83732
C	3.69664	-1.01064	1.46951
C	5.07888	-0.83186	1.34859
H	5.49635	-0.38292	0.45376
C	5.93714	-1.20916	2.38564
H	7.00827	-1.05814	2.27598
C	5.42377	-1.76682	3.55631
H	6.09157	-2.05690	4.36359
C	4.04346	-1.94645	3.68349
H	3.63023	-2.37938	4.59100
C	3.18588	-1.57203	2.65018
H	2.11458	-1.71508	2.74324
N	-1.40098	2.27320	-0.28829
H	-1.50676	1.55057	0.43257
N	-0.13716	0.65501	-1.35467
N	1.09021	-1.91517	-1.13694
N	-1.60855	-2.09296	-0.90307
N	-3.52319	-1.00043	-0.19771
H	-2.89346	-0.55140	0.47888
O	1.48454	-0.24827	0.93190
O	-1.51049	0.12204	1.37044
H	-1.46499	-0.07732	2.31899
Cl	-0.27355	-2.76708	1.91587

^{6}FeBNPAPh2OOHF
Charge: 0
Energy: -2001102.4142594

Fe	-0.20164	-0.94783	0.59745
O	-1.53625	0.15609	1.44910
H	-1.43004	0.16884	2.41262
C	-0.59320	3.45994	2.12920
H	-0.07223	2.52503	1.89680
H	-1.54213	3.20253	2.61774
H	0.01593	4.01834	2.84978
C	-1.52775	5.62471	1.24206
H	-0.89019	6.21995	1.90629
H	-2.47629	5.44291	1.76298
H	-1.74212	6.23189	0.35289
C	0.50762	4.60380	0.17851
H	0.99207	3.68438	-0.15846
H	1.18980	5.11195	0.87086
H	0.37159	5.25309	-0.69591
C	-0.83603	4.30326	0.86328
C	-1.78021	3.53626	-0.10397
H	-2.77324	3.47896	0.35875
H	-1.90766	4.10801	-1.02998
C	-0.58235	1.76068	-1.42228
C	-0.19183	2.59946	-2.49704
H	-0.51577	3.63168	-2.52727
C	0.63780	2.09268	-3.47797
H	0.96289	2.73281	-4.29384
C	1.07759	0.76836	-3.40428
H	1.76533	0.35641	-4.13402
C	0.64104	-0.00114	-2.33244
C	1.04356	-1.46081	-2.27564
H	0.34062	-2.01327	-2.90952
H	2.03802	-1.57901	-2.72242
C	0.35425	-3.39872	-0.97095
H	0.43854	-3.82490	0.03141
H	0.83084	-4.07543	-1.69515
C	-1.11646	-3.22073	-1.27791
C	-1.80003	-4.05913	-2.14661
H	-1.28233	-4.86045	-2.66245
C	-3.17055	-3.82302	-2.33492
H	-3.74132	-4.44251	-3.02188
C	-3.79923	-2.79993	-1.65356
H	-4.85388	-2.60200	-1.79954
C	-3.03891	-1.99527	-0.75931
C	-5.01329	-0.75553	0.06613
H	-5.55364	-1.71003	0.15699
H	-5.36635	-0.27595	-0.86100
C	-5.39974	0.13246	1.27047
C	-6.93062	0.29820	1.24326
H	-7.26355	0.92012	2.08210
H	-7.43937	-0.67061	1.32271

H	-7.26283	0.78150	0.31596
C	-4.73545	1.51855	1.16349
H	-3.64903	1.44607	1.25618
H	-5.09753	2.17469	1.96449
H	-4.96790	1.99607	0.20351
C	-4.97950	-0.54629	2.58867
H	-3.89350	-0.67156	2.64854
H	-5.44019	-1.53700	2.68610
H	-5.29650	0.05888	3.44640
C	2.30716	-2.10243	-0.21484
H	3.11309	-2.48707	-0.85331
H	2.17010	-2.79685	0.61212
C	2.65221	-0.71461	0.42278
C	3.26549	0.27253	-0.58547
C	2.92313	1.62603	-0.48470
H	2.21570	1.91383	0.28329
C	3.45620	2.56830	-1.36193
H	3.16580	3.61162	-1.27083
C	4.34807	2.17385	-2.36197
H	4.75897	2.90593	-3.05238
C	4.71293	0.83064	-2.46212
H	5.41614	0.51071	-3.22720
C	4.18048	-0.10988	-1.57611
H	4.49706	-1.14563	-1.65953
C	3.60568	-0.99179	1.60729
C	4.96637	-0.67492	1.60720
H	5.41282	-0.19043	0.74529
C	5.76265	-0.96414	2.72088
H	6.81900	-0.70686	2.70575
C	5.20585	-1.57159	3.84504
H	5.82475	-1.79413	4.71070
C	3.84367	-1.89102	3.85120
H	3.39900	-2.36398	4.72349
C	3.04831	-1.60255	2.74468
H	1.98992	-1.85091	2.74034
N	-1.38169	2.17560	-0.40664
H	-1.48605	1.50022	0.36030
N	-0.17653	0.46079	-1.37197
N	1.01272	-2.07584	-0.93310
N	-1.70251	-2.20135	-0.62298
N	-3.58715	-1.01413	-0.01252
H	-2.94491	-0.53492	0.63176
O	1.46589	-0.17484	0.94148
F	-0.05078	-2.37689	1.73886

^{6}FeBNPAPh2OOHN$_3$
Charge: 0
Energy: -2041487.9659605

Fe	-0.19599	-0.91483	0.29067
C	-0.97684	3.29268	2.50428
H	-0.43256	2.38179	2.23353
H	-1.96592	2.99518	2.87642
H	-0.43924	3.77679	3.32796
C	-1.84995	5.52616	1.73685
H	-1.29762	6.05089	2.52516
H	-2.84782	5.29057	2.12788
H	-1.97227	6.22094	0.89580
C	0.29708	4.62023	0.78955
H	0.82486	3.73687	0.42096
H	0.89949	5.06543	1.59057
H	0.24090	5.34662	-0.03116
C	-1.10355	4.25157	1.30550
C	-1.93430	3.57482	0.18111
H	-2.95447	3.41759	0.55338
H	-2.02288	4.25255	-0.67472
C	-0.59668	2.03415	-1.28799
C	-0.19197	3.02675	-2.21702
H	-0.53552	4.04685	-2.10711
C	0.67665	2.68400	-3.23331
H	1.01189	3.44217	-3.93589
C	1.14181	1.37041	-3.34085
H	1.85552	1.08149	-4.10352
C	0.69700	0.44625	-2.40463
C	1.11817	-1.00069	-2.55742
H	0.42166	-1.46015	-3.26768
H	2.11378	-1.04379	-3.01417
C	0.47364	-3.13131	-1.58802
H	0.57748	-3.73120	-0.67987
H	0.97100	-3.65585	-2.41685
C	-1.00351	-2.95389	-1.86754
C	-1.66846	-3.70783	-2.82289
H	-1.13071	-4.42688	-3.43114
C	-3.04809	-3.49881	-2.97225
H	-3.60527	-4.05272	-3.72324
C	-3.70352	-2.58688	-2.16943
H	-4.76606	-2.41141	-2.28241
C	-2.96211	-1.86704	-1.19133
C	-4.97532	-0.84165	-0.18401
H	-5.46117	-1.82815	-0.22053
H	-5.37686	-0.25559	-1.02593
C	-5.37557	-0.15821	1.14330
C	-6.91339	-0.07675	1.16768
H	-7.25666	0.39850	2.09364
H	-7.36754	-1.07407	1.11573
H	-7.29509	0.51506	0.32627
C	-4.79015	1.26486	1.22571
H	-3.69939	1.24361	1.28967
H	-5.16679	1.77747	2.11921
H	-5.07344	1.86085	0.34912
C	-4.88621	-0.99455	2.34183
H	-3.79423	-1.06714	2.36551
H	-5.29143	-2.01305	2.30326
H	-5.21253	-0.53748	3.28346
C	2.37507	-1.91532	-0.59186
H	3.20107	-2.18470	-1.26310
H	2.24799	-2.72050	0.13272
C	2.66723	-0.63156	0.24896
C	3.22633	0.54403	-0.57611
C	2.87817	1.84474	-0.19026
H	2.20065	1.96412	0.64695
C	3.37035	2.95238	-0.87700
H	3.07698	3.95104	-0.56457
C	4.22758	2.78263	-1.96721
H	4.60860	3.64586	-2.50655
C	4.59169	1.49354	-2.35524
H	5.26086	1.34465	-3.19915
C	4.09614	0.38505	-1.66352
H	4.39518	-0.60679	-1.98962
C	3.68446	-1.04625	1.33779
C	5.04134	-1.24577	1.05103
H	5.42704	-1.03439	0.05902
C	5.91912	-1.69536	2.03916
H	6.96931	-1.84100	1.79819
C	5.45358	-1.94913	3.33089
H	6.13741	-2.29730	4.10079
C	4.10375	-1.74748	3.62430
H	3.72432	-1.94042	4.62435
C	3.22586	-1.30032	2.63551
H	2.17994	-1.14489	2.86614
N	-1.44015	2.28357	-0.25600
H	-1.54366	1.51079	0.41266
N	-0.15552	0.74911	-1.41005
N	1.08933	-1.81465	-1.32194
N	-1.61624	-2.03559	-1.09638
N	-3.53871	-1.00624	-0.32630
H	-2.91551	-0.59529	0.37916
O	1.46148	-0.24813	0.84805
O	-1.53122	0.03852	1.30734
H	-1.44269	-0.06114	2.26825
N	-0.18855	-2.62849	1.37478
N	-0.08400	-2.54486	2.57831
N	-0.00009	-2.48056	3.73152

^{6}FeBNPAPh2OOHNCS
Charge: 0
Energy: -2246597.9302101

Fe	0.18340	-0.72494	-0.23043
C	1.12722	3.26376	-2.83822
H	0.55431	2.39323	-2.50135
H	2.10376	2.90710	-3.19079
H	0.60162	3.70560	-3.69283
C	2.08593	5.51205	-2.23283
H	1.55360	5.99750	-3.05910
H	3.07448	5.21181	-2.60256
H	2.23359	6.26165	-1.44464
C	-0.09137	4.75811	-1.22273
H	-0.65190	3.92251	-0.79521
H	-0.67811	5.17007	-2.05247
H	-0.00562	5.53620	-0.45364
C	1.29283	4.30093	-1.71157
C	2.09967	3.67466	-0.54208
H	3.10904	3.44191	-0.90417
H	2.22509	4.41014	0.25941
C	0.72124	2.30792	1.05598
C	0.38068	3.38839	1.91054
H	0.76338	4.37996	1.70900
C	-0.47222	3.16850	2.97185
H	-0.75606	3.99499	3.61765
C	-0.98728	1.88906	3.19751
H	-1.68922	1.69260	3.99945
C	-0.60757	0.87363	2.33091
C	-1.08198	-0.53308	2.62253
H	-0.38654	-0.95301	3.35772
H	-2.06760	-0.49305	3.10111
C	-0.56861	-2.77269	1.86672
H	-0.75901	-3.48521	1.06083
H	-1.06130	-3.15625	2.77204
C	0.92562	-2.66126	2.07900
C	1.57287	-3.38808	3.06687
H	1.01081	-4.03136	3.73491
C	2.96564	-3.25669	3.16682
H	3.51080	-3.79487	3.93768
C	3.64893	-2.43981	2.28887
H	4.72282	-2.32319	2.36235
C	2.92374	-1.74141	1.28393
C	4.97173	-0.89178	0.19067

H	5.40435	-1.90102	0.26177
H	5.41420	-0.29592	1.00475
C	5.39406	-0.28335	-1.16555
C	6.93384	-0.27413	-1.20074
H	7.29239	0.14244	-2.14892
H	7.34205	-1.28793	-1.10555
H	7.34785	0.33683	-0.38887
C	4.87380	1.16026	-1.30474
H	3.78283	1.18604	-1.35958
H	5.26553	1.61675	-2.22192
H	5.19152	1.77918	-0.45632
C	4.86020	-1.14638	-2.32536
H	3.76610	-1.17622	-2.33597
H	5.22430	-2.17806	-2.24875
H	5.19509	-0.74096	-3.28748
C	-2.42412	-1.56855	0.78165
H	-3.24146	-1.72757	1.49678
H	-2.36220	-2.45211	0.14594
C	-2.68043	-0.35749	-0.17068
C	-3.16958	0.90637	0.55699
C	-2.74475	2.15449	0.08552
H	-2.05753	2.17738	-0.75187
C	-3.17547	3.33306	0.69120
H	-2.82283	4.28956	0.31494
C	-4.04634	3.28700	1.78245
H	-4.37906	4.20538	2.25897
C	-4.49040	2.05054	2.25184
H	-5.17650	1.99925	3.09359
C	-4.05778	0.87077	1.64065
H	-4.43006	-0.07871	2.01415
C	-3.70603	-0.82822	-1.22682
C	-5.07641	-0.56124	-1.14365
H	-5.46609	0.05234	-0.33853
C	-5.95710	-1.06614	-2.10500
H	-7.01875	-0.84530	-2.02670
C	-5.47871	-1.84252	-3.16011
H	-6.16469	-2.23502	-3.90633
C	-4.10996	-2.11063	-3.25079
H	-3.72337	-2.71685	-4.06568
C	-3.23127	-1.60641	-2.29399
H	-2.16867	-1.81044	-2.36266
N	1.54700	2.44448	-0.00872
H	1.62098	1.61644	-0.61181
N	0.22888	1.05506	1.29126
N	-1.11545	-1.45917	1.46866
N	1.56697	-1.83545	1.22881
N	3.53015	-0.97117	0.35562
H	2.91708	-0.56931	-0.36387
O	-1.46289	-0.08142	-0.81518
O	1.55867	0.06975	-1.32127
H	1.46375	-0.20258	-2.24725
N	0.11931	-2.48870	-1.24003
C	-0.25020	-3.60913	-1.40339
S	-0.78249	-5.12554	-1.58188

^{5}FeMe2PyTACNBrOH
Charge: 0
Energy: -2937495.5418467

H	0.46136	-1.71074	3.29251
H	3.06406	-0.27195	2.52190
H	1.56529	-2.31648	2.08180
C	0.69981	-1.66535	2.22033
H	3.02262	-2.01604	0.74604
H	-0.65913	-3.26620	1.66548
C	2.48619	-0.08231	1.59956
H	1.27218	-3.35196	0.20812
H	4.08987	-0.70402	0.30556
C	0.47860	0.69383	2.75153
C	3.03312	-0.95894	0.46277
N	1.03988	-0.28787	1.81080
C	-0.49137	-2.20282	1.42197
H	2.60916	0.96967	1.32434
H	-1.38689	-1.65502	1.72351
C	0.77194	-2.82120	-0.60751
H	0.35367	-3.60082	-1.25869
H	2.64634	-2.69087	-1.67542
N	-0.31302	-1.99503	-0.02416
N	2.26236	-0.77525	-0.78287
C	1.80303	-2.01994	-1.43315
H	-2.09539	-3.02074	-0.63797
C	2.96195	0.10387	-1.73672
C	-1.58879	-2.04778	-0.75567
H	1.32528	-1.69932	-2.36057
Fe	0.22554	0.21546	-0.46580
H	-1.35418	-1.88128	-1.81270
C	-2.52015	-0.91936	-0.33649
N	-1.93921	0.23393	0.04450
H	-4.35585	-1.98986	-0.69240
C	-3.90807	-1.04609	-0.39488
C	-2.69591	1.29530	0.34970
H	-2.14042	2.19261	0.61062
C	-4.70145	0.05651	-0.07276
C	-4.08878	1.25193	0.30410
H	-5.78454	-0.01885	-0.11659
H	-4.67146	2.13221	0.55551
H	2.28527	0.29896	-2.56989
H	3.90168	-0.34835	-2.09664
H	3.16734	1.05832	-1.24639
H	-0.60321	0.54106	2.81675
H	0.65238	1.69927	2.36498
H	0.91646	0.59221	3.75914
O	-0.13161	-0.00370	-2.33313
H	-0.29827	0.85611	-2.74781
Br	0.75470	2.75924	-0.17028

^{5}FeMe2PyTACNClOH
Charge: 0
Energy: -1610965.1772385

H	0.68717	-0.92961	3.42500
H	3.12733	0.66125	2.42362
H	1.84361	-1.57560	2.28584
C	0.91712	-1.00131	2.35209
H	3.25835	-1.30377	0.89734
H	-0.27619	-2.78848	2.03261
C	2.52690	0.66156	1.49587
H	1.64892	-2.87207	0.56607
H	4.18418	0.03961	0.27058
C	0.44928	1.37359	2.56142
C	3.15931	-0.29820	0.47660
N	1.11304	0.33534	1.75984
C	-0.21629	-1.75499	1.64921
H	2.53332	1.67288	1.07840
H	-1.16133	-1.26354	1.89139
C	1.09548	-2.50465	-0.30342
H	0.75661	-3.40045	-0.84168
H	2.94675	-2.33129	-1.40538
N	-0.06553	-1.72261	0.18573
N	2.37168	-0.36179	-0.76964
C	2.04052	-1.72082	-1.24281
H	-1.74095	-2.98987	-0.25600
C	2.96661	0.45818	-1.83894
C	-1.33272	-1.99670	-0.50992
H	1.53175	-1.57679	-2.19742
Fe	0.24717	0.46031	-0.55750
H	-1.11959	-1.94894	-1.58344
C	-2.36954	-0.91810	-0.22856
N	-1.90328	0.32752	-0.02214
H	-4.09498	-2.19876	-0.39261
C	-3.73896	-1.18430	-0.23794
C	-2.75639	1.34377	0.15134
H	-2.28631	2.31609	0.27639
C	-4.63367	-0.12864	-0.05266
C	-4.13874	1.16131	0.14276
H	-5.70447	-0.31313	-0.06138
H	-4.80358	2.00734	0.28391
H	2.27223	0.46485	-2.68052
H	3.95260	0.07397	-2.15169
H	3.06020	1.48530	-1.47803
H	-0.60896	1.11444	2.66728
H	0.51009	2.32436	2.02994
H	0.89702	1.46577	3.56592
O	-0.09291	-0.06518	-2.37274
H	-0.37083	0.69739	-2.90174
Cl	0.52054	2.86642	-0.51966

^{5}FeMe2PyTACNFOH
Charge: 0
Energy: -1384834.7895075

H	0.69441	1.60250	3.10979
H	3.14696	2.19358	1.23724
H	1.87702	0.40005	2.65149
C	0.94126	0.86504	2.33117
H	3.28609	-0.29356	1.34618
H	-0.23431	-0.72847	3.23368
C	2.51629	1.58694	0.56043
H	1.74813	-1.67547	2.13082
H	4.17719	0.34380	-0.01528
C	0.43200	2.79637	0.92899
C	3.16091	0.20220	0.37850
N	1.12303	1.50695	1.02344
C	-0.17576	-0.18772	2.27212
H	2.47518	2.08365	-0.41347
H	-1.12885	0.32976	2.13312
C	1.17141	-1.98994	1.25594
H	0.85758	-3.02324	1.46290
H	2.99182	-2.56961	0.24417
N	-0.00469	-1.10064	1.13355
N	2.37210	-0.66320	-0.52066
C	2.07080	-2.00822	0.00315
H	-1.62493	-2.43948	1.58479
C	2.93472	-0.72160	-1.88010
C	-1.24211	-1.80584	0.76636
H	1.53442	-2.51783	-0.79912
Fe	0.27335	0.18139	-0.89416
H	-0.98397	-2.41766	-0.10683

C	-2.31257	-0.83342	0.30705
N	-1.88079	0.20680	-0.43309
H	-3.98937	-1.84367	1.20282
C	-3.66726	-1.00476	0.59265
C	-2.76222	1.09422	-0.91258
H	-2.32514	1.89878	-1.49837
C	-4.59028	-0.08690	0.08715
C	-4.13201	0.98553	-0.68051
H	-5.65007	-0.20460	0.29542
H	-4.81640	1.72258	-1.08847
H	2.21510	-1.24380	-2.51439
H	3.91736	-1.22403	-1.90008
H	3.03976	0.30000	-2.25671
H	-0.60959	2.66137	1.23913
H	0.43346	3.09938	-0.11893
H	0.89446	3.57077	1.56684
O	-0.01684	-1.51926	-1.90285
H	-0.83846	-1.49081	-2.41437
F	0.51126	1.76703	-1.81402

^{5}FeMe2PyTACNN$_3$OH
Charge: 0
Energy: -1425223.6165946

H	0.36640	-1.17503	3.41134
H	3.04877	-0.04931	2.49182
H	1.41825	-1.98130	2.27235
C	0.59915	-1.26217	2.33992
H	2.88644	-1.91799	0.87802
H	-0.86359	-2.82221	1.95903
C	2.48394	0.11278	1.55575
H	1.05256	-3.16975	0.50791
H	4.02677	-0.72089	0.30966
C	0.52497	1.15549	2.58148
C	2.95888	-0.89434	0.49704
N	1.02840	0.03274	1.77977
C	-0.63202	-1.80276	1.60446
H	2.70893	1.12421	1.20751
H	-1.48883	-1.17141	1.85082
C	0.57235	-2.70050	-0.35597
H	0.10344	-3.52015	-0.91763
H	2.43326	-2.79594	-1.44833
N	-0.45767	-1.75781	0.14390
N	2.18481	-0.77956	-0.75571
C	1.63599	-2.05237	-1.26928
H	-2.30090	-2.73992	-0.35366
C	2.93884	-0.06776	-1.80527
C	-1.74071	-1.81509	-0.57372
H	1.16542	-1.80068	-2.22142
Fe	0.20211	0.36851	-0.54295
H	-1.50454	-1.77287	-1.64288
C	-2.60426	-0.59788	-0.27587
N	-1.95493	0.55448	-0.02844
H	-4.50363	-1.59193	-0.49766
C	-3.99823	-0.64898	-0.31017
C	-2.64466	1.68451	0.16522
H	-2.03456	2.56869	0.33039
C	-4.72259	0.52686	-0.10643
C	-4.03811	1.71925	0.13321
H	-5.80868	0.51049	-0.13397
H	-4.56705	2.65356	0.29134
H	2.25578	0.12187	-2.63528
H	3.80815	-0.65286	-2.15089
H	3.28146	0.89223	-1.41112
H	-0.55972	1.05370	2.68724
H	0.71575	2.08769	2.04855
H	0.98075	1.18630	3.58572
O	-0.17608	-0.04604	-2.38168
H	-0.37253	0.75205	-2.89395
N	0.61054	2.40457	-0.36037
N	1.74263	2.82246	-0.36049
N	2.83256	3.23402	-0.33824

^{5}FeMe2PyTACNNCSOH
Charge: 0
Energy: -1630335.2852290

H	-0.16504	-1.32728	3.41036
H	2.72280	-1.03653	2.47811
H	0.61030	-2.41423	2.28333
C	0.02988	-1.49104	2.34066
H	2.01908	-2.79351	0.88208
H	-1.81364	-2.58006	1.97714
C	2.22755	-0.72713	1.54065
H	-0.08997	-3.47129	0.52273
H	3.45413	-1.98366	0.29777
C	0.66369	0.84592	2.56551
C	2.38323	-1.83802	0.49154
N	0.81101	-0.37831	1.76574
C	-1.30678	-1.66968	1.61365
H	2.73086	0.17407	1.18256
H	-1.95044	-0.82120	1.85610
C	-0.42080	-2.89164	-0.34414
H	-1.10847	-3.54630	-0.89647
H	1.33017	-3.52120	-1.44191
N	-1.13552	-1.68845	0.15084
N	1.66687	-1.51330	-0.75897
C	0.77936	-2.58009	-1.26588
H	-3.18676	-2.11085	-0.31911
C	2.58610	-1.03516	-1.80793
C	-2.38963	-1.38645	-0.55740
H	0.39559	-2.21023	-2.21845
Fe	0.08762	0.14208	-0.54366
H	-2.16519	-1.42691	-1.62882
C	-2.86822	0.02926	-0.26901
N	-1.91855	0.95018	-0.01826
H	-4.96961	-0.38484	-0.50368
C	-4.21885	0.37651	-0.31318
C	-2.26333	2.22942	0.17116
H	-1.43332	2.90905	0.34442
C	-4.58172	1.70967	-0.11554
C	-3.58864	2.65898	0.12961
H	-5.62746	2.00214	-0.15149
H	-3.83081	3.70528	0.28478
H	1.98346	-0.66716	-2.64006
H	3.26551	-1.83380	-2.15020
H	3.17407	-0.20236	-1.41419
H	-0.40072	1.08851	2.64645
H	1.15875	1.67068	2.05278
H	1.08237	0.73086	3.57927
O	-0.41338	-0.13123	-2.37299
H	-0.33300	0.67484	-2.90376
N	1.25749	1.86229	-0.42906
C	2.38101	2.24031	-0.33278
S	3.93312	2.70498	-0.15401

^{5}FeMe2PyTACNOHBr
Charge: 0
Energy: -2937498.4093767

H	-1.34689	-3.70087	0.55748
H	-3.60232	-2.18661	-0.97479
H	-2.36378	-2.46601	1.25933
C	-1.43551	-2.61460	0.70242
H	-3.48048	-0.80244	1.08929
H	-0.27129	-2.58273	2.53644
C	-2.84514	-1.38423	-0.90923
H	-1.96547	-0.83654	2.66795
H	-4.27649	0.06069	-0.20337
C	-0.94764	-2.70996	-1.68955
C	-3.30412	-0.33766	0.11527
N	-1.50791	-1.91179	-0.59009
C	-0.24009	-2.12976	1.53039
H	-2.75543	-0.90696	-1.88939
H	0.67580	-2.47544	1.04622
C	-1.25561	-0.04899	2.39853
H	-0.87125	0.34508	3.34888
H	-2.87905	1.37281	2.24391
N	-0.16367	-0.65813	1.60316
N	-2.31990	0.76160	0.26392
C	-1.98280	1.09394	1.66245
H	1.49438	-0.64063	2.96375
C	-2.75593	1.95415	-0.48891
C	1.18331	-0.21172	1.99631
H	-1.31947	1.96084	1.61337
Fe	-0.31687	0.15127	-0.65647
H	1.15314	0.88021	2.08623
C	2.20027	-0.53955	0.91877
N	1.72889	-0.56475	-0.33931
H	3.90345	-0.73520	2.22198
C	3.54995	-0.75118	1.19512
C	2.56836	-0.77234	-1.36199
H	2.10183	-0.74817	-2.34286
C	4.42885	-0.96962	0.13344
C	3.93220	-0.97919	-1.17119
H	5.48665	-1.12884	0.32283
H	4.58461	-1.14109	-2.02309
H	-1.97414	2.71311	-0.43510
H	-3.70582	2.35401	-0.09729
H	-2.87744	1.67085	-1.53752
H	0.06497	-3.02132	-1.41454
H	-0.87496	-2.07334	-2.57314
H	-1.55429	-3.60736	-1.90071
O	-0.54750	0.14775	-2.52593
H	-0.26995	0.99689	-2.90281
Br	0.76582	2.58857	-0.14692

^{5}FeMe2PyTACNOHCl
Charge: 0
Energy: -1610968.2941471

H	0.91268	3.39751	1.15993
H	3.31106	2.40675	-0.57012
H	2.04190	2.16044	1.65657
C	1.10649	2.31606	1.11364
H	3.33207	0.67546	1.21594
H	-0.06084	1.85218	2.88656
C	2.63799	1.53449	-0.65995

H	1.80741	0.28896	2.74562
H	4.20762	0.13546	-0.19557
C	0.61846	2.78262	-1.23264
C	3.20080	0.37376	0.17286
N	1.25421	1.86278	-0.27957
C	-0.03956	1.57954	1.81696
H	2.59731	1.23095	-1.71011
H	-0.98274	1.91186	1.37757
C	1.18173	-0.50673	2.33049
H	0.83806	-1.09612	3.19144
H	2.94167	-1.71148	1.96771
N	0.03552	0.11893	1.63160
N	2.33099	-0.82417	0.11165
C	2.02391	-1.42644	1.42358
H	-1.61740	-0.31458	2.92727
C	2.87278	-1.82041	-0.83192
C	-1.25745	-0.52813	1.90644
H	1.45080	-2.33126	1.21033
Fe	0.27562	-0.27409	-0.73449
H	-1.10990	-1.60823	1.79973
C	-2.30087	-0.12091	0.88189
N	-1.83376	0.17789	-0.34187
H	-4.01719	-0.33382	2.16562
C	-3.66591	-0.09958	1.16486
C	-2.68879	0.47960	-1.32708
H	-2.22019	0.68098	-2.28652
C	-4.56161	0.21610	0.14239
C	-4.06724	0.50985	-1.12970
H	-5.63037	0.23192	0.33680
H	-4.73196	0.75606	-1.95144
H	2.15742	-2.63852	-0.92758
H	3.85282	-2.20233	-0.50055
H	2.97388	-1.34500	-1.81106
H	-0.42145	2.93743	-0.92825
H	0.61332	2.30880	-2.21585
H	1.13051	3.75983	-1.26972
O	0.50299	0.10522	-2.57099
H	0.32263	-0.68122	-3.10811
Cl	-0.45661	-2.66319	-0.58736

^{5}FeMe2PyTACNOHF
Charge: 0
Energy: -1384836.9116504

H	0.71777	1.08968	3.30712
H	3.17246	1.92752	1.56648
H	1.88993	-0.03649	2.66568
C	0.95585	0.47738	2.42470
H	3.29818	-0.53595	1.26001
H	-0.22310	-1.22628	3.08577
C	2.54061	1.45351	0.79231
H	1.75710	-2.00037	1.83132
H	4.18036	0.30011	0.00393
C	0.47371	2.61733	1.35842
C	3.16708	0.10811	0.38495
N	1.14137	1.31611	1.22993
C	-0.16815	-0.54867	2.21478
H	2.51317	2.10732	-0.08437
H	-1.11896	-0.01223	2.15995
C	1.16710	-2.17880	0.92755
H	0.85268	-3.23148	0.98111
H	2.95786	-2.61438	-0.20828
N	-0.00495	-1.27913	0.95198
N	2.35420	-0.59525	-0.62407
C	2.04446	-2.00430	-0.32726
H	-1.62813	-2.66959	1.17308
C	2.87083	-0.42465	-1.98975
C	-1.24236	-1.91096	0.47069
H	1.47598	-2.35399	-1.18938
Fe	0.25532	0.34911	-0.82236
H	-0.99012	-2.37668	-0.48699
C	-2.31099	-0.87614	0.17158
N	-1.87273	0.27783	-0.36430
H	-3.99688	-2.03188	0.84906
C	-3.66864	-1.09804	0.40171
C	-2.74899	1.23217	-0.70119
H	-2.30130	2.12308	-1.13399
C	-4.58724	-0.10733	0.04917
C	-4.12162	1.08244	-0.51376
H	-5.64972	-0.26119	0.21638
H	-4.80302	1.87734	-0.80002
H	2.13239	-0.84974	-2.67265
H	3.85454	-0.90586	-2.12883
H	2.95142	0.64599	-2.19811
H	-0.57329	2.44907	1.63106
H	0.49200	3.10962	0.38429
H	0.94446	3.25314	2.12939
O	0.49880	2.08125	-1.58032
H	0.41263	2.07483	-2.54522
F	-0.05579	-1.17195	-2.01236

^{5}FeMe2PyTACNOHN$_3$
Charge: 0
Energy: -1425227.9038083

H	-1.53046	-3.20002	1.38163
H	-3.75894	-1.97917	-0.42551
H	-2.45342	-1.77218	1.78258
C	-1.55596	-2.10777	1.25692
H	-3.51419	-0.13407	1.22065
H	-0.31644	-1.71288	2.99721
C	-2.96012	-1.23023	-0.57732
H	-1.95284	0.10768	2.71894
H	-4.29336	0.42701	-0.23839
C	-1.16026	-2.81183	-1.04618
C	-3.33608	0.06422	0.15986
N	-1.64074	-1.73790	-0.16573
C	-0.30602	-1.50814	1.91212
H	-2.87906	-1.01814	-1.64738
H	0.57340	-2.00393	1.49447
C	-1.20608	0.76744	2.26816
H	-0.78590	1.35144	3.09877
H	-2.73332	2.22604	1.79640
N	-0.16451	-0.06896	1.63154
N	-2.29056	1.10327	0.02118
C	-1.88145	1.74345	1.28557
H	1.53523	0.18391	2.91042
C	-2.65969	2.10148	-0.99845
C	1.20638	0.40011	1.87952
H	-1.15877	2.51323	1.00463
Fe	-0.34692	0.18966	-0.77583
H	1.21838	1.48639	1.74913
C	2.18809	-0.19600	0.88513
N	1.68659	-0.50604	-0.32193
H	3.91459	-0.11640	2.16901
C	3.53882	-0.37221	1.18287
C	2.50338	-0.96780	-1.28021
H	2.01742	-1.16785	-2.23128
C	4.38954	-0.85898	0.19209
C	3.86498	-1.15989	-1.06663
H	5.44762	-0.99440	0.39674
H	4.49576	-1.53302	-1.86696
H	-1.81549	2.77668	-1.14698
H	-3.55923	2.66940	-0.70739
H	-2.84477	1.57826	-1.94036
H	-0.15544	-3.10376	-0.72506
H	-1.08660	-2.41676	-2.06090
H	-1.81776	-3.69810	-1.01562
O	-0.64658	-0.30084	-2.58132
H	-0.39220	0.40761	-3.19131
N	0.44259	2.17168	-0.73542
N	1.59465	2.47176	-0.54045
N	2.69846	2.76839	-0.32091

^{5}FeMe2PyTACNOHNCS
Charge: 0
Energy: -1630339.9107707

H	-2.19629	-2.65185	2.01116
H	-4.21688	-1.30214	0.05888
H	-2.72602	-0.99196	2.13423
C	-1.97669	-1.63251	1.66311
H	-3.42570	0.70595	1.28096
H	-0.54000	-1.23001	3.24048
C	-3.28184	-0.81381	-0.27008
H	-1.72315	0.84381	2.67479
H	-4.15611	1.15420	-0.24128
C	-1.95059	-2.85264	-0.45100
C	-3.28557	0.64891	0.19793
N	-2.08697	-1.53924	0.19615
C	-0.57347	-1.24176	2.13719
H	-3.24112	-0.83892	-1.36289
H	0.12972	-2.00527	1.79608
C	-0.89106	1.20980	2.06642
H	-0.27721	1.82617	2.73572
H	-2.12176	2.84515	1.36762
N	-0.12179	0.04393	1.57116
N	-2.03558	1.35536	-0.17228
C	-1.41832	2.11321	0.93476
H	1.65970	0.04127	2.75351
C	-2.23768	2.20021	-1.36398
C	1.33500	0.19598	1.71046
H	-0.58264	2.66975	0.50843
Fe	-0.44795	-0.15952	-0.81380
H	1.60620	1.22086	1.43673
C	2.08762	-0.75173	0.79263
N	1.42286	-1.20229	-0.28411
H	3.93052	-0.72708	1.90715
C	3.41684	-1.10526	1.02830
C	2.04447	-1.99852	-1.16541
H	1.43748	-2.29228	-2.01748
C	4.06754	-1.93188	0.11343
C	3.37019	-2.39139	-1.00611
H	5.10513	-2.21216	0.27115
H	3.84238	-3.03432	-1.74181
H	-1.27740	2.62061	-1.66497
H	-2.96263	3.00831	-1.17379
H	-2.59713	1.56581	-2.17842

H	-1.02001	-3.31552	-0.10824
H	-1.87245	-2.69874	-1.52844
H	-2.79443	-3.52139	-0.20942
O	-0.96685	-0.88941	-2.47816
H	-0.57084	-0.41217	-3.22257
N	0.87306	1.47176	-1.27011
C	1.57342	2.31457	-0.81353
S	2.49575	3.45680	-0.09213

^{4}FeMe2PyTACNOOHOH2PA
Charge: 0
Energy: -1417271.1681351

H	0.41223	-2.51438	2.62312
H	3.03349	-0.80087	2.48580
H	1.65462	-2.63274	1.40016
C	0.73328	-2.10181	1.65639
H	3.08389	-1.76856	0.20428
H	-0.44845	-3.48924	0.48135
C	2.44335	-0.31366	1.68834
H	1.60720	-2.88917	-0.80969
H	4.08964	-0.34310	0.29985
C	0.36317	-0.04912	2.94700
C	3.04498	-0.68286	0.32262
N	1.01235	-0.65535	1.77489
C	-0.35564	-2.39608	0.61208
H	2.50782	0.77030	1.82035
H	-1.31506	-2.03117	0.98791
C	1.04061	-2.18509	-1.42620
H	0.72549	-2.75395	-2.31408
H	2.85710	-1.45459	-2.36135
N	-0.11649	-1.70327	-0.66044
N	2.28347	-0.09123	-0.80247
C	1.95191	-1.03237	-1.88868
H	-1.78961	-2.50420	-1.75407
C	2.94844	1.11926	-1.30968
C	-1.34724	-1.53503	-1.46652
H	1.42237	-0.44179	-2.64241
Fe	0.22322	0.56028	-0.01029
H	-1.03050	-1.02330	-2.38717
C	-2.34218	-0.68791	-0.71981
N	-1.77106	0.41304	-0.09368
H	-4.07085	-1.86132	-1.14089
C	-3.69150	-0.97005	-0.64488
C	-2.63483	1.25571	0.57872
H	-2.15426	2.11293	1.04207
C	-4.56217	-0.11122	0.05275
C	-3.98932	1.02914	0.66764
H	-5.62568	-0.31459	0.11323
H	-4.60856	1.73488	1.21521
H	2.33532	1.55523	-2.09864
H	3.95746	0.90201	-1.69807
H	3.00751	1.83934	-0.49015
H	-0.70618	-0.27621	2.91021
H	0.47572	1.03594	2.88306
H	0.78158	-0.42416	3.89722
O	0.05982	1.92142	-2.05494
O	0.83687	2.22089	0.85364
H	0.24820	2.66766	-1.42275
H	-0.90423	1.81161	-1.99925
O	0.57005	3.46513	0.07020
H	1.44120	3.89089	0.12425

^{6}FeMePy2CHTACNBr
Charge: 2+
Energy: -3044679.4990504

N	1.86755	-1.41881	-0.88819
C	2.77457	-0.57285	-1.72759
C	3.05174	0.76879	-1.06124
N	1.81066	1.49257	-0.64138
C	1.01884	2.11136	-1.74926
C	0.18183	1.13317	-2.59712
N	-0.32591	-0.05984	-1.84290
C	0.95284	-2.23932	-1.72562
C	-0.02311	-1.36072	-2.53422
C	-1.76067	0.04175	-1.43608
C	-2.07863	-1.15769	-0.54692
C	-1.95689	1.28172	-0.57528
N	-1.03896	1.40819	0.40889
C	-1.18192	2.36981	1.33661
C	-2.23750	3.27955	1.28991
C	-3.16456	3.17957	0.25209
C	-3.02879	2.15557	-0.69423
N	-1.12551	-1.41839	0.37668
C	-1.32147	-2.39194	1.28355
C	-2.48106	-3.16490	1.28680
C	-3.45963	-2.91142	0.32499
C	-3.25823	-1.88589	-0.60773
Fe	0.55151	-0.05607	0.24517
C	2.65413	-2.29722	0.02366
C	2.20845	2.57633	0.30753
H	2.32630	-0.43435	-2.70951
H	3.72336	-1.09618	-1.89196
H	3.65332	1.40262	-1.72578
H	3.63076	0.60475	-0.14887
H	1.68548	2.67876	-2.41200
H	0.35397	2.83033	-1.27140
H	0.77060	0.77318	-3.43922
H	-0.65698	1.68866	-3.03101
H	0.40401	-2.89111	-1.04531
H	1.52951	-2.87977	-2.40594
H	-0.94568	-1.92239	-2.69899
H	0.37723	-1.14527	-3.52576
H	-2.42291	0.06588	-2.30961
H	-0.43655	2.38865	2.12450
H	-2.32611	4.04370	2.05453
H	-3.99207	3.87900	0.18341
H	-3.74801	2.03819	-1.49849
H	-0.53065	-2.53213	2.01271
H	-2.60933	-3.94312	2.03129
H	-4.37239	-3.49876	0.30009
H	-4.00598	-1.66040	-1.36139
H	3.34101	-1.68914	0.61239
H	1.97449	-2.80526	0.70972
H	3.21814	-3.04000	-0.55307
H	2.73689	2.14206	1.15536
H	2.85419	3.30466	-0.19774
H	1.31662	3.08588	0.67105
Br	1.37591	-0.15573	2.48588

^{6}FeMePy2CHTACNCl
Charge: 2+
Energy: -1718151.4451768

N	2.02612	-1.47983	-0.31865
C	3.07621	-0.67650	-1.02106
C	3.26985	0.67896	-0.35339
N	1.99245	1.43492	-0.16239
C	1.40174	2.03561	-1.39743
C	0.68773	1.04665	-2.34130
N	0.04338	-0.11572	-1.64616
C	1.24198	-2.31144	-1.26880
C	0.42524	-1.44093	-2.24594
C	-1.43479	0.01833	-1.46913
C	-1.90662	-1.14953	-0.60534
C	-1.73806	1.28428	-0.67927
N	-0.98006	1.42118	0.43108
C	-1.24638	2.40178	1.30977
C	-2.26745	3.32438	1.08507
C	-3.02504	3.21574	-0.08162
C	-2.76392	2.17041	-0.97743
N	-1.11137	-1.38966	0.46160
C	-1.45878	-2.32424	1.36329
C	-2.61834	-3.08320	1.21546
C	-3.43266	-2.85479	0.10543
C	-3.07483	-1.86632	-0.82097
Fe	0.58658	-0.06379	0.56271
C	2.62676	-2.33297	0.74516
C	2.24786	2.52920	0.82229
H	2.79596	-0.55929	-2.06613
H	4.02707	-1.22150	-1.01422
H	3.98582	1.28334	-0.92536
H	3.68639	0.53155	0.64625
H	2.17768	2.57110	-1.96012
H	0.68540	2.77991	-1.05072
H	1.39460	0.65246	-3.06971
H	-0.06025	1.60314	-2.91693
H	0.57889	-2.93479	-0.66830
H	1.90773	-2.97994	-1.83037
H	-0.47072	-1.99210	-2.54144
H	0.98290	-1.26113	-3.16600
H	-1.95549	0.02647	-2.43399
H	-0.62913	2.42473	2.20177
H	-2.46054	4.10486	1.81306
H	-3.82025	3.92509	-0.28939
H	-3.35422	2.04628	-1.87967
H	-0.79018	-2.44289	2.20962
H	-2.87340	-3.83114	1.95834
H	-4.34035	-3.43268	-0.03900
H	-3.69566	-1.66030	-1.68705
H	3.21255	-1.71132	1.42227
H	1.82861	-2.80427	1.32112
H	3.26632	-3.10514	0.30147
H	2.59661	2.09804	1.76015
H	2.99954	3.22483	0.43034
H	1.32309	3.07497	1.00642
Cl	1.05254	-0.10828	2.71588

^{6}FeMePy2CHTACNF
Charge: 2+
Energy: -1492025.4728910

N	-2.07944	-1.46232	0.09035
C	-3.16752	-0.66231	0.73487
C	-3.31481	0.70248	0.07264
N	-2.01902	1.44144	-0.05276
C	-1.49118	2.04558	1.20690

C	-0.83181	1.05054	2.18825
N	-0.16384	-0.11938	1.52862
C	-1.35900	-2.30515	1.07860
C	-0.59131	-1.44152	2.10362
C	1.32192	-0.00345	1.42034
C	1.82189	-1.17264	0.57166
C	1.68027	1.26197	0.65095
N	0.98340	1.41503	-0.49708
C	1.30806	2.39898	-1.35240
C	2.32834	3.30629	-1.06950
C	3.02184	3.18050	0.13473
C	2.69965	2.13379	1.00845
N	1.08140	-1.39332	-0.53781
C	1.46187	-2.32430	-1.42957
C	2.60251	-3.10003	-1.23005
C	3.35947	-2.89308	-0.07582
C	2.96689	-1.90865	0.84088
Fe	-0.59679	-0.05602	-0.71234
C	-2.60015	-2.28318	-1.03724
C	-2.18933	2.50230	-1.08984
H	-2.94844	-0.55654	1.79592
H	-4.11839	-1.20324	0.66621
H	-4.04663	1.31183	0.61838
H	-3.69064	0.57150	-0.94529
H	-2.29109	2.58679	1.72883
H	-0.75279	2.78442	0.89678
H	-1.57898	0.66386	2.87974
H	-0.11080	1.60295	2.80103
H	-0.66773	-2.93204	0.51465
H	-2.06008	-2.97021	1.59971
H	0.28041	-2.00175	2.45068
H	-1.20035	-1.25838	2.98983
H	1.80092	-0.00594	2.40668
H	0.73714	2.44176	-2.27437
H	2.56899	4.08906	-1.78067
H	3.81379	3.87820	0.38918
H	3.23887	1.99740	1.94041
H	0.83469	-2.42878	-2.30948
H	2.88688	-3.84470	-1.96551
H	4.25019	-3.48524	0.11054
H	3.54408	-1.72037	1.74053
H	-3.09535	-1.63422	-1.76010
H	-1.76296	-2.77327	-1.53805
H	-3.30215	-3.04185	-0.67191
H	-2.39764	2.02780	-2.04998
H	-3.00967	3.17761	-0.81968
H	-1.26973	3.08068	-1.17184
F	-0.99100	-0.11108	-2.42281

^{6}FeMePy2CHTACNN$_3$
Charge: 2+
Energy: -1532413.9190486

N	1.98361	-1.31304	-0.83065
C	2.87108	-0.40490	-1.62148
C	3.09659	0.91794	-0.89797
N	1.83063	1.57607	-0.45154
C	1.02924	2.22455	-1.53190
C	0.22971	1.25939	-2.43165
N	-0.24648	0.01794	-1.73824
C	1.10523	-2.12294	-1.71246
C	0.10479	-1.23811	-2.48642
C	-1.68715	0.05515	-1.34795
C	-1.98123	-1.19463	-0.52138
C	-1.93719	1.24778	-0.43473
N	-1.04161	1.36143	0.57012
C	-1.23076	2.28548	1.52614
C	-2.31206	3.16501	1.49696
C	-3.21882	3.07542	0.44022
C	-3.03393	2.09336	-0.54063
N	-1.03274	-1.47667	0.39874
C	-1.21256	-2.50504	1.24461
C	-2.34863	-3.31024	1.19371
C	-3.32385	-3.03061	0.23525
C	-3.13987	-1.95115	-0.63712
Fe	0.61734	-0.04780	0.36921
C	2.78090	-2.19344	0.06293
C	2.17934	2.60544	0.56902
H	2.42827	-0.23866	-2.60164
H	3.83903	-0.88798	-1.79941
H	3.67840	1.59955	-1.53253
H	3.68112	0.73568	0.00764
H	1.67898	2.84523	-2.16339
H	0.33677	2.89713	-1.02611
H	0.83818	0.95770	-3.28282
H	-0.62095	1.80904	-2.85016
H	0.57180	-2.82345	-1.06886
H	1.70484	-2.71224	-2.41913
H	-0.79663	-1.82279	-2.68547
H	0.50435	-0.96490	-3.46411
H	-2.34126	0.09960	-2.22729
H	-0.49591	2.30495	2.32414
H	-2.43552	3.89874	2.28613
H	-4.06609	3.75176	0.38235
H	-3.73366	1.98636	-1.36336
H	-0.42237	-2.67136	1.96950
H	-2.46182	-4.13357	1.89060
H	-4.21886	-3.64120	0.16605
H	-3.88386	-1.70649	-1.38857
H	3.43182	-1.58017	0.68776
H	2.10516	-2.75281	0.71327
H	3.38992	-2.89566	-0.51925
H	2.67825	2.12335	1.41029
H	2.83925	3.36960	0.14043
H	1.26921	3.08633	0.92690
N	1.30114	-0.20205	2.07576
N	1.72922	-0.40581	3.19325
N	2.13707	-0.59526	4.24782

^{6}FeMePy2CHTACNNCS
Charge: 2+
Energy: -1737522.4335066

N	-1.42378	0.86457	-1.86531
C	-1.89402	-0.26814	-2.72093
C	-2.30555	-1.46734	-1.87443
N	-1.26810	-1.87795	-0.87971
C	-0.08306	-2.59061	-1.44275
C	0.94625	-1.69545	-2.16526
N	1.05371	-0.30524	-1.61442
C	-0.32240	1.62050	-2.51320
C	0.94400	0.75270	-2.67642
C	2.23547	-0.09145	-0.72763
C	2.12052	1.30518	-0.11986
C	2.18490	-1.07384	0.43520
N	0.98181	-1.13285	1.04645
C	0.84280	-1.85132	2.17244
C	1.90129	-2.57658	2.71786
C	3.13594	-2.54905	2.06840
C	3.28467	-1.77693	0.90973
N	0.87937	1.60885	0.31940
C	0.66231	2.77381	0.95258
C	1.68363	3.69952	1.15752
C	2.96388	3.39702	0.69135
C	3.18937	2.17617	0.04378
Fe	-0.55155	0.00252	-0.01963
C	-2.54677	1.77266	-1.51386
C	-1.92093	-2.75512	0.13375
H	-1.10344	-0.54055	-3.41754
H	-2.74631	0.05190	-3.33181
H	-2.56913	-2.31346	-2.52284
H	-3.19609	-1.20829	-1.29582
H	-0.40988	-3.38353	-2.12887
H	0.40041	-3.07847	-0.59658
H	0.69309	-1.62026	-3.22172
H	1.92050	-2.19559	-2.12455
H	-0.11298	2.48011	-1.87538
H	-0.63995	2.00356	-3.49235
H	1.81996	1.40557	-2.65077
H	0.96014	0.27150	-3.65544
H	3.17783	-0.19625	-1.27917
H	-0.13866	-1.83012	2.63472
H	1.75557	-3.14576	3.62954
H	3.97776	-3.11080	2.46140
H	4.23827	-1.71975	0.39462
H	-0.35223	2.94790	1.29643
H	1.47587	4.63180	1.67132
H	3.78047	4.09868	0.83102
H	4.17611	1.91150	-0.32271
H	-3.34910	1.19495	-1.05308
H	-2.19814	2.51208	-0.79001
H	-2.92909	2.28571	-2.40475
H	-2.72147	-2.20210	0.62606
H	-2.33290	-3.65488	-0.33953
H	-1.18777	-3.05545	0.88211
N	-1.86184	0.34781	1.25268
C	-2.74193	0.59132	2.04923
S	-3.89118	0.90625	3.08173

^{6}FeMePy2CHTACNOH
Charge: 2+
Energy: -1476942.1499169

N	-2.06688	-1.49980	0.10577
C	-3.15198	-0.71493	0.77218
C	-3.33194	0.64710	0.11248
N	-2.05253	1.40721	-0.03396
C	-1.51479	2.01187	1.22039
C	-0.82526	1.02461	2.18695
N	-0.14240	-0.12869	1.51442
C	-1.31614	-2.33061	1.08052
C	-0.53994	-1.45871	2.09148
C	1.33824	0.01834	1.40280
C	1.86027	-1.14157	0.55738
C	1.66631	1.29342	0.63762
N	0.96016	1.43909	-0.50428
C	1.25083	2.44744	-1.34225
C	2.24485	3.38109	-1.05234

C	2.95164	3.25616	0.14429
C	2.66390	2.18809	1.00291
N	1.11545	-1.39512	-0.54083
C	1.50951	-2.34146	-1.40927
C	2.66658	-3.09061	-1.20541
C	3.43213	-2.84100	-0.06531
C	3.02460	-1.84668	0.83215
Fe	-0.61151	-0.06778	-0.73087
C	-2.60900	-2.33768	-0.99689
C	-2.26804	2.48120	-1.04662
O	-0.98807	-0.09483	-2.47004
H	-2.91380	-0.60499	1.82865
H	-4.09734	-1.26794	0.72445
H	-4.06694	1.24295	0.66938
H	-3.72047	0.50794	-0.89952
H	-2.31411	2.53859	1.75849
H	-0.79262	2.76375	0.90318
H	-1.55646	0.62102	2.88578
H	-0.10780	1.58776	2.79438
H	-0.62631	-2.94767	0.50388
H	-1.99629	-3.00629	1.61614
H	0.34628	-2.00821	2.41831
H	-1.13279	-1.28826	2.99130
H	1.81989	0.02568	2.38827
H	0.66866	2.49068	-2.25670
H	2.45522	4.18365	-1.75094
H	3.72468	3.97254	0.40482
H	3.21011	2.05401	1.93115
H	0.87326	-2.48781	-2.27613
H	2.95631	-3.84887	-1.92475
H	4.33678	-3.41005	0.12561
H	3.60234	-1.62803	1.72459
H	-3.13657	-1.70064	-1.70719
H	-1.78039	-2.81793	-1.52072
H	-3.28812	-3.10481	-0.60570
H	-2.51341	2.01959	-2.00342
H	-3.07771	3.15128	-0.73331
H	-1.35337	3.06255	-1.15903
H	-0.72233	-0.21494	-3.39416

^{3}FePyTACNBrOH
Charge: 2+
Energy: -2937123.9515787

N	-2.24824	-0.59036	-0.34589
C	-2.62506	-0.93180	1.07024
C	-1.88576	-0.02722	2.03842
N	-0.40893	0.03151	1.75348
C	0.37011	-1.18049	2.17833
C	0.17037	-2.37635	1.25860
N	0.10132	-1.96764	-0.19367
C	-2.21217	-1.81388	-1.21570
C	-0.98694	-2.71124	-0.93253
C	1.43397	-2.09249	-0.86782
C	2.33254	-0.95628	-0.46154
N	1.70730	0.22947	-0.23283
C	2.43733	1.33989	-0.00076
C	3.82746	1.30129	0.04128
C	4.47837	0.08368	-0.15920
C	3.71695	-1.06100	-0.41439
Fe	-0.28364	0.05180	-0.35591
C	-3.23840	0.37018	-0.92718
C	0.15287	1.18815	2.52774
H	-2.41342	-1.98363	1.24850
H	-3.70492	-0.80448	1.19790
H	-2.05333	-0.34235	3.07538
H	-2.25213	0.99563	1.93118
H	0.10434	-1.45009	3.20772
H	1.41874	-0.88237	2.17869
H	-0.74207	-2.91190	1.50776
H	0.99282	-3.08492	1.39884
H	-2.17310	-1.45719	-2.24268
H	-3.14552	-2.37226	-1.08009
H	-0.58859	-3.06250	-1.88434
H	-1.25596	-3.59733	-0.35408
H	1.87903	-3.07109	-0.65987
H	1.88560	2.25989	0.14194
H	4.37950	2.21636	0.22682
H	5.56187	0.02332	-0.12474
H	4.19189	-2.02109	-0.58916
H	-3.38010	1.21120	-0.25131
H	-2.86143	0.73770	-1.88035
H	-4.19076	-0.15098	-1.07587
H	-0.38412	2.10048	2.28076
H	0.05224	0.97971	3.59894
H	1.20711	1.31163	2.28590
H	1.26086	-2.01171	-1.94415
O	-0.22795	-0.09936	-2.09724
H	-0.08754	0.74192	-2.57466
Br	-0.75408	2.43882	-0.43622

^{5}FePyTACNClOH
Charge: 2+
Energy: -1610594.0742191

N	2.49548	0.35049	-0.24431
C	2.89385	-0.00423	1.15531
C	1.97031	-1.05961	1.73860
N	0.51019	-0.75165	1.53662
C	-0.01179	0.46922	2.25179
C	0.31770	1.78987	1.56699
N	0.11369	1.71808	0.08313
C	2.55792	1.82434	-0.51054
C	1.16186	2.46211	-0.67175
C	-1.25025	2.14350	-0.34425
C	-2.27609	1.05091	-0.16009
N	-1.81361	-0.20843	-0.29057
C	-2.67370	-1.24599	-0.32173
C	-4.04478	-1.05875	-0.18347
C	-4.53022	0.23911	-0.00365
C	-3.63343	1.31079	0.00564
Fe	0.32722	-0.35060	-0.54932
C	3.28715	-0.42399	-1.24398
C	-0.26993	-1.92926	2.03625
H	2.89717	0.89241	1.77254
H	3.91978	-0.38950	1.16352
H	2.16339	-1.18563	2.81143
H	2.14072	-2.02115	1.25060
H	0.36557	0.46843	3.28193
H	-1.09404	0.34614	2.29807
H	1.34348	2.09594	1.75415
H	-0.31811	2.57527	1.99042
H	3.11034	1.99658	-1.43641
H	3.13009	2.30508	0.28684
H	0.86810	2.43230	-1.71985
H	1.18209	3.51095	-0.34984
H	-1.54040	3.06535	0.17211
H	-2.23569	-2.22814	-0.46041
H	-4.71160	-1.91366	-0.21506
H	-5.59430	0.41706	0.11813
H	-3.98302	2.33202	0.12065
H	3.22728	-1.48717	-1.01093
H	2.86615	-0.25439	-2.23519
H	4.33488	-0.10155	-1.22369
H	0.08469	-2.83976	1.55765
H	-0.13419	-2.00942	3.12112
H	-1.32595	-1.78682	1.81688
H	-1.19765	2.36417	-1.41485
O	0.31350	0.24216	-2.20374
H	0.16326	-0.43488	-2.89485
Cl	0.54061	-2.47876	-1.06632

^{3}FePyTACNFOH
Charge: 2+
Energy: -1384473.4586805

N	-2.30788	-0.20672	-0.48070
C	-2.83390	0.40130	0.78933
C	-2.00635	1.61908	1.17786
N	-0.52738	1.36633	1.09002
C	0.06198	0.59934	2.22876
C	-0.29189	-0.88004	2.15979
N	-0.23163	-1.40681	0.73785
C	-2.43289	-1.70078	-0.48400
C	-1.38948	-2.35064	0.44805
C	1.09781	-2.05116	0.44212
C	2.13340	-0.99584	0.16097
N	1.64092	0.11706	-0.43375
C	2.45912	1.08619	-0.88656
C	3.83775	0.98398	-0.72857
C	4.36247	-0.13889	-0.08356
C	3.49945	-1.14419	0.36680
Fe	-0.33159	0.15532	-0.58956
C	-2.98878	0.36873	-1.68379
C	0.15912	2.69004	0.99324
H	-2.83183	-0.36007	1.56675
H	-3.87790	0.69661	0.64217
H	-2.27425	1.96393	2.18363
H	-2.21383	2.43344	0.48098
H	-0.26304	1.02157	3.18768
H	1.14311	0.72818	2.16324
H	-1.29299	-1.05610	2.54482
H	0.39070	-1.45728	2.79051
H	-2.26274	-2.02325	-1.50830
H	-3.45394	-1.97503	-0.19551
H	-1.00042	-3.24726	-0.03374
H	-1.82159	-2.66196	1.40076
H	1.38620	-2.72450	1.25515
H	1.97854	1.92654	-1.37434
H	4.48046	1.77234	-1.10540
H	5.43396	-0.23753	0.06120
H	3.88263	-2.03436	0.85521
H	-2.93218	1.45581	-1.64321
H	-2.47430	0.01400	-2.57604
H	-4.03444	0.04326	-1.69121
H	-0.16232	3.19247	0.08228
H	-0.09087	3.30164	1.86727
H	1.23772	2.54004	0.96201

H	0.96818	-2.63881	-0.47012
O	-0.24258	-1.01179	-1.93874
H	0.51216	-0.80932	-2.52314
F	-0.43223	1.57555	-1.54229

^{3}FePyTACNN$_3$OH
Charge: 2+
Energy: -1424865.5307822

N	-2.28147	-0.24075	-0.35363
C	-2.67544	-0.97201	0.89934
C	-1.88985	-0.44741	2.09208
N	-0.41964	-0.33590	1.81251
C	0.33549	-1.62737	1.84815
C	0.07400	-2.49988	0.62625
N	-0.03036	-1.68448	-0.64372
C	-2.31810	-1.13646	-1.55421
C	-1.17084	-2.16084	-1.52040
C	1.26674	-1.66484	-1.39603
C	2.23658	-0.73065	-0.72580
N	1.66393	0.35206	-0.14209
C	2.43631	1.31736	0.39686
C	3.82409	1.22861	0.38492
C	4.42425	0.10733	-0.19216
C	3.61767	-0.88689	-0.75359
Fe	-0.33086	0.32150	-0.17347
C	-3.18738	0.92276	-0.59024
C	0.17430	0.56452	2.84689
H	-2.51738	-2.03738	0.74678
H	-3.74764	-0.83937	1.07742
H	-2.06532	-1.07415	2.97500
H	-2.22739	0.56358	2.32958
H	0.09575	-2.18351	2.76313
H	1.39236	-1.36261	1.89517
H	-0.84720	-3.06457	0.74725
H	0.87683	-3.23701	0.52507
H	-2.21347	-0.49150	-2.42369
H	-3.29298	-1.63568	-1.60390
H	-0.80347	-2.31123	-2.53598
H	-1.50162	-3.13613	-1.15880
H	1.66802	-2.67805	-1.50363
H	1.91371	2.15687	0.83867
H	4.41589	2.02553	0.82227
H	5.50520	0.00760	-0.20830
H	4.05380	-1.76700	-1.21506
H	-3.22913	1.53793	0.30905
H	-2.79992	1.50568	-1.42599
H	-4.19259	0.56195	-0.83327
H	-0.29327	1.54589	2.78793
H	0.01570	0.13750	3.84357
H	1.24483	0.66581	2.67167
H	1.05053	-1.26933	-2.39194
O	-0.35141	0.74530	-1.90925
H	0.40638	1.30061	-2.17067
N	-0.59378	2.01926	0.44673
N	-0.80739	2.96335	-0.32702
N	-1.01426	3.87955	-0.97127

^{3}FePyTACNNCSOH
Charge: 2+
Energy: -1629971.8038643

N	-1.61256	-1.64985	-0.37744
C	-1.72871	-2.27839	0.98078
C	-1.46339	-1.23967	2.05878
N	-0.23520	-0.42483	1.77754
C	1.05598	-1.12228	2.07029
C	1.41420	-2.16265	1.01387
N	1.06554	-1.70319	-0.38716
C	-1.06554	-2.61539	-1.38359
C	0.44904	-2.82725	-1.19471
C	2.26385	-1.12569	-1.08123
C	2.53509	0.25989	-0.56463
N	1.42952	0.95386	-0.19650
C	1.54254	2.24825	0.16235
C	2.77112	2.89738	0.18922
C	3.91869	2.18207	-0.16089
C	3.79716	0.84399	-0.54263
Fe	-0.22728	-0.15602	-0.29908
C	-2.94590	-1.16936	-0.84344
C	-0.29843	0.79892	2.62849
H	-1.03312	-3.11238	1.04285
H	-2.73098	-2.70089	1.10925
H	-1.39320	-1.71167	3.04665
H	-2.29582	-0.53280	2.09018
H	1.02314	-1.59222	3.06149
H	1.82340	-0.34795	2.10157
H	0.89580	-3.09865	1.20569
H	2.48382	-2.38706	1.07070
H	-1.24931	-2.17583	-2.36106
H	-1.61283	-3.56275	-1.31509
H	0.92156	-2.85627	-2.17616
H	0.67650	-3.77589	-0.70429
H	3.12957	-1.78861	-0.98187
H	0.62350	2.75405	0.42943
H	2.82200	3.94105	0.47990
H	4.89357	2.65932	-0.14155
H	4.66727	0.26296	-0.83068
H	-3.39569	-0.54416	-0.07137
H	-2.80707	-0.58690	-1.75391
H	-3.60106	-2.02426	-1.04362
H	-1.19594	1.36688	2.38735
H	-0.32072	0.52023	3.68840
H	0.57883	1.41826	2.44623
H	2.00533	-1.03611	-2.13921
O	-0.21450	-0.10667	-2.08504
H	-0.29799	0.80500	-2.41743
N	-1.41115	1.29972	-0.16968
C	-2.19216	2.19146	-0.28514
S	-3.24747	3.39995	-0.41122

^{3}FePyTACNOHBr
Charge: 2+
Energy: -2937126.9751515

N	-2.33181	-0.07333	-0.03488
C	-2.81849	1.34802	0.11649
C	-1.93618	2.30386	-0.66595
N	-0.47709	2.06953	-0.41288
C	0.03274	2.52404	0.91702
C	-0.37555	1.58542	2.04211
N	-0.22198	0.13234	1.64147
C	-2.52735	-0.85248	1.23916
C	-1.33954	-0.70174	2.22426
C	1.13804	-0.38715	2.03150
C	2.15085	-0.03785	0.97646
N	1.65067	0.08561	-0.27591
C	2.47445	0.22990	-1.33246
C	3.85307	0.28827	-1.16591
C	4.38326	0.20072	0.12347
C	3.51940	0.03591	1.20937
Fe	-0.31846	-0.00665	-0.42073
C	-3.08723	-0.73433	-1.14923
C	0.29666	2.75557	-1.48856
H	-2.85455	1.59867	1.17358
H	-3.84714	1.41578	-0.25131
H	-2.19445	3.34497	-0.43715
H	-2.08261	2.14655	-1.73602
H	-0.31394	3.54361	1.12622
H	1.12014	2.55656	0.83747
H	-1.40749	1.74645	2.34004
H	0.23462	1.78321	2.92855
H	-2.61514	-1.90115	0.96015
H	-3.47708	-0.54737	1.69090
H	-0.94044	-1.69344	2.42992
H	-1.64546	-0.26368	3.17850
H	1.41930	-0.01991	3.02324
H	1.99738	0.29924	-2.30187
H	4.49230	0.39984	-2.03504
H	5.45601	0.25056	0.28248
H	3.90160	-0.05374	2.22122
H	-3.00250	-0.12122	-2.04617
H	-2.66401	-1.71984	-1.33729
H	-4.13946	-0.83323	-0.86167
H	0.01923	2.33457	-2.45386
H	0.07028	3.82795	-1.47134
H	1.36316	2.61340	-1.32134
H	1.07573	-1.47757	2.07866
O	-0.44483	0.07671	-2.15806
H	-0.44634	-0.79443	-2.60296
Br	-0.07440	-2.44927	-0.40293

^{3}FePyTACNOHCl
Charge: 2+
Energy: -1610598.5613636

N	-2.32900	-0.27857	-0.22226
C	-2.83313	0.92295	0.53694
C	-1.96508	2.13500	0.25036
N	-0.50049	1.82692	0.36828
C	0.02005	1.67613	1.76387
C	-0.37472	0.34502	2.38444
N	-0.22737	-0.79196	1.39578
C	-2.51100	-1.54204	0.57381
C	-1.34394	-1.79879	1.56039
C	1.13125	-1.43469	1.50963
C	2.14664	-0.65701	0.71912
N	1.64900	0.00936	-0.34894
C	2.47380	0.60082	-1.23460
C	3.85262	0.57555	-1.05961
C	4.38069	-0.07298	0.05913
C	3.51509	-0.69781	0.96087
Fe	-0.32041	-0.03016	-0.52527
C	-3.06422	-0.39597	-1.52328
C	0.25709	2.92226	-0.30824
H	-2.86273	0.68324	1.59701
H	-3.86523	1.13116	0.23752
H	-2.22701	2.96772	0.91395

H	-2.11908	2.46200	-0.77945
H	-0.32926	2.50829	2.38714
H	1.10631	1.74741	1.69757
H	-1.40300	0.35929	2.73458
H	0.24719	0.14697	3.26268
H	-2.55195	-2.36280	-0.13958
H	-3.47758	-1.49401	1.08657
H	-0.93594	-2.78634	1.35276
H	-1.67229	-1.79022	2.60319
H	1.41318	-1.55017	2.56073
H	1.99835	1.09191	-2.07435
H	4.49335	1.05649	-1.79078
H	5.45335	-0.10132	0.22397
H	3.89587	-1.22622	1.82904
H	-2.99247	0.55056	-2.05848
H	-2.61413	-1.19005	-2.11747
H	-4.11446	-0.63364	-1.32282
H	-0.02644	2.95980	-1.35878
H	0.02073	3.87660	0.17591
H	1.32626	2.73486	-0.22472
H	1.06320	-2.42996	1.06322
O	-0.43855	0.79247	-2.05815
H	-0.42069	0.17753	-2.81942
Cl	-0.10720	-2.07503	-1.43675

^{3}FePyTACNOHF
Charge: 2+
Energy: -1384475.8996609

N	-2.29996	-0.23805	-0.50027
C	-2.84450	0.31704	0.78564
C	-2.06085	1.55583	1.19593
N	-0.57260	1.35528	1.09638
C	0.05856	0.59483	2.22465
C	-0.23775	-0.89889	2.15990
N	-0.22133	-1.41281	0.73589
C	-2.36628	-1.73450	-0.54607
C	-1.38315	-2.35155	0.46176
C	1.09289	-2.05169	0.37528
C	2.13256	-0.99410	0.12707
N	1.64744	0.15641	-0.39499
C	2.48041	1.12933	-0.80735
C	3.85911	0.99728	-0.67701
C	4.37484	-0.16763	-0.10523
C	3.49879	-1.17843	0.30244
Fe	-0.32434	0.19321	-0.57205
C	-3.01357	0.33270	-1.68343
C	0.06905	2.70664	1.03276
H	-2.80476	-0.45851	1.54786
H	-3.90058	0.57466	0.65462
H	-2.33171	1.87068	2.21032
H	-2.29773	2.37657	0.51648
H	-0.27174	1.00679	3.18575
H	1.13205	0.76527	2.14320
H	-1.21207	-1.11702	2.59144
H	0.49825	-1.44575	2.75703
H	-2.09722	-2.02389	-1.55930
H	-3.39343	-2.06136	-0.34622
H	-1.00173	-3.29121	0.05980
H	-1.86570	-2.58968	1.41062
H	1.39116	-2.76985	1.14571
H	2.01391	2.00452	-1.24319
H	4.50857	1.79481	-1.02137
H	5.44636	-0.29380	0.01531
H	3.87078	-2.10164	0.73494
H	-2.98318	1.42064	-1.63302
H	-2.51146	-0.00794	-2.58923
H	-4.05191	-0.01571	-1.68429
H	-0.28779	3.23453	0.15027
H	-0.18581	3.27055	1.93673
H	1.15052	2.59371	0.97453
H	0.93796	-2.58746	-0.56470
O	-0.42018	1.63642	-1.53845
H	-0.34531	1.40725	-2.48839
F	-0.16098	-0.91531	-1.92903

^{3}FePyTACNOHN$_3$
Charge: 2+
Energy: -1424866.2353750

N	2.35051	0.57517	-0.03111
C	3.01442	-0.77454	0.00538
C	2.27319	-1.75457	-0.88930
N	0.78997	-1.72807	-0.66551
C	0.31905	-2.43006	0.56698
C	0.60823	-1.63666	1.83454
N	0.36410	-0.15481	1.64126
C	2.43458	1.26539	1.29725
C	1.43819	0.67193	2.31804
C	-1.01277	0.22983	2.10107
C	-2.03018	-0.14307	1.05605
N	-1.57277	-0.08630	-0.21899
C	-2.41318	-0.26067	-1.25810
C	-3.76242	-0.52936	-1.05398
C	-4.24247	-0.62365	0.25422
C	-3.36369	-0.42764	1.32433
Fe	0.36611	0.29630	-0.39216
C	2.98164	1.43316	-1.08079
C	0.14047	-2.36749	-1.84854
H	3.05621	-1.11441	1.03777
H	4.05142	-0.67819	-0.33240
H	2.66046	-2.77162	-0.75272
H	2.42290	-1.47618	-1.93400
H	0.77202	-3.42709	0.63550
H	-0.75670	-2.56774	0.45220
H	1.63854	-1.77470	2.15178
H	-0.01785	-2.00792	2.65190
H	2.19399	2.31170	1.12063
H	3.46533	1.20911	1.66554
H	0.96297	1.49336	2.85415
H	1.93622	0.05158	3.06606
H	-1.23537	-0.21215	3.07774
H	-1.97049	-0.17876	-2.24351
H	-4.41769	-0.66085	-1.90824
H	-5.28963	-0.84023	0.44181
H	-3.71089	-0.48099	2.35119
H	2.96539	0.90283	-2.03270
H	2.41707	2.36178	-1.16596
H	4.01516	1.65798	-0.79633
H	0.37054	-1.78766	-2.74068
H	0.51082	-3.39283	-1.96132
H	-0.93864	-2.39463	-1.70315
H	-1.02695	1.31778	2.21228
O	0.42105	0.43239	-2.14413
H	0.43317	1.34940	-2.47729
N	0.07893	2.10435	-0.03728
N	-0.95110	2.64856	-0.45802
N	-1.87473	3.21708	-0.81379

^{3}FePyTACNOHNCS
Charge: 2+
Energy: -1629971.7867396

N	2.22387	0.77930	-0.00607
C	3.16046	-0.39190	0.09951
C	2.66541	-1.51635	-0.79248
N	1.19727	-1.77708	-0.60959
C	0.85040	-2.54333	0.62737
C	0.91058	-1.68306	1.88513
N	0.37316	-0.29094	1.64255
C	2.11060	1.51159	1.29519
C	1.22909	0.75294	2.31633
C	-1.06703	-0.19659	2.04385
C	-1.94065	-0.81739	0.98392
N	-1.45924	-0.70992	-0.27691
C	-2.20426	-1.09993	-1.32768
C	-3.46940	-1.65157	-1.15078
C	-3.96374	-1.80408	0.14623
C	-3.18863	-1.37853	1.22944
Fe	0.36465	0.06942	-0.40540
C	2.69794	1.71331	-1.07258
C	0.74457	-2.57321	-1.79256
H	3.22854	-0.69519	1.14209
H	4.16759	-0.08767	-0.20385
H	3.23961	-2.43495	-0.62221
H	2.78972	-1.23027	-1.83835
H	1.50832	-3.41450	0.73520
H	-0.16376	-2.91724	0.48404
H	1.93242	-1.59926	2.24706
H	0.34077	-2.16569	2.68575
H	1.66198	2.47846	1.06938
H	3.11250	1.69887	1.69894
H	0.58346	1.47212	2.82215
H	1.83004	0.27603	3.09355
H	-1.23278	-0.64104	3.03129
H	-1.75149	-0.95684	-2.30165
H	-4.04782	-1.95665	-2.01605
H	-4.94225	-2.24301	0.31478
H	-3.55129	-1.47129	2.24811
H	2.79972	1.16372	-2.00721
H	1.96227	2.50580	-1.20864
H	3.65949	2.14977	-0.78115
H	0.86632	-1.97272	-2.69166
H	1.33713	-3.49207	-1.86393
H	-0.30484	-2.83810	-1.67396
H	-1.32216	0.86506	2.10859
O	0.42940	0.20994	-2.17228
H	0.09599	1.06982	-2.48799
N	-0.42911	1.79074	-0.22812
C	-1.02132	2.82140	-0.27331
S	-1.82133	4.22174	-0.31401

^{6}FemepBrOH
Charge: 1+
Energy: -2984475.3165680

Fe	0.01253	0.12583	-0.51094
C	2.93217	1.24900	0.16105

H	2.37607	2.16148	0.34171
N	2.19497	0.17249	-0.16667
N	0.59946	-2.04430	-0.18726
C	4.31968	1.19932	0.25151
N	-0.45309	-0.17205	1.76351
N	-2.12481	-0.22728	-0.36606
C	4.96449	-0.01042	-0.00662
C	4.19925	-1.12632	-0.34745
H	4.66578	-2.08463	-0.55236
C	2.81461	-0.99775	-0.42723
C	1.91818	-2.13515	-0.85212
H	1.73531	-2.04281	-1.92751
H	2.39483	-3.10661	-0.66010
C	-0.36978	-2.93440	-0.86167
H	-0.49219	-2.59130	-1.88990
H	-1.33572	-2.87498	-0.35921
C	0.69468	-2.31604	1.26776
H	1.65316	-1.93033	1.62280
C	-0.44702	-1.63630	2.01598
H	-1.40293	-2.04175	1.67588
C	0.51329	0.53424	2.63162
H	0.55117	1.58342	2.33306
H	1.50702	0.10447	2.50077
C	-1.81109	0.38544	1.95364
H	-1.72115	1.47700	1.94108
H	-2.23212	0.09018	2.92536
C	-2.72435	-0.02057	0.82152
C	-4.10621	-0.12364	0.96360
H	-4.56500	0.03754	1.93396
C	-4.87931	-0.42622	-0.15808
C	-4.24956	-0.62437	-1.38859
C	-2.86485	-0.51670	-1.45110
H	-2.29988	-0.65166	-2.36660
H	6.04561	-0.08650	0.05839
H	4.87483	2.09207	0.51791
H	-5.95865	-0.50645	-0.07187
H	-4.81670	-0.85745	-2.28312
H	0.22624	0.45963	3.68984
H	-0.02170	-3.97641	-0.85076
H	0.68525	-3.39748	1.46247
H	-0.37064	-1.84436	3.09243
O	0.06785	-0.23088	-2.31525
H	0.11832	0.54758	-2.89592
Br	-0.26933	2.59749	-0.37655

^{6}FemepClOH
Charge: 1+
Energy: -1657947.6719184

Fe	0.00432	-0.20830	-0.63472
C	-2.92294	-1.41638	-0.31580
H	-2.37686	-2.34632	-0.42425
N	-2.17294	-0.30027	-0.30739
N	-0.53523	1.79158	0.31498
C	-4.30929	-1.37709	-0.20305
N	0.48398	-0.58278	1.62281
N	2.15154	0.05878	-0.41458
C	-4.93547	-0.13672	-0.07686
C	-4.15513	1.02029	-0.07198
H	-4.60817	2.00178	0.02514
C	-2.77309	0.90267	-0.19929
C	-1.85628	2.09920	-0.27690
H	-1.68209	2.32631	-1.33360
H	-2.31181	2.97857	0.19961
C	0.44904	2.82058	-0.08344
H	0.55856	2.78874	-1.16828
H	1.41619	2.59940	0.36903
C	-0.61544	1.63266	1.78765
H	-1.58088	1.18109	2.02771
C	0.51381	0.74101	2.29403
H	1.47773	1.20818	2.07816
C	-0.49972	-1.49216	2.24765
H	-0.56778	-2.39982	1.64565
H	-1.48124	-1.01705	2.26388
C	1.82567	-1.20685	1.62131
H	1.70307	-2.24068	1.28157
H	2.25811	-1.22917	2.63188
C	2.74751	-0.50403	0.65300
C	4.13164	-0.47665	0.80854
H	4.58812	-0.92765	1.68393
C	4.90960	0.12919	-0.17897
C	4.28290	0.69627	-1.29056
C	2.89586	0.64077	-1.37112
H	2.33233	1.05330	-2.20055
H	-6.01498	-0.06928	0.01806
H	-4.87828	-2.30028	-0.21483
H	5.99056	0.15830	-0.08112
H	4.85405	1.17231	-2.08009
H	-0.20817	-1.74831	3.27590
H	0.12390	3.82105	0.23362
H	-0.57953	2.61108	2.28662
H	0.44524	0.62659	3.38502
O	-0.04538	0.67134	-2.25299
H	-0.11884	0.09921	-3.03590
Cl	0.19343	-2.44176	-1.11273

^{6}FemepFOH
Charge: 1+
Energy: -1431823.7739280

Fe	-0.00498	-0.05079	-0.77228
C	2.88390	1.08333	-1.11181
H	2.31366	1.79907	-1.69382
N	2.15244	0.13221	-0.50900
N	0.50080	-1.32104	1.08835
C	4.26970	1.12625	-0.99276
N	-0.49794	1.38667	0.99841
N	-2.16546	-0.15827	-0.49700
C	4.90278	0.15004	-0.22075
C	4.13532	-0.83957	0.39711
H	4.59856	-1.61316	1.00129
C	2.75357	-0.82476	0.22074
C	1.82997	-1.88845	0.76728
H	1.67156	-2.63177	-0.02098
H	2.27392	-2.39249	1.63741
C	-0.49255	-2.40591	1.23530
H	-0.58237	-2.92071	0.27753
H	-1.46417	-1.98088	1.49058
C	0.55337	-0.44514	2.28412
H	1.52342	0.05807	2.29162
C	-0.56613	0.59416	2.24718
H	-1.53711	0.09319	2.27824
C	0.51029	2.46335	1.06832
H	0.61692	2.89280	0.07109
H	1.47359	2.04853	1.36715
C	-1.81191	1.94982	0.62251
H	-1.63499	2.62828	-0.21892
H	-2.25561	2.53015	1.44416
C	-2.75174	0.86441	0.15267
C	-4.13321	0.92033	0.32123
H	-4.58213	1.74941	0.85891
C	-4.91888	-0.10084	-0.21673
C	-4.30256	-1.14922	-0.90246
C	-2.91624	-1.14149	-1.02105
H	-2.35824	-1.91543	-1.53692
H	5.98186	0.15791	-0.10015
H	4.83444	1.90617	-1.49180
H	-5.99819	-0.07779	-0.10016
H	-4.88059	-1.95777	-1.33650
H	0.21699	3.24208	1.78652
H	-0.19455	-3.11581	2.01959
H	0.48844	-1.03901	3.20668
H	-0.50677	1.24414	3.13198
O	0.02459	-1.62508	-1.74238
H	0.16447	-1.54117	-2.70024
F	0.01852	1.41585	-1.81287

^{6}FemepN_3OH
Charge: 1+
Energy: -1472207.2626415

Fe	0.03440	0.38669	-0.41691
C	2.88965	1.44495	0.40372
H	2.28431	2.27831	0.74442
N	2.20408	0.40916	-0.10852
N	0.69033	-1.81988	-0.53560
C	4.27872	1.44441	0.48340
N	-0.39055	-0.40384	1.74864
N	-2.10974	-0.06025	-0.33178
C	4.97253	0.32737	0.01471
C	4.25677	-0.74465	-0.52053
H	4.76565	-1.62784	-0.89344
C	2.86671	-0.66663	-0.57636
C	2.00624	-1.73764	-1.20480
H	1.81225	-1.44775	-2.24280
H	2.52132	-2.70897	-1.20426
C	-0.25949	-2.58284	-1.37205
H	-0.40039	-2.04304	-2.30961
H	-1.22302	-2.64960	-0.86496
C	0.80205	-2.37533	0.83393
H	1.75510	-2.04774	1.25664
C	-0.34801	-1.88579	1.71068
H	-1.29791	-2.24033	1.30297
C	0.57754	0.15241	2.71520
H	0.59895	1.23805	2.60152
H	1.57495	-0.23377	2.50214
C	-1.75078	0.08777	2.05454
H	-1.66916	1.16534	2.23378
H	-2.15220	-0.37717	2.96670
C	-2.68327	-0.12392	0.88438
C	-4.05458	-0.32024	1.03138
H	-4.49160	-0.37975	2.02318
C	-4.84631	-0.43103	-0.11312
C	-4.24465	-0.34979	-1.37024
C	-2.86711	-0.16535	-1.43708
H	-2.32127	-0.09267	-2.37162
H	6.05645	0.28965	0.06599
H	4.79892	2.29854	0.90305

H	-5.91805	-0.58005	-0.02330
H	-4.82702	-0.42862	-2.28176
H	0.30713	-0.10748	3.74859
H	0.11179	-3.59793	-1.57195
H	0.81790	-3.47425	0.81105
H	-0.25415	-2.30147	2.72420
O	0.03498	0.38225	-2.26600
H	0.11994	1.22602	-2.73904
N	-0.18023	2.20069	0.23767
N	-0.79739	3.12658	-0.26063
N	-1.37652	4.01733	-0.69840

^{6}FemepNCSOH
Charge: 1+
Energy: -1677315.4606026

Fe	0.08096	-0.08906	-0.65258
C	2.81220	1.46605	-0.28980
H	2.14222	2.31536	-0.36238
N	2.22319	0.25890	-0.32227
N	0.87383	-2.04460	0.21702
C	4.19116	1.61286	-0.17741
N	-0.42979	0.12000	1.64549
N	-2.02713	-0.61769	-0.42162
C	4.97923	0.46364	-0.09534
C	4.36417	-0.78875	-0.13335
H	4.94764	-1.70185	-0.07135
C	2.97817	-0.85524	-0.25782
C	2.22340	-2.15738	-0.38193
H	2.07796	-2.36451	-1.44701
H	2.79000	-2.98779	0.06231
C	0.02825	-3.17460	-0.22609
H	-0.08461	-3.11424	-1.30926
H	-0.95942	-3.09392	0.22923
C	0.94097	-1.94523	1.69583
H	1.84261	-1.38643	1.95778
C	-0.28904	-1.23002	2.24490
H	-1.18720	-1.80280	2.00128
C	0.44005	1.10890	2.31447
H	0.37748	2.05844	1.78033
H	1.47570	0.76850	2.28450
C	-1.83797	0.56915	1.68432
H	-1.85783	1.63501	1.43365
H	-2.26268	0.46423	2.69342
C	-2.67679	-0.17740	0.67200
C	-4.04879	-0.36610	0.82616
H	-4.54779	-0.01021	1.72200
C	-4.76006	-1.00942	-0.18742
C	-4.07951	-1.45320	-1.32308
C	-2.70787	-1.23774	-1.40172
H	-2.10615	-1.54738	-2.24924
H	6.05821	0.54015	-0.00136
H	4.63096	2.60394	-0.15443
H	-5.83046	-1.16344	-0.09042
H	-4.59762	-1.95599	-2.13241
H	0.14255	1.26043	3.36178
H	0.47642	-4.13785	0.05456
H	1.03313	-2.94237	2.14857
H	-0.23139	-1.16688	3.34104
O	0.21734	-0.90390	-2.30523
H	0.22449	-0.31415	-3.07748
N	-0.29363	1.79512	-0.90717
C	-0.74768	2.87570	-0.64840
S	-1.35516	4.30007	-0.25866

^{6}FemepOHBr
Charge: 1+
Energy: -2984475.3181556

Fe	0.01245	0.12605	-0.51101
C	-2.86506	-0.51738	-1.45083
H	-2.30025	-0.65254	-2.36640
N	-2.12487	-0.22767	-0.36598
N	-0.45280	-0.17157	1.76347
C	-4.24974	-0.62509	-1.38810
N	0.59949	-2.04421	-0.18728
N	2.19522	0.17261	-0.16663
C	-4.87932	-0.42667	-0.15753
C	-4.10607	-0.12381	0.96395
H	-4.56469	0.03756	1.93436
C	-2.72421	-0.02073	0.82162
C	-1.81096	0.38557	1.95365
H	-1.72128	1.47715	1.94109
H	-2.23182	0.09020	2.92541
C	0.51344	0.53502	2.63154
H	0.55116	1.58417	2.33289
H	1.50723	0.10535	2.50080
C	-0.44629	-1.63580	2.01620
H	-1.40218	-2.04157	1.67643
C	0.69529	-2.31557	1.26783
H	1.65391	-1.92989	1.62245
C	-0.36969	-2.93475	-0.86094
H	-0.49328	-2.59192	-1.88911
H	-1.33529	-2.87598	-0.35771
C	1.91791	-2.13470	-0.85274
H	1.73451	-2.04139	-1.92796
H	2.39456	-3.10636	-0.66169
C	2.81458	-0.99766	-0.42743
C	4.19922	-1.12656	-0.34762
H	4.66554	-2.08493	-0.55275
C	4.96466	-0.01090	-0.00654
C	4.32010	1.19895	0.25177
C	2.93262	1.24894	0.16127
H	2.37673	2.16151	0.34209
H	-5.95865	-0.50690	-0.07117
H	-4.81701	-0.85837	-2.28249
H	6.04577	-0.08722	0.05853
H	4.87542	2.09153	0.51836
H	-0.02106	-3.97659	-0.85030
H	0.22632	0.46048	3.68974
H	-0.36963	-1.84359	3.09269
H	0.68581	-3.39698	1.46279
O	0.06748	-0.23093	-2.31527
H	0.11661	0.54784	-2.89566
Br	-0.26972	2.59747	-0.37701

^{6}FemepOHCl
Charge: 1+
Energy: -1657947.6675949

Fe	0.00437	-0.20805	-0.63510
C	2.89676	0.64033	-1.37041
H	2.33378	1.05294	-2.20019
N	2.15190	0.05822	-0.41449
N	0.48335	-0.58288	1.62234
C	4.28380	0.69597	-1.28898
N	-0.53522	1.79157	0.31474
N	-2.17306	-0.30031	-0.30850
C	4.90984	0.12888	-0.17707
C	4.13126	-0.47718	0.80989
H	4.58727	-0.92821	1.68551
C	2.74728	-0.50470	0.65344
C	1.82485	-1.20758	1.62107
H	1.70179	-2.24119	1.28082
H	2.25686	-1.23052	2.63181
C	-0.50077	-1.49202	2.24696
H	-0.56920	-2.39947	1.64470
H	-1.48208	-1.01648	2.26333
C	0.51358	0.74081	2.29383
H	1.47768	1.20766	2.07812
C	-0.61534	1.63291	1.78752
H	-1.58095	1.18178	2.02769
C	0.44916	2.82012	-0.08426
H	0.55905	2.78667	-1.16903
H	1.41613	2.59940	0.36886
C	-1.85632	2.09915	-0.27715
H	-1.68208	2.32624	-1.33385
H	-2.31183	2.97854	0.19931
C	-2.77308	0.90263	-0.19936
C	-4.15500	1.02028	-0.07069
H	-4.60787	2.00177	0.02727
C	-4.93544	-0.13667	-0.07529
C	-4.30943	-1.37701	-0.20266
C	-2.92320	-1.41634	-0.31674
H	-2.37729	-2.34628	-0.42614
H	5.99072	0.15809	-0.07845
H	4.85533	1.17218	-2.07813
H	-6.01484	-0.06921	0.02073
H	-4.87848	-2.30017	-0.21434
H	0.12397	3.82098	0.23152
H	-0.20929	-1.74851	3.27514
H	0.44482	0.62620	3.38479
H	-0.57887	2.61139	2.28629
O	-0.04343	0.67307	-2.25291
H	-0.11668	0.10101	-3.03592
Cl	0.19290	-2.44140	-1.11372

^{6}FemepOHF
Charge: 1+
Energy: -1431823.7716689

Fe	-0.00495	-0.05064	-0.77191
C	-2.91560	-1.14222	-1.02158
H	-2.35693	-1.91582	-1.53723
N	-2.16543	-0.15853	-0.49733
N	-0.49884	1.38768	0.99770
C	-4.30189	-1.15071	-0.90325
N	0.50072	-1.31973	1.08950
N	2.15270	0.13206	-0.50852
C	-4.91897	-0.10265	-0.21761
C	-4.13400	0.91892	0.32050
H	-4.58344	1.74774	0.85814
C	-2.75241	0.86374	0.15225
C	-1.81343	1.94977	0.62245
H	-1.63773	2.62932	-0.21834
H	-2.25746	2.52905	1.44469
C	0.50908	2.46488	1.06563
H	0.61549	2.89206	0.06741

H	1.47243	2.05089	1.36543
C	-0.56594	0.59627	2.24726
H	-1.53684	0.09522	2.27947
C	0.55371	-0.44284	2.28446
H	1.52369	0.06052	2.29107
C	-0.49290	-2.40417	1.23738
H	-0.58298	-2.91971	0.28002
H	-1.46441	-1.97873	1.49243
C	1.82968	-1.88780	0.76877
H	1.67101	-2.63164	-0.01895
H	2.27350	-2.39136	1.63925
C	2.75362	-0.82485	0.22144
C	4.13543	-0.84031	0.39733
H	4.59847	-1.61387	1.00170
C	4.90320	0.14860	-0.22127
C	4.27032	1.12479	-0.99348
C	2.88444	1.08253	-1.11203
H	2.31440	1.79827	-1.69420
H	-5.99832	-0.08026	-0.10130
H	-4.87943	-1.95957	-1.33736
H	5.98232	0.15596	-0.10106
H	4.83527	1.90422	-1.49307
H	-0.19505	-3.11359	2.02217
H	0.21543	3.24495	1.78222
H	-0.50608	1.24711	3.13139
H	0.48928	-1.03590	3.20759
O	0.02508	-1.62570	-1.74104
H	0.16622	-1.54221	-2.69875
F	0.01992	1.41506	-1.81374

^{6}FemepOHN$_3$
Charge: 1+
Energy: -1472207.2599306

Fe	0.03459	0.38673	-0.41657
C	-2.86721	-0.16462	-1.43709
H	-2.32129	-0.09184	-2.37156
N	-2.10988	-0.05998	-0.33170
N	-0.39098	-0.40452	1.74860
C	-4.24479	-0.34880	-1.37042
N	0.69015	-1.81967	-0.53629
N	2.20418	0.40880	-0.10794
C	-4.84659	-0.43030	-0.11338
C	-4.05492	-0.32006	1.03120
H	-4.49202	-0.37985	2.02296
C	-2.68356	-0.12396	0.88435
C	-1.75114	0.08706	2.05468
H	-1.66947	1.16453	2.23453
H	-2.15268	-0.37835	2.96655
C	0.57717	0.15120	2.71544
H	0.59859	1.23689	2.60233
H	1.57456	-0.23488	2.50215
C	-0.34852	-1.88647	1.70992
H	-1.29844	-2.24073	1.30202
C	0.80158	-2.37571	0.83302
H	1.75459	-2.04838	1.25602
C	-0.25974	-2.58205	-1.37317
H	-0.40029	-2.04189	-2.31056
H	-1.22340	-2.64864	-0.86632
C	2.00617	-1.73741	-1.20531
H	1.81238	-1.44725	-2.24327
H	2.52111	-2.70881	-1.20496
C	2.86673	-0.66672	-0.57645
C	4.25681	-0.74472	-0.52100
H	4.76564	-1.62770	-0.89450
C	4.97265	0.32706	0.01460
C	4.27890	1.44385	0.48401
C	2.88982	1.44439	0.40464
H	2.28452	2.27756	0.74587
H	-5.91837	-0.57913	-0.02371
H	-4.82710	-0.42723	-2.28203
H	6.05658	0.28937	0.06559
H	4.79917	2.29778	0.90397
H	0.11124	-3.59720	-1.57334
H	0.30676	-0.10924	3.74870
H	-0.25474	-2.30263	2.72326
H	0.81735	-3.47462	0.80964
O	0.03489	0.38354	-2.26564
H	0.11578	1.22790	-2.73835
N	-0.17981	2.20051	0.23897
N	-0.79618	3.12654	-0.26010
N	-1.37448	4.01753	-0.69857

^{6}FemepOHNCS
Charge: 1+
Energy: -1677315.4600316

Fe	0.08138	-0.08901	-0.65254
C	-2.70716	-1.23879	-1.40162
H	-2.10525	-1.54851	-2.24898
N	-2.02667	-0.61841	-0.42155
N	-0.42972	0.12022	1.64531
C	-4.07876	-1.45452	-1.32314
N	0.87491	-2.04418	0.21744
N	2.22335	0.25964	-0.32209
C	-4.75956	-1.01069	-0.18766
C	-4.04857	-0.36706	0.82591
H	-4.54777	-0.01113	1.72162
C	-2.67659	-0.17808	0.67190
C	-1.83808	0.56879	1.68422
H	-1.85845	1.63466	1.43363
H	-2.26268	0.46365	2.69334
C	0.43964	1.10960	2.31416
H	0.37680	2.05896	1.77972
H	1.47544	0.76960	2.28445
C	-0.28842	-1.22961	2.24504
H	-1.18636	-1.80278	2.00153
C	0.94187	-1.94451	1.69620
H	1.84331	-1.38538	1.95816
C	0.02981	-3.17456	-0.22560
H	-0.08291	-3.11424	-1.30879
H	-0.95795	-3.09416	0.22958
C	2.22458	-2.15658	-0.38135
H	2.07932	-2.36404	-1.44639
H	2.79146	-2.98667	0.06313
C	2.97885	-0.85412	-0.25756
C	4.36485	-0.78695	-0.13339
H	4.94876	-1.69976	-0.07132
C	4.97931	0.46575	-0.09581
C	4.19068	1.61459	-0.17799
C	2.81178	1.46710	-0.29011
H	2.14132	2.31603	-0.36273
H	-5.82995	-1.16490	-0.09079
H	-4.59665	-1.95757	-2.13245
H	6.05827	0.54280	-0.00207
H	4.63004	2.60587	-0.15537
H	0.47831	-4.13760	0.05521
H	0.14192	1.26131	3.36137
H	-0.23083	-1.16617	3.34117
H	1.03429	-2.94153	2.14916
O	0.21796	-0.90427	-2.30498
H	0.22334	-0.31485	-3.07751
N	-0.29404	1.79484	-0.90774
C	-0.74962	2.87473	-0.64874
S	-1.35911	4.29808	-0.25850

^{3}FeMePy2CHTACNOH
Charge: 3+
Energy: -1476623.9815443

N	-1.93881	-1.45137	-0.00844
C	-3.12403	-0.73261	0.58952
C	-3.28191	0.61616	-0.07122
N	-1.97410	1.36563	-0.10649
C	-1.54991	2.01117	1.19198
C	-0.91671	1.03468	2.19314
N	-0.20274	-0.12132	1.50928
C	-1.29812	-2.33632	1.01572
C	-0.61399	-1.47520	2.08633
C	1.30971	0.01405	1.46131
C	1.79462	-1.14152	0.59846
C	1.63719	1.27671	0.69411
N	0.89534	1.38548	-0.43822
C	1.17258	2.34598	-1.33980
C	2.18970	3.27297	-1.11361
C	2.92249	3.20196	0.07325
C	2.64778	2.17764	0.99224
N	1.01208	-1.31815	-0.49752
C	1.33525	-2.24069	-1.42324
C	2.46417	-3.04486	-1.27189
C	3.26389	-2.88570	-0.13754
C	2.92490	-1.91350	0.81616
Fe	-0.53756	-0.02854	-0.50342
C	-2.35790	-2.25074	-1.20412
C	-2.12379	2.43859	-1.14752
O	-0.78980	-0.03357	-2.20834
H	-2.97665	-0.63740	1.66385
H	-4.02513	-1.33779	0.44461
H	-4.04168	1.22113	0.43669
H	-3.59380	0.49535	-1.11068
H	-2.41231	2.51121	1.64778
H	-0.83110	2.78359	0.92390
H	-1.67135	0.61365	2.85401
H	-0.20880	1.57322	2.83023
H	-0.58237	-2.97476	0.50128
H	-2.05945	-2.98620	1.46392
H	0.26728	-1.99049	2.47258
H	-1.26533	-1.29537	2.94071
H	1.73559	0.00259	2.46868
H	0.57307	2.36331	-2.24261
H	2.39620	4.03262	-1.86098
H	3.70908	3.92251	0.27869
H	3.21839	2.08135	1.91088
H	0.68157	-2.32415	-2.28450
H	2.70560	-3.77787	-2.03519
H	4.14427	-3.50569	0.00609
H	3.53128	-1.76558	1.70459
H	-2.82754	-1.59681	-1.93765

H	-1.48215	-2.71776	-1.65092
H	-3.06218	-3.02762	-0.88720
H	-2.24934	1.97399	-2.12497
H	-3.00640	3.04218	-0.90765
H	-1.25154	3.08726	-1.14715
H	-0.03812	0.00964	-2.83335

[4]FePyTACNOOH
Charge: 2+
Energy: -1368979.9152150

N	-2.32899	-0.16908	-0.46102
C	-2.82072	0.48043	0.80366
C	-1.97225	1.69628	1.12401
N	-0.50114	1.39838	1.03624
C	0.06692	0.64300	2.19687
C	-0.29777	-0.83771	2.16746
N	-0.24517	-1.40135	0.76928
C	-2.47480	-1.66300	-0.40545
C	-1.40643	-2.32734	0.49846
C	1.08171	-2.03511	0.48396
C	2.11244	-0.97881	0.17878
N	1.63821	0.13787	-0.42881
C	2.47750	1.07943	-0.90377
C	3.85302	0.95842	-0.74566
C	4.35909	-0.16232	-0.08239
C	3.47763	-1.14305	0.38295
Fe	-0.32248	0.15478	-0.64586
C	-3.05913	0.37074	-1.64986
C	0.21424	2.70677	0.91983
H	-2.80133	-0.25557	1.60396
H	-3.86656	0.77741	0.67372
H	-2.21592	2.09602	2.11552
H	-2.16686	2.48113	0.39021
H	-0.26318	1.09664	3.13951
H	1.14944	0.76040	2.13914
H	-1.29605	-0.99798	2.56786
H	0.38518	-1.39266	2.81903
H	-2.36117	-2.02126	-1.42611
H	-3.48909	-1.90255	-0.06604
H	-1.03867	-3.21946	-0.00830
H	-1.82850	-2.65604	1.45057
H	1.39224	-2.69067	1.30442
H	2.01691	1.91859	-1.41194
H	4.50756	1.72887	-1.13862
H	5.42879	-0.27870	0.06256
H	3.84505	-2.03366	0.88261
H	-2.97799	1.45763	-1.65996
H	-2.60575	-0.02924	-2.55580
H	-4.11124	0.07114	-1.59696
H	-0.09492	3.20491	0.00102
H	-0.02835	3.33504	1.78414
H	1.28948	2.53739	0.89733
H	0.96690	-2.64200	-0.41830
O	-0.39677	1.45187	-1.62841
O	-0.22369	-1.09639	-1.89652
H	-0.09702	-0.70066	-2.78060

[5]FemepOOH
Charge: 1+
Energy: -1416321.4633081

Fe	0.01580	-0.05863	-0.69263
C	-2.94125	-1.24172	-0.88467
H	-2.38277	-2.07038	-1.30713
N	-2.19287	-0.22985	-0.42256
N	-0.50710	1.44528	0.85729
C	-4.33207	-1.21186	-0.82868
N	0.50211	-1.23203	1.09460
N	2.18302	0.18882	-0.46836
O	-0.09912	1.02324	-1.89789
C	-4.95277	-0.09057	-0.27380
C	-4.16755	0.96476	0.19364
H	-4.61915	1.85337	0.62369
C	-2.78176	0.86175	0.08806
C	-1.83465	1.97682	0.46573
H	-1.67454	2.60033	-0.42021
H	-2.25524	2.60818	1.26064
C	0.48253	2.54379	0.87262
H	0.58543	2.92572	-0.14451
H	1.45089	2.16394	1.19768
C	-0.56883	0.72911	2.16004
H	-1.53736	0.22837	2.22259
C	0.55410	-0.29693	2.25288
H	1.52237	0.20822	2.23373
C	-0.47728	-2.32162	1.30800
H	-0.57587	-2.87722	0.37452
H	-1.44771	-1.89727	1.56451
C	1.83902	-1.81693	0.81776
H	1.68853	-2.58898	0.05652
H	2.25664	-2.28854	1.71782
C	2.77777	-0.78169	0.24647
C	4.16382	-0.84623	0.37513
H	4.62137	-1.63113	0.96907
C	4.94224	0.10829	-0.28205
C	4.31597	1.09498	-1.04700
C	2.92596	1.09931	-1.11485
H	2.36642	1.82419	-1.69703
O	0.09345	-1.61271	-1.63143
H	-6.03522	-0.03623	-0.20828
H	-4.91084	-2.04614	-1.21016
H	6.02462	0.07906	-0.20112
H	4.88982	1.84455	-1.58104
H	-0.14909	-2.99112	2.11424
H	0.16578	3.35112	1.54646
H	-0.51031	1.43843	2.99688
H	0.49153	-0.85025	3.19952
H	0.10154	-1.44107	-2.58787

[6]FeMeN4PyBr
Charge: 2+
Energy: -3138118.5751779

C	-0.61637	-2.94448	3.29573
C	0.59881	-3.59897	3.09393
C	1.42886	-3.19907	2.03891
C	1.00643	-2.15721	1.22538
N	-0.16938	-1.52366	1.42883
C	1.76201	-1.65776	-0.00000
C	1.00643	-2.15721	-1.22538
C	1.42886	-3.19907	-2.03891
C	0.59881	-3.59897	-3.09393
C	-0.61637	-2.94448	-3.29573
C	-0.96935	-1.90341	-2.43813
N	-0.16938	-1.52366	-1.42883
N	1.69471	-0.15916	-0.00000
C	2.22843	0.47001	-1.23889
C	2.22843	0.47001	1.23889
C	1.34447	1.59129	1.74431
C	1.34447	1.59129	-1.74431
C	1.84943	2.61821	-2.53654
C	0.96991	3.56959	-3.05802
C	-0.39198	3.46981	-2.76738
C	-0.82479	2.42727	-1.95648
N	0.02685	1.50767	-1.45786
N	0.02685	1.50767	1.45786
C	-0.82479	2.42727	1.95648
C	-0.39198	3.46981	2.76738
C	0.96991	3.56959	3.05802
C	1.84943	2.61821	2.53654
C	-0.96935	-1.90341	2.43813
H	2.79500	-2.02382	-0.00000
H	-1.28529	-3.23162	4.09966
H	0.90175	-4.41144	3.74716
H	2.38025	-3.68876	1.85743
H	2.38025	-3.68876	-1.85743
H	0.90175	-4.41144	-3.74716
H	-1.28529	-3.23162	-4.09966
H	-1.90288	-1.36064	-2.53886
H	3.25153	0.82730	-1.08032
H	2.28185	-0.29463	-2.01984
H	2.28185	-0.29463	2.01984
H	3.25153	0.82730	1.08032
H	2.91309	2.66924	-2.74741
H	1.34418	4.37675	-3.68016
H	-1.10819	4.18663	-3.15387
H	-1.86705	2.30586	-1.68464
H	-1.86705	2.30586	1.68464
H	-1.10819	4.18663	3.15387
H	1.34418	4.37675	3.68016
H	2.91309	2.66924	2.74741
H	-1.90288	-1.36064	2.53886
Fe	-0.53751	0.05803	0.00000
Br	-2.93040	0.14073	0.00000

[6]FeMeN4PyCl
Charge: 2+
Energy: -1811590.5748810

C	-0.84044	-2.93229	3.28402
C	0.38088	-3.57855	3.09183
C	1.21709	-3.17536	2.04250
C	0.79478	-2.13688	1.22477
N	-0.38569	-1.51079	1.42184
C	1.55018	-1.63396	0.00000
C	0.79478	-2.13688	-1.22477
C	1.21709	-3.17536	-2.04250
C	0.38088	-3.57855	-3.09183
C	-0.84044	-2.93229	-3.28402
C	-1.19305	-1.89349	-2.42337
N	-0.38569	-1.51079	-1.42184
N	1.47546	-0.13565	0.00000
C	2.00237	0.49812	-1.23950
C	2.00237	0.49812	1.23950
C	1.10260	1.60533	1.74902
C	1.10260	1.60533	-1.74902
C	1.58769	2.63484	-2.55020
C	0.69038	3.56975	-3.07179

C	-0.66863	3.45232	-2.77313
C	-1.08174	2.40857	-1.95362
N	-0.21183	1.50609	-1.45620
N	-0.21183	1.50609	1.45620
C	-1.08174	2.40857	1.95362
C	-0.66863	3.45232	2.77313
C	0.69038	3.56975	3.07179
C	1.58769	2.63484	2.55020
C	-1.19305	-1.89349	2.42337
H	2.58441	-1.99645	0.00000
H	-1.51366	-3.22405	4.08268
H	0.68380	-4.38852	3.74816
H	2.17220	-3.66055	1.86860
H	2.17220	-3.66055	-1.86860
H	0.68380	-4.38852	-3.74816
H	-1.51366	-3.22405	-4.08268
H	-2.13042	-1.35494	-2.51386
H	3.01983	0.87096	-1.08040
H	2.06856	-0.26737	-2.01873
H	2.06856	-0.26737	2.01873
H	3.01983	0.87096	1.08040
H	2.64918	2.70088	-2.76773
H	1.04909	4.37868	-3.70077
H	-1.39685	4.15676	-3.15993
H	-2.11984	2.27087	-1.67267
H	-2.11984	2.27087	1.67267
H	-1.39685	4.15676	3.15993
H	1.04909	4.37868	3.70077
H	2.64918	2.70088	2.76773
H	-2.13042	-1.35494	2.51386
Fe	-0.77276	0.06293	0.00000
Cl	-2.97785	0.16386	0.00000

^{6}FeMeN4PyF
Charge: 2+
Energy: -1585464.6907478

C	-0.97045	-2.91663	3.28824
C	0.25237	-3.56128	3.09953
C	1.08892	-3.16079	2.04951
C	0.66591	-2.12758	1.22508
N	-0.51668	-1.50365	1.41822
C	1.42726	-1.63020	-0.00000
C	0.66591	-2.12758	-1.22508
C	1.08892	-3.16079	-2.04951
C	0.25237	-3.56128	-3.09953
C	-0.97045	-2.91663	-3.28824
C	-1.32275	-1.88181	-2.42270
N	-0.51668	-1.50365	-1.41822
N	1.37571	-0.13111	-0.00000
C	1.90463	0.49932	-1.24079
C	1.90463	0.49932	1.24079
C	0.99483	1.59397	1.76561
C	0.99483	1.59397	-1.76561
C	1.46132	2.61630	-2.58716
C	0.54791	3.53568	-3.10948
C	-0.80735	3.41436	-2.79217
C	-1.20173	2.37880	-1.95333
N	-0.31434	1.49238	-1.45978
N	-0.31434	1.49238	1.45978
C	-1.20173	2.37880	1.95333
C	-0.80735	3.41436	2.79217
C	0.54791	3.53568	3.10948
C	1.46132	2.61630	2.58716
C	-1.32275	-1.88181	2.42270
H	2.45497	-2.01107	-0.00000
H	-1.64310	-3.20539	4.08845
H	0.55658	-4.36740	3.76003
H	2.04575	-3.64419	1.88012
H	2.04575	-3.64419	-1.88012
H	0.55658	-4.36740	-3.76003
H	-1.64310	-3.20539	-4.08845
H	-2.25967	-1.34173	-2.51507
H	2.91636	0.88624	-1.07892
H	1.98629	-0.27052	-2.01458
H	1.98629	-0.27052	2.01458
H	2.91636	0.88624	1.07892
H	2.51934	2.69005	-2.81881
H	0.89206	4.33885	-3.75385
H	-1.54383	4.11020	-3.17886
H	-2.23203	2.23068	-1.64684
H	-2.23203	2.23068	1.64684
H	-1.54383	4.11020	3.17886
H	0.89206	4.33885	3.75385
H	2.51934	2.69005	2.81881
H	-2.25967	-1.34173	2.51507
Fe	-0.89306	0.07438	0.00000
F	-2.62595	0.37737	0.00000

^{6}FeMeN4PyN_3
Charge: 2+
Energy: -1625852.8658714

C	-2.95105	-3.31311	0.63427
C	-3.57243	-3.09917	-0.59641
C	-3.14877	-2.03698	-1.40410
C	-2.11906	-1.22648	-0.94457
N	-1.51975	-1.43778	0.24654
C	-1.59636	0.00003	-1.68374
C	-2.11904	1.22652	-0.94454
C	-3.14874	2.03705	-1.40406
C	-3.57239	3.09922	-0.59635
C	-2.95100	3.31313	0.63434
C	-1.92111	2.45699	1.02143
N	-1.51972	1.43780	0.24657
N	-0.10203	0.00001	-1.57594
C	0.54060	1.23714	-2.09615
C	0.54058	-1.23712	-2.09617
C	1.64456	-1.74107	-1.18820
C	1.64456	1.74109	-1.18815
C	2.68830	2.52699	-1.67020
C	3.62240	3.04188	-0.76901
C	3.49074	2.75151	0.59074
C	2.43193	1.94787	0.99676
N	1.52898	1.45716	0.12572
N	1.52898	-1.45718	0.12568
C	2.43194	-1.94790	0.99670
C	3.49077	-2.75150	0.59065
C	3.62243	-3.04183	-0.76910
C	2.68831	-2.52694	-1.67027
C	-1.92114	-2.45699	1.02138
H	-1.93758	0.00004	-2.72559
H	-3.25384	-4.12575	1.28555
H	-4.37520	-3.75014	-0.92859
H	-3.60964	-1.84809	-2.36841
H	-3.60962	1.84818	-2.36837
H	-4.37516	3.75021	-0.92851
H	-3.25378	4.12577	1.28563
H	-1.39857	2.57519	1.96491
H	0.91986	1.08030	-3.11189
H	-0.22019	2.02066	-2.16534
H	-0.22022	-2.02063	-2.16535
H	0.91982	-1.08027	-3.11192
H	2.76613	2.73679	-2.73247
H	4.44223	3.65843	-1.12454
H	4.19532	3.13251	1.32187
H	2.28367	1.67190	2.03517
H	2.28369	-1.67196	2.03512
H	4.19536	-3.13251	1.32177
H	4.44226	-3.65835	-1.12466
H	2.76614	-2.73670	-2.73256
H	-1.39861	-2.57521	1.96486
Fe	0.06485	-0.00002	0.67747
N	0.13260	-0.00004	2.53050
N	-0.08110	-0.00010	3.72594
N	-0.27431	-0.00016	4.85606

^{6}FeMeN4PyNCS
Charge: 2+
Energy: -1830961.1267467

C	-2.93326	-3.30325	0.68521
C	-3.64573	-3.09669	-0.49636
C	-3.28583	-2.03887	-1.34020
C	-2.22439	-1.22597	-0.96520
N	-1.53576	-1.43246	0.17744
C	-1.76226	0.00005	-1.74534
C	-2.22439	1.22603	-0.96514
C	-3.28582	2.03895	-1.34008
C	-3.64571	3.09673	-0.49619
C	-2.93325	3.30321	0.68540
C	-1.87665	2.44549	0.98835
N	-1.53576	1.43245	0.17752
N	-0.26409	0.00005	-1.75955
C	0.33442	1.23716	-2.32890
C	0.33443	-1.23702	-2.32898
C	1.50420	-1.74376	-1.50892
C	1.50419	1.74386	-1.50880
C	2.50672	2.53177	-2.06879
C	3.50561	3.04835	-1.24095
C	3.47826	2.75810	0.12491
C	2.45505	1.95233	0.61046
N	1.49016	1.45996	-0.19021
N	1.49017	-1.45995	-0.19030
C	2.45506	-1.95237	0.61034
C	3.47828	-2.75810	0.12474
C	3.50563	-3.04826	-1.24115
C	2.50673	-2.53162	-2.06896
C	-1.87666	-2.44554	0.98821
H	-2.18763	0.00008	-2.75580
H	-3.18663	-4.11128	1.36277
H	-4.47121	-3.74950	-0.76277
H	-3.81982	-1.85491	-2.26701
H	-3.81981	1.85505	-2.26691
H	-4.47120	3.74955	-0.76256
H	-3.18662	4.11121	1.36300
H	-1.28511	2.55388	1.89149
H	0.63477	1.08035	-3.37076

H	-0.43059	2.01965	-2.33988
H	-0.43058	-2.01952	-2.34001
H	0.63477	-1.08014	-3.37083
H	2.50321	2.74175	-3.13388
H	4.29491	3.66637	-1.65774
H	4.23556	3.14082	0.80032
H	2.38563	1.67658	1.65721
H	2.38564	-1.67668	1.65711
H	4.23558	-3.14085	0.80012
H	4.29493	-3.66624	-1.65797
H	2.50324	-2.74153	-3.13406
H	-1.28512	-2.55399	1.89135
Fe	0.07634	-0.00002	0.48035
N	0.32137	-0.00007	2.33298
C	0.42206	-0.00011	3.53996
S	0.55866	-0.00018	5.11192

[2]FeMeN4PyOH
Charge: 2+
Energy: -1570381.1026007

C	-2.71468	3.27298	-1.06421
C	-3.44425	3.13585	0.11739
C	-3.13922	2.09139	1.00002
C	-2.11716	1.21939	0.65549
N	-1.41623	1.35820	-0.49385
C	-1.66987	0.00013	1.45027
C	-2.11777	-1.21884	0.65538
C	-3.14030	-2.09033	0.99982
C	-3.44588	-3.13454	0.11709
C	-2.71638	-3.27195	-1.06452
C	-1.69547	-2.36176	-1.33726
N	-1.41691	-1.35791	-0.49398
N	-0.15547	-0.00024	1.40563
C	0.48767	-1.24737	1.93395
C	0.48829	1.24650	1.93415
C	1.56147	1.74204	0.98737
C	1.56122	-1.74264	0.98747
C	2.58142	-2.60130	1.38325
C	3.47510	-3.07567	0.41960
C	3.32425	-2.67445	-0.90897
C	2.28972	-1.80211	-1.23339
N	1.43366	-1.35346	-0.29952
N	1.43400	1.35263	-0.29953
C	2.28985	1.80145	-1.23352
C	3.32409	2.67418	-0.90929
C	3.47485	3.07567	0.41922
C	2.58139	2.60114	1.38297
C	-1.69427	2.36226	-1.33704
H	-2.06477	0.00018	2.47105
H	-2.92645	4.07167	-1.76666
H	-4.23947	3.83503	0.35645
H	-3.68262	1.96487	1.93077
H	-3.68363	-1.96361	1.93059
H	-4.24148	-3.83332	0.35608
H	-2.92857	-4.07046	-1.76704
H	-1.08145	-2.41480	-2.22977
H	0.88803	-1.07742	2.93777
H	-0.28221	-2.01925	2.02669
H	-0.28134	2.01852	2.02785
H	0.88925	1.07590	2.93761
H	2.67273	-2.89713	2.42366
H	4.27859	-3.74745	0.70513
H	3.99861	-3.02249	-1.68372
H	2.11191	-1.43507	-2.23794
H	2.11208	1.43424	-2.23802
H	3.99831	3.02233	-1.68412
H	4.27810	3.74780	0.70460
H	2.67264	2.89716	2.42333
H	-1.08025	2.41503	-2.22957
Fe	0.03309	-0.00023	-0.62383
O	0.24014	-0.00028	-2.39542
H	-0.60743	-0.00023	-2.87442

[5]FeMeOPyNMe3Br
Charge: 3+
Energy: -2961109.7584616

Fe	0.83425	-0.01822	-0.31348
N	-1.06724	0.11392	-0.44930
C	-1.83716	-1.02027	-0.40933
N	0.69130	2.10206	-0.18964
N	0.99583	-0.01849	1.85227
N	0.39201	-2.09511	-0.17054
C	-3.02051	1.48752	-0.31328
H	-3.50130	2.46099	-0.30234
C	-1.66467	1.35343	-0.42614
C	-0.69903	2.47265	-0.65759
H	-0.64124	2.65579	-1.73629
H	-1.00586	3.41098	-0.18350
C	1.67909	2.88859	-1.01034
H	1.43151	3.95459	-0.92909
H	2.68850	2.72414	-0.63706
H	1.61460	2.57873	-2.05453
C	0.90700	2.38560	1.28635
H	1.98219	2.49461	1.43039
H	0.44765	3.35060	1.52859
C	0.34967	1.28849	2.18965
H	-0.73029	1.18345	2.07055
H	0.54744	1.54667	3.23727
C	2.38591	-0.10511	2.40112
H	2.33929	-0.09201	3.49655
H	2.86867	-1.02332	2.07059
H	2.98493	0.73538	2.05455
C	0.18852	-1.22832	2.20387
H	0.35890	-1.50304	3.25205
H	-0.86950	-0.98407	2.09108
C	0.59217	-2.39352	1.30425
H	0.02202	-3.29331	1.56161
H	1.64805	-2.63240	1.43416
C	1.24681	-3.01809	-0.99914
H	1.21260	-2.70607	-2.04421
H	2.27460	-2.99626	-0.64078
H	0.85290	-4.03814	-0.90792
C	-3.83944	0.31485	-0.24865
C	-3.20545	-0.96510	-0.30209
H	-3.78765	-1.87953	-0.28416
C	-1.04367	-2.27418	-0.61045
H	-1.47521	-3.14289	-0.10197
H	-1.03214	-2.49837	-1.68299
O	-5.11375	0.52218	-0.15479
C	-6.10934	-0.55656	-0.11403
H	-7.06434	-0.04057	-0.03969
H	-6.05228	-1.13262	-1.04119
H	-5.93455	-1.17657	0.76889
Br	3.01078	-0.17591	-1.03104

[6]FeMeOPyNMe3BrOH
Charge: 3+
Energy: -3008705.1070579

Fe	1.05385	-0.38245	0.06135
N	-0.83977	-0.13370	-0.11999
C	-1.62708	-0.08351	0.99340
N	0.98684	0.12646	-1.97373
N	1.10989	2.80412	0.04933
N	0.59773	0.14778	2.04121
C	-2.75252	0.01467	-1.53784
H	-3.20741	0.05016	-2.52289
C	-1.39770	-0.08999	-1.37128
C	-0.38917	-0.24491	-2.47277
H	-0.35292	-1.29988	-2.76364
H	-0.64185	0.33359	-3.36817
C	2.02657	-0.67004	-2.72127
H	1.99066	-0.40974	-3.78552
H	3.01136	-0.43648	-2.31750
H	1.82371	-1.73269	-2.59742
C	1.32004	1.57872	-2.16222
H	2.39162	1.67734	-1.98800
H	1.12905	1.83383	-3.21143
C	0.54918	2.60387	-1.29329
H	-0.50947	2.36249	-1.20319
H	0.63673	3.57275	-1.80637
C	2.38422	3.49556	0.16772
H	2.17476	4.58084	0.14064
H	2.87054	3.26669	1.11704
H	3.04220	3.25563	-0.66864
C	0.30456	2.61839	1.26344
H	0.29594	3.59269	1.77348
H	-0.71821	2.37696	0.97587
C	0.89276	1.60206	2.27398
H	0.50738	1.86925	3.26520
H	1.97824	1.69770	2.30525
C	1.47307	-0.64046	2.98307
H	1.29507	-1.70440	2.83424
H	2.51741	-0.41229	2.77172
H	1.23591	-0.36783	4.01797
C	-3.59950	0.04517	-0.38766
C	-2.99681	0.01494	0.90490
H	-3.59864	0.05191	1.80570
C	-0.84874	-0.21671	2.27168
H	-1.26838	0.37671	3.09157
H	-0.87221	-1.26658	2.58220
O	-4.87488	0.11154	-0.62569
C	-5.88142	0.10644	0.43735
H	-6.83366	0.14238	-0.08789
H	-5.79637	-0.81777	1.01473
H	-5.75606	0.99350	1.06384
O	2.71115	0.13830	0.21904
H	3.42213	-0.53356	0.28751
Br	1.12613	-2.75789	0.08168

[5]FeMeOPyNMe3Cl
Charge: 3+
Energy: -1634579.5610596

Fe	-1.08141	0.04437	-0.50680
N	0.81816	-0.12022	-0.47627

C	1.60350	1.00335	-0.39911
N	-0.98855	-2.06727	-0.32733
N	-1.43203	0.09230	1.64885
N	-0.61875	2.10959	-0.36213
C	2.73126	-1.52245	-0.16502
H	3.19310	-2.50296	-0.09911
C	1.39075	-1.36985	-0.38412
C	0.42625	-2.47797	-0.66982
H	0.45380	-2.68725	-1.74496
H	0.67307	-3.40957	-0.14971
C	-1.93314	-2.81662	-1.22874
H	-1.74467	-3.89183	-1.11469
H	-2.96315	-2.59622	-0.95393
H	-1.75727	-2.52291	-2.26488
C	-1.34119	-2.32269	1.12726
H	-2.42667	-2.41118	1.17543
H	-0.92272	-3.29092	1.42411
C	-0.84511	-1.22023	2.06054
H	0.24305	-1.13623	2.03784
H	-1.14260	-1.45648	3.08985
C	-2.86944	0.21372	2.04506
H	-2.93571	0.22753	3.13971
H	-3.29912	1.12977	1.64344
H	-3.44360	-0.62580	1.65713
C	-0.63896	1.29818	2.04035
H	-0.89782	1.60049	3.06272
H	0.42062	1.03509	2.02730
C	-0.94262	2.44766	1.08183
H	-0.38042	3.34375	1.36765
H	-2.00104	2.70729	1.11263
C	-1.40707	2.99491	-1.29078
H	-1.27243	2.65450	-2.31888
H	-2.46306	2.96149	-1.02867
H	-1.03682	4.02326	-1.19211
C	3.56344	-0.36165	-0.05963
C	2.95800	0.92741	-0.18632
H	3.55368	1.83225	-0.14152
C	0.84971	2.26573	-0.68492
H	1.25003	3.13629	-0.15462
H	0.92997	2.47377	-1.75776
O	4.82242	-0.58748	0.13559
C	5.83289	0.47432	0.23230
H	6.76908	-0.05716	0.39008
H	5.85798	1.03168	-0.70763
H	5.60242	1.11531	1.08700
Cl	-3.02611	0.20933	-1.29350

^{6}FeMeOPyNMe3ClOH
Charge: 3+
Energy: -1682174.5787200

Fe	-1.06630	-0.02397	-0.77810
N	0.78199	-0.14685	-0.26344
C	1.56163	0.97304	-0.27131
N	-1.06465	-1.97816	-0.01677
N	-1.51143	0.34754	2.36649
N	-0.67562	2.00890	-0.43300
C	2.66675	-1.51671	0.24559
H	3.11455	-2.48573	0.44326
C	1.33100	-1.37909	-0.02021
C	0.34467	-2.50226	-0.15969
H	0.43295	-2.91706	-1.16917
H	0.52231	-3.31941	0.54808
C	-2.00075	-2.81542	-0.85201
H	-1.98768	-3.84917	-0.48730
H	-3.00881	-2.40957	-0.77232
H	-1.67590	-2.78749	-1.89136
C	-1.57439	-1.99746	1.39556
H	-2.64967	-1.82692	1.34146
H	-1.41723	-3.00673	1.79451
C	-0.93276	-1.00258	2.39574
H	0.14756	-0.92812	2.27541
H	-1.13853	-1.39864	3.40091
C	-2.85801	0.53109	2.88501
H	-2.77710	0.64069	3.98231
H	-3.31411	1.43816	2.48567
H	-3.48310	-0.33809	2.67563
C	-0.68918	1.54205	2.13082
H	-0.79976	2.16759	3.02848
H	0.35541	1.24239	2.05272
C	-1.14833	2.41297	0.93380
H	-0.79805	3.43504	1.12141
H	-2.23724	2.43951	0.89153
C	-1.44917	2.82000	-1.44248
H	-1.15256	2.51925	-2.44660
H	-2.51435	2.63583	-1.30554
H	-1.23548	3.88510	-1.29553
C	3.50685	-0.36087	0.23014
C	2.91295	0.91218	-0.01942
H	3.50930	1.81737	-0.02952
C	0.80462	2.21514	-0.64714
H	1.14841	3.10566	-0.10935
H	0.95370	2.39993	-1.71616
O	4.76712	-0.57482	0.45932
C	5.77127	0.49060	0.43244
H	6.71279	-0.01656	0.63305
H	5.78677	0.95073	-0.55889
H	5.55307	1.21824	1.21858
O	-2.76980	0.17691	-0.44102
H	-3.39545	0.15509	-1.19679
Cl	-0.88834	-0.26567	-2.93084

^{3}FeMeOPyNMe3F
Charge: 3+
Energy: -1408454.1722949

Fe	-0.95531	-0.02632	0.51870
N	0.82806	0.11595	-0.05088
C	1.59822	-1.02303	-0.13062
N	-0.95147	2.02922	0.26816
N	-2.40978	-0.15089	-0.96174
N	-0.61848	-2.05696	0.28376
C	2.75935	1.50964	-0.18875
H	3.23616	2.48406	-0.23730
C	1.39995	1.36598	-0.15273
C	0.38621	2.46547	-0.29931
H	0.70400	3.39456	0.18242
H	0.26522	2.68074	-1.36682
C	-1.18372	2.68216	1.60401
H	-1.26994	3.76615	1.46809
H	-2.09572	2.28637	2.04901
H	-0.33578	2.45993	2.25631
C	-2.08801	2.29778	-0.69072
H	-2.99901	2.40212	-0.10039
H	-1.92898	3.24939	-1.20976
C	-2.19914	1.14937	-1.69588
H	-1.28862	1.05015	-2.29366
H	-3.04210	1.31346	-2.37930
C	-3.78973	-0.26608	-0.39488
H	-4.49049	-0.33154	-1.23792
H	-3.87668	-1.15503	0.22525
H	-4.02800	0.60262	0.21422
C	-1.98349	-1.40035	-1.69013
H	-2.78401	-1.70315	-2.37726
H	-1.09886	-1.15340	-2.28411
C	-1.68934	-2.51220	-0.68086
H	-1.37293	-3.42589	-1.19587
H	-2.57387	-2.76420	-0.09491
C	-0.75295	-2.73144	1.62264
H	0.04248	-2.37175	2.27968
H	-1.71978	-2.48390	2.05906
H	-0.66396	-3.81599	1.49393
C	3.58756	0.33721	-0.16285
C	2.96786	-0.95498	-0.16203
H	3.56213	-1.86126	-0.19694
C	0.77534	-2.27360	-0.27110
H	0.69971	-2.51231	-1.33806
H	1.23597	-3.13607	0.21923
O	4.86185	0.55702	-0.16976
C	5.88001	-0.50318	-0.15752
H	6.82647	0.03282	-0.13172
H	5.75171	-1.11341	0.74045
H	5.79127	-1.09253	-1.07409
F	-2.06112	-0.11018	1.79241

^{6}FeMeOPyNMe3FOH
Charge: 3+
Energy: -1456044.7735687

Fe	-1.05246	0.01499	-0.94750
N	0.77431	-0.13053	-0.33153
C	1.54986	0.98962	-0.25912
N	-1.06697	-1.97363	-0.33054
N	-1.69070	0.19271	2.16465
N	-0.69049	2.01296	-0.48197
C	2.65473	-1.52382	0.12592
H	3.10303	-2.50195	0.27090
C	1.32562	-1.37431	-0.16524
C	0.35228	-2.49008	-0.41356
H	0.50154	-2.86177	-1.43261
H	0.48613	-3.33753	0.26756
C	-1.93335	-2.72028	-1.31461
H	-1.90108	-3.79220	-1.08721
H	-2.95778	-2.35777	-1.23561
H	-1.55588	-2.54128	-2.32253
C	-1.67367	-2.09055	1.03824
H	-2.74417	-1.92165	0.92393
H	-1.53176	-3.12298	1.37931
C	-1.10514	-1.15669	2.13982
H	-0.01990	-1.07096	2.09216
H	-1.36991	-1.61784	3.10230
C	-3.06265	0.33722	2.62499
H	-3.03727	0.38125	3.72967
H	-3.50549	1.26423	2.25764
H	-3.66850	-0.52165	2.33263
C	-0.86825	1.40654	2.04328
H	-1.04051	1.98045	2.96514
H	0.18245	1.11922	2.01375

C	-1.25947	2.34240	0.86838
H	-0.93002	3.35439	1.13245
H	-2.34325	2.36390	0.75629
C	-1.40684	2.83274	-1.52679
H	-1.07219	2.51330	-2.51491
H	-2.48019	2.67098	-1.43282
H	-1.17772	3.89427	-1.37752
C	3.48734	-0.36578	0.21291
C	2.89420	0.91816	0.02486
H	3.48617	1.82424	0.08642
C	0.79919	2.24877	-0.58811
H	1.09277	3.09998	0.03598
H	1.01098	2.51696	-1.62845
O	4.74098	-0.58883	0.46725
C	5.73891	0.48038	0.54016
H	6.67608	-0.03429	0.74198
H	5.78567	1.00025	-0.42014
H	5.48938	1.15757	1.36133
O	-2.77055	0.19017	-0.61193
H	-3.37437	0.21448	-1.38562
F	-0.86036	-0.06563	-2.67449

^{5}FeMeOPyNMe3N$_3$
Charge: 3+
Energy: -1448853.0099653

Fe	0.98722	-0.03265	-0.27760
N	-0.88738	0.10370	-0.48363
C	-1.66138	-1.02583	-0.44660
N	0.87170	2.05634	-0.18059
N	1.11690	-0.01840	1.86125
N	0.56119	-2.07811	-0.13884
C	-2.83594	1.48672	-0.40432
H	-3.31257	2.46198	-0.41195
C	-1.47860	1.34610	-0.48394
C	-0.49401	2.45411	-0.69641
H	-0.40095	2.62870	-1.77401
H	-0.80294	3.39958	-0.23928
C	1.91922	2.77581	-0.97892
H	1.76082	3.85790	-0.89697
H	2.90668	2.52889	-0.58961
H	1.84338	2.48218	-2.02772
C	1.04244	2.37799	1.29674
H	2.11137	2.50311	1.47037
H	0.56651	3.34190	1.50579
C	0.47267	1.28855	2.19974
H	-0.60618	1.18665	2.06607
H	0.65766	1.54676	3.24960
C	2.51350	-0.10201	2.38962
H	2.49074	-0.08131	3.48538
H	2.99011	-1.02182	2.05442
H	3.10721	0.73413	2.02368
C	0.31241	-1.22446	2.22946
H	0.47430	-1.48682	3.28204
H	-0.74555	-0.98463	2.10409
C	0.72552	-2.39256	1.33983
H	0.14312	-3.28890	1.57852
H	1.77578	-2.64152	1.49367
C	1.47031	-2.95740	-0.94729
H	1.41408	-2.66954	-1.99902
H	2.49262	-2.85478	-0.58414
H	1.15555	-4.00271	-0.84315
C	-3.66004	0.31919	-0.34500
C	-3.03196	-0.96286	-0.37141
H	-3.61841	-1.87430	-0.35497
C	-0.86191	-2.28308	-0.60936
H	-1.30220	-3.14295	-0.09441
H	-0.82617	-2.52826	-1.67662
O	-4.93737	0.53259	-0.27914
C	-5.92800	-0.54733	-0.24574
H	-6.88692	-0.03542	-0.19826
H	-5.85195	-1.13665	-1.16314
H	-5.77240	-1.15646	0.64831
N	2.73846	-0.16811	-0.76270
N	3.59496	-0.23572	-1.63467
N	4.43876	-0.30185	-2.40601

^{6}FeMeOPyNMe3N$_3$OH
Charge: 3+
Energy: -1496443.7114210

Fe	-1.11907	0.44682	0.05349
N	0.81297	0.31412	-0.12204
C	1.59737	0.31929	0.98891
N	-0.99663	-0.04129	-1.97301
N	-0.98392	-2.70229	0.08923
N	-0.61963	0.02167	2.03712
C	2.73543	0.21905	-1.53134
H	3.19336	0.18710	-2.51489
C	1.37595	0.27748	-1.36714
C	0.36403	0.38322	-2.47194
H	0.28528	1.43335	-2.77077
H	0.64114	-0.18966	-3.36376
C	-2.06444	0.69710	-2.73099
H	-2.01308	0.44120	-3.79561
H	-3.04034	0.41881	-2.33344
H	-1.90888	1.76849	-2.60751
C	-1.25343	-1.51185	-2.14475
H	-2.31825	-1.66658	-1.97320
H	-1.03939	-1.77199	-3.18814
C	-0.43452	-2.48471	-1.25620
H	0.61008	-2.18833	-1.16802
H	-0.47112	-3.46254	-1.75768
C	-2.20841	-3.47677	0.21469
H	-1.92531	-4.54495	0.21087
H	-2.71443	-3.25894	1.15593
H	-2.87458	-3.29504	-0.62939
C	-0.19782	-2.44542	1.30393
H	-0.14052	-3.40712	1.83369
H	0.81224	-2.15675	1.01528
C	-0.84020	-1.44180	2.29747
H	-0.43964	-1.67216	3.29179
H	-1.91843	-1.59560	2.32799
C	-1.52866	0.78846	2.95687
H	-1.39930	1.85472	2.77307
H	-2.56109	0.50354	2.75493
H	-1.28168	0.56476	4.00111
C	3.57865	0.23090	-0.38074
C	2.97228	0.26837	0.90729
H	3.57142	0.27273	1.81040
C	0.80973	0.45188	2.26215
H	1.24964	-0.10307	3.09827
H	0.78947	1.50845	2.54810
O	4.85942	0.19609	-0.61481
C	5.85212	0.24365	0.45591
H	6.81142	0.22358	-0.05729
H	5.74029	1.17387	1.01919
H	5.74490	-0.63537	1.09723
O	-2.69195	-0.32761	0.21346
H	-3.49890	0.22037	0.27265
N	-1.36340	2.29884	0.04631
N	-1.93365	3.37636	0.07405
N	-2.44387	4.40387	0.09756

^{5}FeMeOPyNMe3NCS
Charge: 3+
Energy: -1653972.2082365

Fe	0.73225	-0.00294	-0.16156
N	-1.11430	0.08778	-0.49651
C	-1.86157	-1.05690	-0.49252
N	0.59051	2.07988	-0.12191
N	0.72928	0.06084	1.97003
N	0.35980	-2.05131	-0.00276
C	-3.08744	1.42895	-0.59267
H	-3.58265	2.39265	-0.65515
C	-1.72473	1.31589	-0.57099
C	-0.74611	2.43952	-0.73473
H	-0.58423	2.59579	-1.80696
H	-1.10670	3.38606	-0.31987
C	1.66980	2.81087	-0.86155
H	1.48411	3.89025	-0.81639
H	2.63336	2.59418	-0.40153
H	1.67722	2.48853	-1.90434
C	0.64827	2.44393	1.35248
H	1.69891	2.59974	1.59896
H	0.13741	3.40010	1.50689
C	0.04308	1.36183	2.24223
H	-1.02280	1.23632	2.04130
H	0.15436	1.64423	3.29611
C	2.08966	0.01570	2.58515
H	2.00394	0.06052	3.67706
H	2.60125	-0.90339	2.30233
H	2.68926	0.85563	2.23675
C	-0.07466	-1.15084	2.31961
H	0.02022	-1.38293	3.38725
H	-1.12587	-0.93463	2.11748
C	0.41537	-2.33333	1.48876
H	-0.17237	-3.23102	1.70793
H	1.45370	-2.56532	1.72775
C	1.33586	-2.93615	-0.71795
H	1.35446	-2.67335	-1.77725
H	2.32762	-2.80127	-0.28772
H	1.03585	-3.98474	-0.60836
C	-3.88792	0.24545	-0.56493
C	-3.23580	-1.02256	-0.51709
H	-3.80375	-1.94550	-0.51983
C	-1.02267	-2.29858	-0.56666
H	-1.48289	-3.15677	-0.06675
H	-0.90579	-2.56427	-1.62312
O	-5.17337	0.43222	-0.59400
C	-6.13351	-0.67180	-0.60464
H	-7.10712	-0.18713	-0.63729
H	-5.97882	-1.28069	-1.49915
H	-6.02789	-1.25774	0.31209
N	2.57415	-0.11778	-0.63035
C	3.69409	-0.18799	-1.04165
S	5.20445	-0.28102	-1.58765

^{6}FeMeOPyNMe3NCSOH
Charge: 3+
Energy: -1701559.8161458

Fe	1.19070	0.20134	0.06585
N	-0.74931	-0.48552	-0.12574
C	-1.48466	-0.78323	0.97605
N	0.68413	0.67658	-2.03533
N	-0.44660	3.01220	0.10021
N	0.35245	0.43162	2.10294
C	-2.57165	-1.12313	-1.53804
H	-3.00976	-1.25299	-2.52249
C	-1.29711	-0.64205	-1.36420
C	-0.36422	-0.28449	-2.49676
H	0.14353	-1.19609	-2.82946
H	-0.90806	0.10911	-3.36365
C	1.95371	0.47842	-2.80530
H	1.80292	0.68154	-3.87213
H	2.71618	1.15158	-2.41031
H	2.28670	-0.55374	-2.68115
C	0.26927	2.10395	-2.17718
H	1.15986	2.71212	-2.02190
H	-0.07522	2.26940	-3.20580
C	-0.86748	2.60477	-1.24566
H	-1.67730	1.88176	-1.15690
H	-1.27200	3.51218	-1.71725
C	0.34469	4.22505	0.23180
H	-0.35679	5.07747	0.24140
H	0.90384	4.22405	1.16723
H	1.02148	4.34109	-0.61425
C	-1.06584	2.45863	1.31066
H	-1.54270	3.31101	1.81582
H	-1.84875	1.76108	1.01570
C	-0.08359	1.83980	2.34159
H	-0.58158	1.89325	3.31798
H	0.81874	2.44812	2.39355
C	1.48612	0.12693	3.03360
H	1.83858	-0.88852	2.84271
H	2.29837	0.83003	2.84305
H	1.16944	0.20740	4.08021
C	-3.33866	-1.48203	-0.39198
C	-2.77099	-1.27807	0.89596
H	-3.32565	-1.50901	1.79801
C	-0.75256	-0.55882	2.27915
H	-1.43420	-0.25176	3.08139
H	-0.30415	-1.50774	2.59231
O	-4.53146	-1.95725	-0.63097
C	-5.42628	-2.38910	0.43629
H	-6.31248	-2.75638	-0.07733
H	-4.95604	-3.19310	1.00918
H	-5.68064	-1.53679	1.07260
O	2.11890	1.73843	0.23811
H	3.07772	1.89811	0.29575
N	2.32131	-1.49008	0.05036
C	3.04814	-2.42931	0.04248
S	4.04894	-3.71032	0.03241

^{3}FeMeOPyNMe3OH
Charge: 3+
Energy: -1393378.6768864

Fe	-1.17187	0.05754	-0.55553
N	0.70262	-0.10371	-0.44475
C	1.48723	1.01249	-0.30570
N	-1.11064	-2.02923	-0.36078
N	-1.65561	0.12576	1.38446
N	-0.74717	2.10376	-0.43647
C	2.60050	-1.52860	-0.14609
H	3.05946	-2.51189	-0.11295
C	1.26693	-1.36026	-0.38513
C	0.29211	-2.44371	-0.73922
H	0.31195	-2.57784	-1.82666
H	0.53525	-3.40943	-0.28465
C	-2.08092	-2.74959	-1.25166
H	-1.93624	-3.83193	-1.15317
H	-3.10191	-2.50744	-0.95386
H	-1.90986	-2.45461	-2.28849
C	-1.42150	-2.31963	1.09468
H	-2.48449	-2.55081	1.16702
H	-0.87938	-3.21143	1.42461
C	-1.05780	-1.12869	1.97088
H	0.02177	-0.98502	2.03003
H	-1.44441	-1.26187	2.98873
C	-3.15318	0.15361	1.54477
H	-3.37666	0.17080	2.61794
H	-3.56604	1.03717	1.06438
H	-3.59598	-0.73195	1.09526
C	-1.02454	1.39276	1.91322
H	-1.46275	1.62396	2.89120
H	0.04134	1.19935	2.05067
C	-1.26727	2.51433	0.91746
H	-0.78498	3.44114	1.24653
H	-2.33134	2.72790	0.80920
C	-1.44069	2.87411	-1.52409
H	-1.11020	2.49952	-2.49445
H	-2.51685	2.73694	-1.43568
H	-1.18630	3.93664	-1.43013
C	3.43302	-0.37400	0.02418
C	2.83759	0.92114	-0.06978
H	3.43789	1.82000	0.01499
C	0.74848	2.29615	-0.55862
H	1.07733	3.10609	0.10013
H	0.96101	2.61157	-1.58568
O	4.68655	-0.61374	0.24225
C	5.69358	0.44141	0.40611
H	6.62587	-0.09634	0.56563
H	5.74293	1.03659	-0.50933
H	5.44298	1.04857	1.27961
O	-2.62795	0.24867	-1.42789
H	-3.37624	-0.32628	-1.68532

^{6}FeMeOPyNMe3OHBr
Charge: 3+
Energy: -3008690.6859867

Fe	0.89554	-0.03334	-0.39482
N	-1.24447	0.14594	-0.11117
C	-1.99269	-1.00699	-0.20262
N	0.58135	2.17064	-0.08121
N	1.11103	-0.04145	1.77504
N	0.24715	-2.13736	-0.04083
C	-3.19934	1.48715	-0.12558
H	-3.69614	2.45452	-0.11587
C	-1.78735	1.34972	-0.12114
C	-0.85875	2.53457	-0.20179
H	-1.02405	2.99705	-1.18312
H	-1.13434	3.29426	0.54210
C	1.37803	2.94535	-1.08834
H	1.23891	4.02228	-0.93708
H	2.43342	2.70030	-0.97808
H	1.04792	2.66446	-2.08972
C	1.10989	2.39314	1.30312
H	2.19951	2.37788	1.23805
H	0.82124	3.38485	1.67331
C	0.61227	1.30314	2.23654
H	-0.47925	1.27429	2.26289
H	0.95810	1.48733	3.25988
C	2.50438	-0.25347	2.30101
H	2.46030	-0.29823	3.39502
H	2.92259	-1.18081	1.91583
H	3.15159	0.56795	2.00085
C	0.22548	-1.16335	2.24842
H	0.42796	-1.36614	3.30670
H	-0.81169	-0.83227	2.17444
C	0.46596	-2.41319	1.41805
H	-0.18245	-3.22930	1.75877
H	1.49424	-2.75870	1.53380
C	1.07043	-3.06315	-0.88577
H	0.97216	-2.77022	-1.93205
H	2.11585	-2.98412	-0.59049
H	0.73221	-4.09815	-0.75722
C	-4.00344	0.28447	-0.14389
C	-3.36926	-0.98773	-0.18663
H	-3.94348	-1.90583	-0.24732
C	-1.17927	-2.25285	-0.44869
H	-1.64708	-3.13331	0.00996
H	-1.19760	-2.41096	-1.53438
O	-5.28167	0.51507	-0.14395
C	-6.32254	-0.52599	-0.17537
H	-7.25673	0.02241	-0.07242
H	-6.26222	-1.03447	-1.14417
H	-6.15968	-1.21676	0.65741
O	0.43080	-0.04895	-2.08994
H	1.11751	-0.09600	-2.78695
Br	3.21245	-0.15839	-0.84515

^{6}FeMeOPyNMe3OHCl
Charge: 3+
Energy: -1682168.8358663

Fe	0.93636	-0.00513	-0.92906
N	-0.88926	0.12606	-0.24942
C	-1.66074	-0.99701	-0.21746
N	0.92955	2.02372	-0.27887
N	1.53616	-0.15111	2.20953
N	0.58521	-2.03925	-0.40217
C	-2.80285	1.50858	0.08473
H	-3.26321	2.48490	0.20169
C	-1.45967	1.36495	-0.14823
C	-0.50122	2.49334	-0.39061
H	-0.64545	2.84466	-1.41735
H	-0.66965	3.34870	0.27377
C	1.77752	2.83912	-1.22245
H	1.66883	3.90267	-0.97762
H	2.82164	2.54422	-1.13065
H	1.43462	2.65806	-2.24152
C	1.48978	2.15245	1.10883

H	2.57103	2.03819	1.03086
H	1.29089	3.17387	1.45607
C	0.93086	1.19057	2.18854
H	-0.15153	1.08668	2.12725
H	1.17640	1.64535	3.15914
C	2.89367	-0.27928	2.72230
H	2.82729	-0.30612	3.82526
H	3.35516	-1.20793	2.38356
H	3.50389	0.57861	2.43637
C	0.71845	-1.37104	2.11184
H	0.88417	-1.91878	3.05072
H	-0.33174	-1.08599	2.06648
C	1.11260	-2.34402	0.97086
H	0.74705	-3.33800	1.25706
H	2.19805	-2.40542	0.89179
C	1.28613	-2.92814	-1.39872
H	0.97759	-2.63450	-2.40250
H	2.36456	-2.81406	-1.30084
H	1.00469	-3.97180	-1.21362
C	-3.62686	0.34437	0.16359
C	-3.01701	-0.93576	0.01261
H	-3.60204	-1.84694	0.06562
C	-0.90382	-2.25563	-0.52846
H	-1.21593	-3.10644	0.08810
H	-1.10241	-2.51872	-1.57251
O	-4.89109	0.56052	0.37185
C	-5.88488	-0.51321	0.42456
H	-6.83025	-0.00234	0.59534
H	-5.89981	-1.04162	-0.53220
H	-5.65425	-1.18267	1.25796
O	0.57257	0.07716	-2.66935
H	1.16233	0.05472	-3.45130
Cl	3.07869	-0.19288	-0.68449

^{4}FeMeOPyNMe3OHF
Charge: 3+
Energy: -1456040.9114676

Fe	-1.11701	0.05021	-0.52916
N	0.75478	-0.12362	-0.23978
C	1.53126	1.00313	-0.24491
N	-1.09639	-2.00750	-0.27252
N	-1.57871	0.12774	1.50651
N	-0.70368	2.07335	-0.33480
C	2.65126	-1.53556	-0.00454
H	3.11729	-2.51532	0.04646
C	1.29942	-1.37217	-0.19810
C	0.31829	-2.45965	-0.53129
H	0.40947	-2.65877	-1.60449
H	0.51569	-3.39681	-0.00087
C	-2.03444	-2.65847	-1.24757
H	-2.04204	-3.74025	-1.06642
H	-3.03477	-2.25057	-1.10416
H	-1.69337	-2.45686	-2.26305
C	-1.54290	-2.28831	1.14944
H	-2.62939	-2.37296	1.13227
H	-1.14769	-3.25907	1.46681
C	-1.09074	-1.17236	2.07281
H	-0.00218	-1.13035	2.14918
H	-1.48950	-1.32184	3.08295
C	-3.05322	0.28475	1.76087
H	-3.21668	0.32110	2.84325
H	-3.42597	1.19595	1.30071
H	-3.60644	-0.54664	1.33232
C	-0.83300	1.31568	2.03577
H	-1.18462	1.56963	3.04261
H	0.22471	1.05434	2.11060
C	-1.05611	2.47732	1.08446
H	-0.46103	3.35101	1.37025
H	-2.10059	2.78862	1.07796
C	-1.52007	2.86307	-1.31712
H	-1.24672	2.56740	-2.33006
H	-2.57662	2.65894	-1.14512
H	-1.31690	3.93120	-1.17319
C	3.48175	-0.36670	0.09595
C	2.89171	0.93047	-0.05462
H	3.49963	1.82859	-0.05634
C	0.76367	2.23562	-0.63118
H	1.14363	3.14835	-0.16069
H	0.86872	2.35025	-1.71574
O	4.74122	-0.60231	0.28465
C	5.78252	0.43361	0.37868
H	6.69620	-0.12157	0.58073
H	5.84297	0.95491	-0.58137
H	5.53950	1.11149	1.20153
O	-0.75422	-0.00755	-2.26429
H	-1.58595	0.04786	-2.78831
F	-2.79105	0.20360	-0.87339

^{3}FeMeOPyNMe3OHMeCN$_3$cis
Charge: 3+
Energy: -1476767.3360323

Fe	0.82572	-0.01116	-0.33790
O	0.91110	-0.02390	-2.08282
N	-1.02655	0.10390	-0.34309
C	-1.77089	-1.03829	-0.36495
N	0.73264	2.06049	-0.13408
N	0.92625	-0.00265	1.77499
N	0.47333	-2.05172	-0.10935
C	-2.98024	1.46085	-0.32763
H	-3.47078	2.42861	-0.35790
C	-1.61840	1.33825	-0.38919
C	-0.63299	2.44201	-0.64401
H	-0.55164	2.58186	-1.72748
H	-0.94539	3.39997	-0.21638
C	1.77653	2.77181	-0.93699
H	1.61337	3.85393	-0.87416
H	2.75976	2.53105	-0.53659
H	1.71474	2.44048	-1.97362
C	0.87813	2.39845	1.33276
H	1.94209	2.52569	1.53235
H	0.39717	3.36031	1.53963
C	0.28950	1.29180	2.19021
H	-0.78995	1.20854	2.05599
H	0.47750	1.48436	3.25263
C	2.31169	-0.07664	2.35778
H	2.23451	-0.05815	3.45000
H	2.80740	-0.99238	2.04648
H	2.91119	0.76609	2.02387
C	0.14915	-1.21123	2.20849
H	0.32198	-1.41327	3.27170
H	-0.91485	-1.00562	2.08112
C	0.60073	-2.38650	1.35912
H	0.02147	-3.28819	1.58488
H	1.64738	-2.62617	1.54660
C	1.40751	-2.89744	-0.91770
H	1.37107	-2.57279	-1.95765
H	2.41933	-2.77537	-0.53525
H	1.11299	-3.95019	-0.83757
C	-3.78590	0.28124	-0.25883
C	-3.14475	-0.99348	-0.30528
H	-3.72021	-1.91174	-0.32194
C	-0.93741	-2.26743	-0.59193
H	-1.36411	-3.16395	-0.13091
H	-0.89290	-2.44912	-1.67149
O	-5.06806	0.47799	-0.18695
C	-6.03844	-0.61723	-0.14830
H	-7.00517	-0.12323	-0.07575
H	-5.97181	-1.19446	-1.07422
H	-5.85642	-1.23652	0.73385
N	2.84481	-0.13920	-0.43461
C	3.94888	-0.20810	-0.78104
C	5.33347	-0.29467	-1.21289
H	5.81516	-1.16998	-0.76089
H	5.36900	-0.38913	-2.30546
H	5.87800	0.60880	-0.91337
H	0.08353	0.03183	-2.59955

^{3}FeMeOPyNMe3OHMeCN$_3$trans
Charge: 3+
Energy: -1476766.0245501

Fe	1.17019	0.06327	0.07775
N	-0.75995	0.17619	-0.11562
C	-1.56212	0.18011	0.98843
O	2.89420	-0.00756	0.25492
N	1.03355	-0.13812	-2.09418
N	1.12477	-2.14791	0.04796
N	0.59408	-0.18508	2.17280
C	-2.67573	0.17189	-1.54525
H	-3.12497	0.19490	-2.53290
C	-1.31774	0.21037	-1.36825
C	-0.31454	0.40918	-2.47249
H	-0.19501	1.48612	-2.62803
H	-0.64314	-0.02455	-3.42347
C	2.12025	0.61350	-2.78814
H	2.02814	0.48550	-3.87393
H	3.08528	0.23297	-2.45329
H	2.03739	1.67140	-2.53798
C	1.16193	-1.61619	-2.37288
H	2.22654	-1.83748	-2.45164
H	0.71350	-1.84375	-3.34706
C	0.51176	-2.46041	-1.28576
H	-0.56089	-2.27781	-1.21861
H	0.66025	-3.52657	-1.50018
C	2.50177	-2.70648	0.17760
H	2.42075	-3.80101	0.15077
H	2.95632	-2.39248	1.11342
H	3.13349	-2.36257	-0.63700
C	0.26413	-2.49047	1.22836
H	0.37490	-3.56054	1.44591
H	-0.77558	-2.30929	0.95448
C	0.68221	-1.66775	2.43944
H	0.05724	-1.92188	3.30364
H	1.71402	-1.88375	2.71753
C	1.50849	0.55874	3.08863
H	1.46528	1.62136	2.84838

H	2.52585	0.19378	2.94695
H	1.20167	0.40516	4.13069
C	-3.52962	0.12642	-0.40374
C	-2.93590	0.14381	0.89011
H	-3.54442	0.14644	1.78679
C	-0.80986	0.33938	2.28364
H	-1.32203	-0.13267	3.12948
H	-0.74183	1.41040	2.50040
O	-4.80754	0.08267	-0.65122
C	-5.81076	0.05626	0.41021
H	-6.76410	0.02032	-0.11310
H	-5.73757	0.96922	1.00717
H	-5.67687	-0.84035	1.02129
N	1.27153	2.28185	0.10614
C	1.39061	3.43616	0.12319
C	1.54419	4.88335	0.14469
H	0.56917	5.36523	0.00809
H	1.96966	5.19787	1.10504
H	2.21672	5.19757	-0.66232
H	3.38972	0.83491	0.31179

[2]FeMeOPyNMe3OHN$_3$
Charge: 3+
Energy: -1496440.3778397

Fe	0.91663	-0.03040	-0.25915
N	-0.93123	0.10748	-0.32358
C	-1.68798	-1.02784	-0.35310
N	0.85131	2.04216	-0.06853
N	0.98608	-0.01164	1.85089
N	0.54069	-2.06487	-0.02813
C	-2.86502	1.49077	-0.36431
H	-3.34396	2.46387	-0.41117
C	-1.50414	1.35059	-0.38988
C	-0.49515	2.43974	-0.62090
H	-0.38059	2.57404	-1.70210
H	-0.80535	3.40379	-0.20555
C	1.93000	2.73287	-0.84477
H	1.78628	3.81841	-0.79304
H	2.89966	2.48740	-0.40894
H	1.89135	2.40296	-1.88341
C	0.96422	2.38905	1.40166
H	2.02368	2.51238	1.62708
H	0.48338	3.35474	1.58960
C	0.34896	1.28995	2.24734
H	-0.72770	1.21357	2.08806
H	0.51371	1.48357	3.31338
C	2.35916	-0.09648	2.46677
H	2.25411	-0.06587	3.55624
H	2.85582	-1.01957	2.17783
H	2.98057	0.73419	2.14067
C	0.18202	-1.20694	2.27646
H	0.32933	-1.40238	3.34471
H	-0.87590	-0.98654	2.12414
C	0.63365	-2.39409	1.44670
H	0.03663	-3.28623	1.66360
H	1.67269	-2.64789	1.65779
C	1.48750	-2.92543	-0.80779
H	1.47878	-2.61241	-1.85231
H	2.49163	-2.81996	-0.39433
H	1.18382	-3.97580	-0.72982
C	-3.68732	0.31946	-0.30972
C	-3.06154	-0.96578	-0.32905
H	-3.64962	-1.87610	-0.35170
C	-0.86137	-2.26895	-0.54536
H	-1.30888	-3.15550	-0.08485
H	-0.79172	-2.46369	-1.62135
O	-4.96626	0.53296	-0.27366
C	-5.95951	-0.54511	-0.25175
H	-6.91757	-0.03124	-0.20798
H	-5.87831	-1.12962	-1.17186
H	-5.81029	-1.15943	0.63990
O	1.08465	-0.05521	-2.00773
H	0.28780	0.00290	-2.56918
N	2.96248	-0.19675	-0.26087
N	3.60487	-0.22994	-1.29980
N	4.24866	-0.26675	-2.25288

[4]FeMeOPyNMe3OHNCS
Charge: 3+
Energy: -1701561.9090028

Fe	0.64448	0.00379	-0.29707
N	-1.20834	0.10086	-0.27842
C	-1.93821	-1.04755	-0.34091
N	0.53142	2.07443	-0.11612
N	0.74704	0.02764	1.81410
N	0.31204	-2.03734	-0.06083
C	-3.17510	1.43504	-0.36231
H	-3.67426	2.39644	-0.42875
C	-1.81067	1.32450	-0.37292
C	-0.83576	2.43101	-0.64070
H	-0.75138	2.53016	-1.72786
H	-1.15613	3.39747	-0.23877
C	1.56025	2.80602	-0.91834
H	1.39046	3.88611	-0.83952
H	2.55210	2.57314	-0.53240
H	1.48330	2.50021	-1.96194
C	0.67061	2.42651	1.34782
H	1.73280	2.57082	1.54756
H	0.17569	3.38325	1.54570
C	0.09806	1.32087	2.21707
H	-0.98032	1.22443	2.08613
H	0.28703	1.52688	3.27678
C	2.12735	-0.03494	2.40514
H	2.04667	-0.01392	3.49701
H	2.63136	-0.94938	2.10117
H	2.72289	0.81258	2.07417
C	-0.02944	-1.18074	2.25210
H	0.14187	-1.37752	3.31655
H	-1.09277	-0.97635	2.12105
C	0.42268	-2.36208	1.41155
H	-0.16435	-3.25872	1.63742
H	1.46613	-2.60715	1.61180
C	1.25302	-2.89479	-0.84645
H	1.20277	-2.60951	-1.89747
H	2.26611	-2.75689	-0.47023
H	0.97179	-3.94869	-0.73796
C	-3.96942	0.24695	-0.31215
C	-3.31342	-1.02082	-0.33286
H	-3.87712	-1.94526	-0.37905
C	-1.08810	-2.26161	-0.56966
H	-1.50812	-3.17394	-0.13415
H	-1.02256	-2.40657	-1.65323
O	-5.25564	0.42986	-0.28835
C	-6.21648	-0.67419	-0.28616
H	-7.18967	-0.18933	-0.24572
H	-6.11137	-1.24733	-1.21114
H	-6.05839	-1.29495	0.59962
O	0.54995	-0.01561	-2.05132
H	1.41343	-0.06041	-2.50794
N	2.60804	-0.10010	-0.40897
C	3.77053	-0.16277	-0.63409
S	5.36901	-0.24782	-0.92243

[5]FePyNMe3BrOCOcy22bCPCAcis
Charge: 2+
Energy: -3155620.3043343

Fe	-0.42190	-0.04728	-0.02977
N	-2.56038	0.05911	-0.26034
C	-3.15534	1.26019	-0.39439
O	1.30751	-1.14281	0.27511
N	-1.19175	-2.22648	0.36222
N	-0.75809	0.15274	2.11906
N	-0.88342	2.21719	-0.03049
C	-4.69928	-1.00892	-0.25163
H	-5.27692	-1.92627	-0.20374
C	-3.30881	-1.06162	-0.21497
C	-2.54923	-2.35399	-0.21835
H	-2.42737	-2.65121	-1.26624
H	-3.11422	-3.15315	0.27928
C	-0.34678	-3.31157	-0.21506
H	-0.82796	-4.28481	-0.05542
H	0.63319	-3.30847	0.25349
H	-0.22447	-3.13031	-1.28393
C	-1.18124	-2.29738	1.85021
H	-0.15757	-2.52725	2.14902
H	-1.81558	-3.12265	2.20120
C	-1.63787	-0.99706	2.50781
H	-2.66161	-0.75560	2.22296
H	-1.62044	-1.11504	3.59826
C	0.50279	0.11775	2.91479
H	0.26433	0.20890	3.98080
H	1.15236	0.93659	2.61415
H	1.02275	-0.82150	2.73743
C	-1.44116	1.47630	2.30044
H	-1.37937	1.77644	3.35365
H	-2.49690	1.35139	2.05936
C	-0.80417	2.54769	1.42334
H	-1.28156	3.51696	1.62100
H	0.25466	2.65021	1.66417
C	0.06244	3.08358	-0.79722
H	0.10273	2.73370	-1.82928
H	1.05637	3.02124	-0.36634
H	-0.28843	4.12304	-0.77237
C	2.12244	-0.15790	0.25179
C	-4.54170	1.38531	-0.43484
H	-4.99358	2.36699	-0.53354
C	-2.23719	2.42826	-0.59871
H	-2.68005	3.35666	-0.21546
H	-2.11817	2.55263	-1.68083
O	1.66712	1.00344	0.21330
C	3.62602	-0.47438	0.23747
H	3.74705	-1.53886	0.46099
C	4.10708	-0.19424	-1.20696
H	3.88869	0.84941	-1.45980
H	3.58836	-0.83384	-1.92955

C	4.35793	0.38481	1.27414
H	4.02259	0.15242	2.29327
H	4.13724	1.44128	1.08305
C	5.63879	-0.45891	-1.27584
H	5.95733	-0.23134	-2.30126
H	5.83549	-1.52421	-1.10377
C	5.88632	0.12139	1.17526
H	6.38784	0.76368	1.90811
H	6.09912	-0.91750	1.45655
C	6.37981	0.39333	-0.24874
H	6.26461	1.45800	-0.48952
H	7.45627	0.16784	-0.30058
C	-5.32498	0.23395	-0.35597
H	-6.40810	0.30334	-0.38127
Br	-0.16874	-0.21891	-2.41616

^{5}FePyNMe3BrOCOcy22bCPCAtrans
Charge: 2+
Energy: -3155622.5757492

Fe	0.19082	-0.36344	0.09053
N	0.79997	1.61509	0.09764
C	0.78114	2.30785	-1.05829
N	1.33219	-0.12461	2.10787
N	3.57112	-0.42338	-0.33905
N	0.79955	0.05973	-2.12294
C	1.35203	3.57064	1.33392
H	1.58100	4.04465	2.28290
C	1.08048	2.20668	1.27553
C	1.03580	1.29079	2.47619
H	0.01399	1.30905	2.86686
H	1.70232	1.64547	3.27297
C	0.72797	-1.04488	3.12671
H	1.18394	-0.87541	4.10993
H	0.89814	-2.07549	2.81382
H	-0.34310	-0.86680	3.17734
C	2.78715	-0.41842	2.08309
H	2.89756	-1.50215	2.02310
H	3.23354	-0.09483	3.03345
C	3.62882	0.23775	0.96642
H	3.38176	1.29018	0.83752
H	4.67664	0.17416	1.29255
C	4.32810	-1.66412	-0.49204
H	5.38899	-1.39436	-0.61654
H	3.99144	-2.21214	-1.37141
H	4.21840	-2.29061	0.39248
C	3.30971	0.35440	-1.55220
H	4.24436	0.33678	-2.13065
H	3.11020	1.38676	-1.27045
C	2.21412	-0.21078	-2.48291
H	2.41529	0.20366	-3.48038
H	2.32833	-1.29379	-2.55049
C	-0.04147	-0.78030	-3.03738
H	-1.09110	-0.61536	-2.80851
H	0.19372	-1.83098	-2.86494
H	0.16073	-0.52126	-4.08403
C	1.04379	3.67454	-1.06750
H	1.03148	4.22982	-1.99979
C	0.42466	1.49514	-2.28085
H	0.86375	1.92717	-3.18942
H	-0.66369	1.52600	-2.39129
O	-1.40858	-0.13331	1.39075
O	-1.66066	-0.11789	-0.74514
C	-2.22963	-0.05369	0.40799
C	-4.33047	-1.35112	0.30615
H	-4.06832	-1.66137	-0.71384
H	-3.90229	-2.08698	0.99703
C	-3.70144	0.05273	0.57298
H	-3.89054	0.32418	1.61840
C	-5.85726	-1.28339	0.45962
H	-6.10485	-1.05843	1.50614
H	-6.27940	-2.27062	0.24114
C	-6.47178	-0.21774	-0.45901
H	-7.55445	-0.16708	-0.30261
H	-6.31806	-0.50875	-1.50796
C	-5.83971	1.16040	-0.21522
H	-6.08823	1.50640	0.79777
H	-6.25164	1.90085	-0.90979
C	-4.31226	1.11465	-0.37268
H	-3.87393	2.09882	-0.16203
H	-4.05077	0.85427	-1.40642
C	1.32268	4.31002	0.14704
H	1.52988	5.37576	0.16658
Br	1.08552	-2.62123	-0.12051

^{3}FePyNMe3BrOCOcy23bPAAtrans
Charge: 2+
Energy: -3104871.7387474

Fe	-0.78536	0.05453	-0.08174
N	1.13191	-0.05798	0.12094
C	1.87881	-0.28459	-0.98400
N	-0.66993	0.42343	1.99080
N	-0.98852	-2.02962	0.53077
N	-0.33181	-0.81070	-1.93851
C	3.08419	0.13611	1.45865
H	3.56635	0.33929	2.40863
C	1.71806	0.20806	1.31310
C	0.77247	0.66937	2.37726
H	0.91157	1.74538	2.48230
H	0.97444	0.19982	3.34546
C	-1.49184	1.58750	2.45944
H	-1.34071	1.71229	3.53832
H	-2.54246	1.40002	2.25136
H	-1.16205	2.48418	1.93954
C	-1.16906	-0.83568	2.63922
H	-2.25454	-0.84423	2.53367
H	-0.93727	-0.81236	3.71027
C	-0.54775	-2.04261	1.95931
H	0.54307	-2.00603	1.99657
H	-0.86322	-2.97085	2.44835
C	-2.34334	-2.67439	0.45173
H	-2.23491	-3.73731	0.69583
H	-2.76862	-2.56453	-0.54206
H	-3.02844	-2.21052	1.15622
C	-0.06507	-2.75611	-0.39244
H	-0.20265	-3.83959	-0.29756
H	0.96390	-2.52926	-0.11563
C	-0.37578	-2.31288	-1.81381
H	0.32379	-2.76257	-2.52647
H	-1.37694	-2.63122	-2.10322
C	-1.24552	-0.35241	-3.03191
H	-1.28451	0.73617	-3.01767
H	-2.24479	-0.74507	-2.85581
H	-0.86504	-0.71079	-3.99573
C	3.88640	-0.16351	0.33063
C	3.25457	-0.36069	-0.92476
H	3.82634	-0.54712	-1.82526
C	1.05780	-0.32985	-2.23893
H	1.50875	-0.94379	-3.02563
H	0.96690	0.69219	-2.61737
O	5.18335	-0.21809	0.54330
C	6.10992	-0.47428	-0.54039
H	7.09489	-0.46008	-0.07752
H	6.03755	0.31641	-1.29317
H	5.91566	-1.45736	-0.97997
O	-0.62044	1.67621	-0.87594
O	0.73493	2.85371	0.49804
C	0.04280	2.79276	-0.49684
C	-0.21193	3.92803	-1.46012
H	0.43169	4.76978	-1.20043
H	-0.03158	3.61247	-2.49199
H	-1.26351	4.22751	-1.38831
Br	-3.16419	0.30113	-0.25472

^{5}FePyNMe3ClOCOcy22bCPCAcis
Charge: 2+
Energy: -1829096.4108987

Fe	0.47276	0.07258	-0.18040
N	2.48314	-0.42391	-0.55135
C	2.88769	-1.69683	-0.41380
O	-2.19651	2.36467	0.58534
N	1.44271	2.08988	-0.36876
N	1.07647	0.40819	1.98729
N	0.58010	-2.05805	0.46527
C	4.68848	0.27987	-1.09538
H	5.37517	1.07189	-1.37550
C	3.33689	0.55140	-0.90748
C	2.68488	1.88373	-1.17457
H	2.38801	1.88844	-2.22900
H	3.38179	2.71686	-1.02353
C	0.55955	3.06291	-1.07761
H	1.06874	4.02756	-1.19389
H	-0.35330	3.20617	-0.49972
H	0.30059	2.66044	-2.05720
C	1.73843	2.58170	1.01370
H	0.83345	3.07004	1.38006
H	2.52479	3.34626	0.98324
C	2.14213	1.44939	1.95240
H	3.06924	0.98355	1.61591
H	2.32465	1.85188	2.95717
C	-0.04719	0.85909	2.85459
H	0.30914	1.03212	3.87755
H	-0.83172	0.10462	2.86810
H	-0.48011	1.77877	2.46225
C	1.58518	-0.91246	2.45612
H	1.63672	-0.94069	3.55216
H	2.60105	-1.04594	2.08048
C	0.67868	-2.03413	1.95736
H	1.03516	-3.00320	2.32888
H	-0.33417	-1.89515	2.34028
C	-0.65613	-2.77228	0.03922
H	-0.73910	-2.71745	-1.04700
H	-1.51748	-2.27059	0.47928
H	-0.62978	-3.82022	0.36179
C	-2.29912	1.16292	0.39177
C	4.22544	-2.04164	-0.58469

H	4.54862	-3.07055	-0.46496
C	1.77475	-2.68653	-0.17430
H	2.11618	-3.54955	0.40986
H	1.46121	-3.06114	-1.15463
O	-1.46717	0.21762	0.40683
C	-3.85962	0.75400	0.04391
H	-4.43930	1.67743	0.09597
C	-3.81749	0.20150	-1.37450
H	-3.12225	-0.64163	-1.43093
H	-3.49978	0.95606	-2.10142
C	-4.30663	-0.23917	1.10411
H	-4.32693	0.20782	2.10393
H	-3.63368	-1.10313	1.11790
C	-5.27425	-0.26546	-1.72241
H	-5.23194	-0.68819	-2.73352
H	-5.93665	0.60707	-1.75961
C	-5.75535	-0.69973	0.71951
H	-6.06539	-1.43513	1.47137
H	-6.43846	0.15406	0.79692
C	-5.77454	-1.27752	-0.69444
H	-5.16693	-2.19120	-0.73749
H	-6.80372	-1.56983	-0.94876
C	5.13410	-1.03435	-0.92197
H	6.18451	-1.27355	-1.05650
Cl	-0.09075	-0.14592	-2.34075

[5]FePyNMe3ClOCOcy22bCPCAtrans
Charge: 2+
Energy: -1829094.6383978

Fe	-0.25895	-0.59632	-0.03157
N	-0.93484	1.36082	-0.18709
C	-0.93477	2.14070	0.91248
N	-1.39854	-0.53484	-2.06055
N	-3.63374	-0.72484	0.40426
N	-0.87675	-0.01731	2.13974
C	-1.53880	3.20305	-1.56674
H	-1.77888	3.59748	-2.54882
C	-1.22919	1.85543	-1.40595
C	-1.15576	0.85592	-2.53725
H	-0.13683	0.88251	-2.93472
H	-1.83781	1.12731	-3.35359
C	-0.75605	-1.51847	-2.99202
H	-1.22982	-1.47490	-3.98052
H	-0.86659	-2.51899	-2.57166
H	0.30318	-1.29022	-3.07686
C	-2.83819	-0.88458	-2.00805
H	-2.90231	-1.96331	-1.85991
H	-3.29880	-0.65902	-2.97983
C	-3.71166	-0.17373	-0.94834
H	-3.51225	0.89552	-0.90339
H	-4.75479	-0.31206	-1.26768
C	-4.25918	-2.01972	0.64587
H	-5.34168	-1.84792	0.76030
H	-3.86941	-2.47072	1.55749
H	-4.08959	-2.69100	-0.19500
C	-3.39842	0.14366	1.55757
H	-4.33056	0.12419	2.14081
H	-3.24380	1.16157	1.20424
C	-2.27834	-0.31528	2.51978
H	-2.49757	0.15851	3.48668
H	-2.34970	-1.39426	2.66283
C	-0.00688	-0.77379	3.09794
H	1.03601	-0.56917	2.87093
H	-0.19066	-1.84097	2.96649
H	-0.23135	-0.48066	4.13102
C	-1.23577	3.49631	0.81889
H	-1.23845	4.12051	1.70661
C	-0.55366	1.43610	2.19398
H	-1.01155	1.91951	3.06685
H	0.53236	1.51470	2.30255
O	1.33237	-0.38703	-1.35027
O	1.58605	-0.19654	0.77727
C	2.14886	-0.19316	-0.37975
C	4.30282	-1.39221	-0.22488
H	4.05994	-1.65784	0.81240
H	3.90123	-2.18099	-0.87196
C	3.61437	-0.03177	-0.56090
H	3.78625	0.18943	-1.62112
C	5.82460	-1.27035	-0.39397
H	6.05643	-1.09177	-1.45298
H	6.28873	-2.22617	-0.12651
C	6.39966	-0.13242	0.46134
H	7.47841	-0.04581	0.29392
H	6.26410	-0.37259	1.52556
C	5.70954	1.20343	0.14912
H	5.93779	1.50411	-0.88297
H	6.09463	1.99653	0.79955
C	4.18612	1.10333	0.32085
H	3.70616	2.05597	0.06150
H	3.94176	0.88888	1.36920
C	-1.53188	4.03055	-0.43936
H	-1.76878	5.08556	-0.53902
Cl	-1.06811	-2.65446	0.32083

[5]FePyNMe3ClOCOcy23bPAAtrans
Charge: 2+
Energy: -1778351.5477746

Fe	1.12549	0.59730	0.06505
N	-0.88926	0.27572	-0.12983
C	-1.67121	0.23548	0.96994
N	0.88563	-0.22200	-2.10167
N	0.70814	-2.77411	0.03784
N	0.46565	-0.20505	2.15133
C	-2.80393	0.12900	-1.54221
H	-3.25378	0.08271	-2.52808
C	-1.44159	0.22243	-1.36891
C	-0.44538	0.31554	-2.50166
H	-0.30082	1.37572	-2.72950
H	-0.82205	-0.17306	-3.40945
C	1.96132	0.36539	-2.96373
H	1.84246	0.03309	-4.00250
H	2.93003	0.04297	-2.57934
H	1.90934	1.44965	-2.91298
C	0.98503	-1.69345	-2.25017
H	2.03816	-1.95716	-2.14474
H	0.67714	-1.97264	-3.26734
C	0.14322	-2.57234	-1.29596
H	-0.87633	-2.20480	-1.19437
H	0.10194	-3.57021	-1.75634
C	1.88123	-3.63224	0.15545
H	1.53164	-4.67680	0.12507
H	2.39507	-3.45302	1.09900
H	2.56777	-3.45960	-0.67233
C	-0.10308	-2.56353	1.23645
H	-0.23121	-3.55800	1.68797
H	-1.08423	-2.20001	0.93644
C	0.53717	-1.67499	2.32805
H	0.03980	-1.94781	3.26922
H	1.59134	-1.93596	2.42994
C	1.35069	0.39351	3.20185
H	1.31151	1.47702	3.12779
H	2.37565	0.06719	3.02004
H	1.02920	0.07391	4.20094
C	-3.64499	0.11305	-0.40093
C	-3.05050	0.14765	0.88271
H	-3.64879	0.11552	1.78499
C	-0.91867	0.32976	2.27840
H	-1.46688	-0.16002	3.09377
H	-0.82582	1.39043	2.52973
O	-4.93987	0.04276	-0.64023
C	-5.89601	0.05358	0.44556
H	-6.87145	0.01871	-0.03629
H	-5.79785	0.97469	1.02804
H	-5.76050	-0.82762	1.08047
O	1.03530	2.38382	1.13556
O	1.28781	2.36695	-1.00435
C	1.20500	3.06530	0.06602
C	1.33280	4.54824	0.06743
H	0.96581	4.96449	-0.87340
H	0.80695	4.97797	0.92253
H	2.39750	4.80108	0.15738
Cl	3.02246	-0.57898	0.26122

[5]FePyNMe3FOCOcy22bCPCAcis
Charge: 2+
Energy: -1602970.9902566

Fe	0.49397	0.08004	-0.31501
N	2.52226	-0.41678	-0.63015
C	2.92675	-1.69093	-0.50777
O	-2.19264	2.32171	0.49838
N	1.47823	2.08468	-0.39160
N	1.00032	0.34479	1.89732
N	0.57997	-2.07106	0.25009
C	4.74831	0.30585	-1.05949
H	5.44408	1.10714	-1.28568
C	3.38955	0.56941	-0.91980
C	2.74821	1.91255	-1.15925
H	2.49335	1.96479	-2.22321
H	3.43895	2.73746	-0.94733
C	0.58673	3.03135	-1.12241
H	1.07988	4.00100	-1.26209
H	-0.33030	3.17394	-0.55050
H	0.33759	2.59381	-2.09049
C	1.71613	2.54038	1.01203
H	0.79784	3.02124	1.35450
H	2.50567	3.30166	1.03764
C	2.07628	1.37663	1.93372
H	3.01139	0.91272	1.61656
H	2.22642	1.74886	2.95522
C	-0.14098	0.77704	2.75147
H	0.18815	0.90674	3.78982
H	-0.93422	0.03212	2.71579
H	-0.55223	1.71647	2.38344
C	1.47434	-1.00095	2.33248
H	1.47642	-1.07769	3.42729

H	2.50485	-1.13238	1.99717
C	0.57830	-2.09028	1.74477
H	0.88878	-3.07666	2.11205
H	-0.45461	-1.93617	2.06295
C	-0.62937	-2.74958	-0.29383
H	-0.64531	-2.62045	-1.37801
H	-1.51549	-2.27402	0.12484
H	-0.62508	-3.81744	-0.04413
C	-2.30321	1.12615	0.26929
C	4.27162	-2.02913	-0.63293
H	4.59269	-3.06008	-0.52538
C	1.81230	-2.69121	-0.32320
H	2.13226	-3.54591	0.28484
H	1.55660	-3.08118	-1.31425
O	-1.48338	0.17462	0.22970
C	-3.88243	0.73910	-0.04155
H	-4.44923	1.66707	0.05292
C	-3.89638	0.22094	-1.47262
H	-3.21685	-0.63153	-1.57113
H	-3.59383	0.98986	-2.19123
C	-4.30337	-0.27548	1.00893
H	-4.28189	0.14679	2.01945
H	-3.64027	-1.14675	0.97711
C	-5.36937	-0.21997	-1.78125
H	-5.36981	-0.61810	-2.80306
H	-6.02127	0.66126	-1.77355
C	-5.76946	-0.71031	0.66538
H	-6.06204	-1.46159	1.40846
H	-6.43931	0.14858	0.78910
C	-5.84760	-1.25149	-0.76135
H	-5.25421	-2.17138	-0.84892
H	-6.88862	-1.52438	-0.98598
C	5.19027	-1.01220	-0.90636
H	6.24604	-1.24572	-1.00392
F	0.06592	0.07549	-2.02689

^{3}FePyNMe3FOCOcy22bCPCAtrans
Charge: 2+
Energy: -1602943.9779255

Fe	-0.25480	-0.52474	0.06328
N	-0.98992	1.21101	-0.42261
C	-1.13352	2.14704	0.53535
N	-1.43087	-1.07394	-1.74464
N	-3.48107	-1.00509	0.63660
N	-0.96325	0.20850	2.06113
C	-1.95363	2.62650	-2.06582
H	-2.29351	2.78641	-3.08381
C	-1.41713	1.39946	-1.68596
C	-1.26221	0.18115	-2.56201
H	-0.24658	0.17152	-2.96362
H	-1.95716	0.20084	-3.40941
C	-0.69422	-2.22039	-2.38198
H	-1.19456	-2.52428	-3.30894
H	-0.68033	-3.04188	-1.66462
H	0.32916	-1.92938	-2.59509
C	-2.85551	-1.51015	-1.70976
H	-2.86526	-2.56726	-1.44226
H	-3.28696	-1.44232	-2.71699
C	-3.76858	-0.73360	-0.76394
H	-3.72908	0.34323	-0.93062
H	-4.80391	-1.06521	-0.94742
C	-3.34004	-2.37886	1.08868
H	-3.90515	-3.04902	0.43766
H	-3.69488	-2.47543	2.11671
H	-2.26546	-2.64004	1.04275
C	-3.47672	0.07884	1.60781
H	-4.42198	0.00695	2.17084
H	-3.47782	1.03025	1.07516
C	-2.32798	-0.03645	2.60692
H	-2.53053	0.66456	3.42727
H	-2.32771	-1.03327	3.04910
C	-0.02951	-0.39163	3.07557
H	0.99430	-0.11740	2.84372
H	-0.12225	-1.47629	3.00689
H	-0.28815	-0.04407	4.08278
C	-1.66179	3.39510	0.21763
H	-1.77403	4.15544	0.98357
C	-0.69429	1.68233	1.90162
H	-1.17113	2.26358	2.69933
H	0.38548	1.82467	1.98354
O	1.19827	-0.51942	-1.24426
O	1.44721	0.12792	0.77692
C	2.02462	-0.11206	-0.34603
C	4.15449	-1.30930	-0.04126
H	3.92082	-1.41937	1.02588
H	3.73026	-2.17424	-0.56422
C	3.48531	0.00359	-0.56137
H	3.64497	0.06392	-1.64524
C	5.67583	-1.23862	-0.24235
H	5.89627	-1.21851	-1.31853
H	6.12777	-2.15415	0.15515
C	6.27970	0.00040	0.43387
H	7.35738	0.04249	0.24429
H	6.15438	-0.08158	1.52298
C	5.60775	1.28956	-0.06074
H	5.82712	1.43413	-1.12783
H	6.01413	2.16101	0.46403
C	4.08498	1.24423	0.13982
H	3.61728	2.15720	-0.24998
H	3.85195	1.18956	1.21099
C	-2.05241	3.63877	-1.10423
H	-2.46257	4.60626	-1.37750
F	-0.30070	-2.19909	0.63251

^{3}FePyNMe3FOCOcy23bPAAtrans
Charge: 2+
Energy: -1552212.4797804

Fe	-1.32806	-0.17646	0.23691
N	0.67615	-0.19696	0.39217
C	1.53705	0.85152	0.37375
N	-1.14694	-2.15720	-0.16497
N	-0.69997	0.04387	-2.13946
N	0.04410	2.62044	-0.70115
C	2.53773	-1.71581	0.41004
H	2.92363	-2.72940	0.41480
C	1.18200	-1.46175	0.39297
C	0.15767	-2.56787	0.44310
H	-0.03953	-2.78570	1.49717
H	0.52922	-3.48591	-0.02567
C	-2.27479	-2.89489	0.48944
H	-2.17911	-3.96836	0.29161
H	-3.21245	-2.51740	0.08296
H	-2.25086	-2.70120	1.56061
C	-1.22883	-2.35216	-1.64594
H	-2.27963	-2.22628	-1.91047
H	-0.94470	-3.38255	-1.89318
C	-0.36087	-1.37766	-2.43060
H	0.69140	-1.53714	-2.18100
H	-0.47061	-1.59335	-3.50262
C	-1.91188	0.46761	-2.88686
H	-1.72729	0.47668	-3.96978
H	-2.22254	1.46082	-2.55731
H	-2.73774	-0.20238	-2.65881
C	0.46365	0.87252	-2.50593
H	0.62125	0.87257	-3.59605
H	1.35752	0.44061	-2.05726
C	0.35285	2.35460	-2.10656
H	1.32788	2.82308	-2.31248
H	-0.39483	2.87090	-2.70752
C	-1.02278	3.53938	-0.35897
H	-1.66063	3.05119	0.39389
H	-1.58998	3.82450	-1.24307
H	-0.58746	4.43187	0.11771
C	3.44354	-0.63577	0.44162
C	2.91222	0.67509	0.39979
H	3.56635	1.53794	0.39128
C	0.97495	2.26227	0.38284
H	1.79984	2.98665	0.31819
H	0.43979	2.43325	1.31772
O	4.72456	-0.94206	0.48421
C	5.73594	0.09074	0.54478
H	6.68241	-0.44383	0.60200
H	5.59819	0.70480	1.44008
H	5.70802	0.70377	-0.36166
O	-1.51243	-0.62633	2.40581
O	-1.48280	1.34760	1.47958
C	-1.65981	0.61082	2.54781
C	-2.04700	1.26109	3.83592
H	-3.13507	1.40402	3.83519
H	-1.78292	0.61751	4.67687
H	-1.58091	2.24451	3.93515
F	-2.95752	-0.11182	-0.29824

^{5}FePyNMe3N$_3$OCOcy22bCPCAcis
Charge: 2+
Energy: -1643360.2227085

Fe	0.49533	0.05706	-0.21463
N	2.66315	-0.03120	-0.44361
C	3.25887	-1.22217	-0.64271
O	-1.21889	1.15353	0.04160
N	1.29902	2.21287	0.34125
N	0.82735	-0.27949	1.91223
N	0.97528	-2.19050	-0.36645
C	4.80656	1.02612	-0.33732
H	5.38668	1.93568	-0.21988
C	3.41577	1.07910	-0.31153
C	2.66248	2.37376	-0.21679
H	2.55553	2.76206	-1.23591
H	3.23002	3.12329	0.35079
C	0.46627	3.34433	-0.15367
H	0.93978	4.30133	0.10046
H	-0.52489	3.29830	0.28862
H	0.37045	3.26638	-1.23840
C	1.27986	2.17490	1.83072
H	0.25635	2.39080	2.14132

H	1.91775	2.96795	2.24455
C	1.72234	0.82628	2.38920
H	2.74291	0.59572	2.08472
H	1.70809	0.86111	3.48539
C	-0.43640	-0.27715	2.70774
H	-0.20107	-0.39958	3.77113
H	-1.08161	-1.08892	2.38118
H	-0.96188	0.66480	2.55898
C	1.49055	-1.62293	2.01748
H	1.40794	-1.99307	3.04649
H	2.55183	-1.49595	1.80116
C	0.85645	-2.62324	1.05756
H	1.31598	-3.61116	1.19596
H	-0.20895	-2.72391	1.26745
C	0.03446	-2.96797	-1.22454
H	0.02490	-2.52318	-2.22136
H	-0.96759	-2.92983	-0.80932
H	0.36775	-4.01119	-1.29307
C	-2.04249	0.16323	0.08694
C	4.64533	-1.35086	-0.67708
H	5.09656	-2.32586	-0.83038
C	2.34132	-2.37801	-0.91646
H	2.77373	-3.32272	-0.56225
H	2.24723	-2.46230	-2.00460
O	-1.54587	-0.98672	-0.00519
C	-3.52535	0.43006	0.20934
H	-3.65169	1.48735	0.46731
C	-4.17567	0.16572	-1.16808
H	-3.97114	-0.87051	-1.46491
H	-3.74576	0.82213	-1.93860
C	-4.14957	-0.46185	1.30694
H	-3.69485	-0.24454	2.28156
H	-3.93555	-1.51088	1.06860
C	-5.70017	0.40985	-1.08764
H	-6.13885	0.19778	-2.06847
H	-5.88937	1.46935	-0.87249
C	-5.67196	-0.22569	1.36747
H	-6.09619	-0.89064	2.12935
H	-5.86920	0.80247	1.69891
C	-6.32698	-0.46855	0.00532
H	-6.22821	-1.52682	-0.27140
H	-7.40199	-0.25411	0.06454
C	5.43047	-0.20919	-0.51735
H	6.51365	-0.28030	-0.53433
N	0.31155	0.28144	-2.10034
N	-0.71128	0.65870	-2.66098
N	-1.63529	1.00340	-3.24315

^{5}FePyNMe3N$_3$OCOcy22bCPCAtrans
Charge: 2+
Energy: -1643360.9305769

Fe	-0.67501	-0.61390	0.01120
N	-1.05202	1.32615	-0.24030
C	-0.87253	2.17837	0.79438
N	-1.75198	-0.69099	-1.99510
N	-2.89050	-0.79473	0.66054
N	-0.71583	0.17026	2.26432
C	-1.83505	3.08222	-1.63738
H	-2.21835	3.41316	-2.59705
C	-1.52018	1.74060	-1.43799
C	-1.61148	0.69873	-2.52571
H	-0.67791	0.74284	-3.09180
H	-2.42958	0.92999	-3.21872
C	-1.13425	-1.67168	-2.93440
H	-1.67462	-1.66850	-3.88928
H	-1.19565	-2.66546	-2.48870
H	-0.09095	-1.41540	-3.09819
C	-3.17167	-1.07867	-1.77457
H	-3.20280	-2.16701	-1.70144
H	-3.78282	-0.79919	-2.64257
C	-3.73029	-0.44478	-0.51624
H	-3.74862	0.64320	-0.61045
H	-4.76459	-0.77581	-0.35534
C	-3.15598	-2.19189	1.10061
H	-4.19349	-2.28587	1.44452
H	-2.47655	-2.46624	1.90572
H	-2.98115	-2.88420	0.27936
C	-3.15033	0.16396	1.76847
H	-4.13894	-0.02885	2.20628
H	-3.17413	1.16976	1.34641
C	-2.08221	0.05682	2.84062
H	-2.24452	0.82566	3.60753
H	-2.14824	-0.90725	3.34726
C	0.24780	-0.53601	3.15115
H	1.25245	-0.45182	2.74403
H	-0.02752	-1.59169	3.19899
H	0.22008	-0.11261	4.16344
C	-1.16602	3.52942	0.64402
H	-1.02413	4.21174	1.47558
C	-0.29548	1.58144	2.05612
H	-0.54755	2.20010	2.92683
H	0.79332	1.58353	1.95204
O	0.97835	-0.15176	-1.64125
O	1.24334	-0.35442	0.50270
C	1.75932	-0.11919	-0.66703
C	4.05194	-1.05398	-0.27221
H	3.79133	-1.25351	0.77515
H	3.79320	-1.94986	-0.85141
C	3.23659	0.16288	-0.76835
H	3.43982	0.33030	-1.83224
C	5.55969	-0.76156	-0.38964
H	5.82564	-0.64728	-1.44900
H	6.11930	-1.62515	-0.01445
C	5.93826	0.51111	0.38208
H	7.00558	0.72095	0.25052
H	5.77832	0.34682	1.45714
C	5.10846	1.71703	-0.07943
H	5.35237	1.95775	-1.12305
H	5.35278	2.60601	0.51323
C	3.60024	1.43587	0.03427
H	3.02088	2.29364	-0.33151
H	3.32965	1.27523	1.08732
C	-1.64915	3.98334	-0.58689
H	-1.88954	5.03346	-0.72263
N	-0.43088	-2.43825	0.12367
N	0.67783	-2.97409	0.20382
N	1.67305	-3.52430	0.27766

^{5}FePyNMe3N$_3$OCOcy23bPAAtrans
Charge: 2+
Energy: -1592609.8051467

Fe	-0.67616	-0.01579	-0.10100
N	1.34878	0.00655	-0.53617
C	2.08380	-1.09653	-0.30916
N	-0.28988	2.20386	-0.30709
N	-0.29221	0.42754	2.03770
N	-0.05039	-2.09641	0.54092
C	3.32861	1.31202	-0.78565
H	3.82290	2.26058	-0.96474
C	1.95574	1.19403	-0.76326
C	1.00528	2.34087	-1.03872
H	0.77769	2.32662	-2.11017
H	1.47875	3.30728	-0.82370
C	-1.36787	2.89437	-1.05775
H	-1.17958	3.97149	-1.15345
H	-2.31754	2.74601	-0.53733
H	-1.44436	2.45620	-2.05584
C	-0.20844	2.73003	1.08600
H	-1.22815	2.95514	1.40842
H	0.34767	3.67680	1.11615
C	0.43447	1.73060	2.04971
H	1.46850	1.54142	1.75611
H	0.45484	2.15723	3.06141
C	-1.53849	0.52067	2.83475
H	-1.32386	0.74323	3.88816
H	-2.08335	-0.42399	2.78430
H	-2.17572	1.31246	2.43631
C	0.56077	-0.69249	2.53038
H	0.60080	-0.69995	3.62780
H	1.57715	-0.52416	2.16968
C	0.04401	-2.04215	2.02815
H	0.68770	-2.84614	2.41038
H	-0.95759	-2.22815	2.42397
C	-1.02939	-3.13015	0.12233
H	-1.12142	-3.11412	-0.96638
H	-2.00399	-2.89623	0.55833
H	-0.72960	-4.13663	0.44172
C	4.11776	0.15581	-0.57279
C	3.47043	-1.07385	-0.31676
H	4.03116	-1.98118	-0.12920
C	1.27284	-2.36003	-0.09838
H	1.84260	-3.10568	0.47109
H	1.07967	-2.79190	-1.08641
O	5.42848	0.33546	-0.61509
C	6.32596	-0.77834	-0.42508
H	7.32563	-0.35960	-0.52832
H	6.15895	-1.53976	-1.19366
H	6.20186	-1.20394	0.57608
O	-1.60172	-0.43133	-1.94809
O	-3.74007	-0.40862	-1.24983
C	-2.79985	-0.54411	-2.20284
C	-3.38192	-0.83488	-3.54622
H	-3.07090	-0.04448	-4.23832
H	-2.95997	-1.77739	-3.91189
H	-4.47028	-0.89801	-3.51580
N	-3.13073	-0.12686	0.03436
N	-4.09448	-0.01297	0.84431
N	-4.85472	0.11374	1.67269

^{5}FePyNMe3NCSOCOcy22bCPCAcis
Charge: 2+
Energy: -1848470.8327910

Fe	0.54783	0.04828	0.06271
N	2.68291	0.46986	-0.28278
C	3.22927	0.23912	-1.49245

O	-1.15062	0.00403	1.38552
N	1.46274	0.47683	2.16906
N	1.14728	-2.00064	0.52649
N	0.98069	-0.62694	-2.12517
C	4.85837	0.93387	0.60572
H	5.47123	1.21335	1.45651
C	3.47752	0.82394	0.74642
C	2.76948	1.16531	2.02438
H	2.57096	2.24289	2.00821
H	3.40757	0.97458	2.89742
C	0.61767	1.30873	3.07329
H	1.15336	1.51023	4.00964
H	-0.31529	0.79653	3.28757
H	0.39250	2.25226	2.57227
C	1.59502	-0.90383	2.72129
H	0.60649	-1.19277	3.08104
H	2.27163	-0.90572	3.58672
C	2.08908	-1.91383	1.68740
H	3.07271	-1.63224	1.31004
H	2.19080	-2.89856	2.16002
C	-0.02619	-2.84958	0.88508
H	0.30678	-3.86673	1.12172
H	-0.72655	-2.87638	0.05269
H	-0.53779	-2.42129	1.74502
C	1.80721	-2.53488	-0.70725
H	1.85248	-3.62996	-0.66183
H	2.83433	-2.16884	-0.73185
C	1.05019	-2.10953	-1.96403
H	1.51787	-2.56787	-2.84604
H	0.02063	-2.46701	-1.91742
C	-0.07413	-0.26983	-3.11643
H	-0.21767	0.81237	-3.09942
H	-1.01041	-0.75047	-2.85022
H	0.23192	-0.58272	-4.12281
C	-1.93288	-0.31863	0.43469
C	4.60203	0.32886	-1.70895
H	5.01146	0.12863	-2.69376
C	2.25819	-0.04077	-2.60166
H	2.71013	-0.67305	-3.37733
H	2.02192	0.91852	-3.07554
O	-1.38042	-0.57572	-0.68402
C	-3.42842	-0.33403	0.60181
H	-3.64399	-0.08572	1.64670
C	-4.07028	0.71442	-0.32244
H	-3.78155	0.51298	-1.36103
H	-3.67274	1.73360	-0.08017
C	-4.00447	-1.74284	0.27536
H	-3.56130	-2.48508	0.95038
H	-3.71450	-2.00915	-0.74881
C	-5.59504	0.74725	-0.16959
H	-6.02541	1.49335	-0.84498
H	-5.86129	1.03749	0.85434
C	-5.53389	-1.72762	0.41081
H	-5.92318	-2.71891	0.14581
H	-5.80662	-1.55280	1.46003
C	-6.17134	-0.65743	-0.47831
H	-5.99656	-0.89559	-1.53580
H	-7.25733	-0.62687	-0.33059
C	5.42929	0.67884	-0.64159
H	6.50381	0.75006	-0.77921
N	0.02381	2.01023	-0.40507
C	-0.93082	2.70991	-0.46050
S	-2.26680	3.63494	-0.53297

[5]FePyNMe3NCSOCOcy22bCPCAtrans
Charge: 2+
Energy: -1848469.7435663

Fe	-0.90541	0.59681	0.07039
N	-1.36347	-1.44444	-0.06003
C	-1.61831	-2.00477	-1.25314
N	-1.36558	0.09713	2.20242
N	-3.07707	1.06001	0.08191
N	-1.29119	0.31136	-2.13094
C	-2.00706	-3.43387	1.07770
H	-2.15538	-3.97421	2.00690
C	-1.53914	-2.12504	1.08926
C	-1.13193	-1.37000	2.33351
H	-0.05487	-1.51134	2.46757
H	-1.63141	-1.76709	3.22553
C	-0.44725	0.84678	3.10333
H	-0.62944	0.59078	4.15429
H	-0.60352	1.91635	2.95533
H	0.58195	0.60726	2.83485
C	-2.78850	0.47541	2.47000
H	-2.79151	1.51562	2.79980
H	-3.19503	-0.12070	3.29641
C	-3.66458	0.31505	1.23038
H	-3.74101	-0.73654	0.94927
H	-4.67972	0.67313	1.44586
C	-3.29017	2.52658	0.23988
H	-4.36280	2.75065	0.28701
H	-2.83986	3.05954	-0.59583
H	-2.79954	2.87998	1.14568
C	-3.60989	0.59074	-1.22968
H	-4.58663	1.04721	-1.43430
H	-3.76062	-0.48940	-1.17058
C	-2.63332	0.93231	-2.34991
H	-3.04415	0.61785	-3.31804
H	-2.48192	2.01227	-2.40093
C	-0.26647	1.01981	-2.94940
H	0.71369	0.59013	-2.74097
H	-0.26123	2.07459	-2.67289
H	-0.48626	0.92241	-4.01978
C	-2.09106	-3.31347	-1.33893
H	-2.30218	-3.75860	-2.30579
C	-1.28826	-1.14750	-2.45146
H	-1.96131	-1.36115	-3.29063
H	-0.27529	-1.41565	-2.76457
O	1.05614	-0.05622	0.50210
O	1.67437	-1.19385	-1.38093
C	1.81689	-0.66452	-0.29903
C	4.11177	0.40826	-0.50254
H	4.09809	0.13326	-1.56239
H	3.65668	1.39947	-0.38712
C	3.39516	-0.64551	0.31852
H	3.27709	-0.33319	1.35878
C	5.59339	0.46257	0.00845
H	5.60878	0.82151	1.04468
H	6.11560	1.20709	-0.60373
C	6.23950	-0.91934	-0.09097
H	7.26545	-0.86558	0.29980
H	6.31499	-1.22279	-1.14292
C	5.45405	-1.96586	0.70018
H	5.46884	-1.72553	1.77043
H	5.88100	-2.96946	0.58797
C	3.97404	-2.03803	0.19643
H	3.42271	-2.76813	0.79942
H	3.94463	-2.36267	-0.84824
C	-2.28575	-4.03121	-0.15735
H	-2.65861	-5.05021	-0.19561
N	-0.25562	2.35261	0.05724
C	0.72833	3.05689	0.05965
S	2.01321	3.97552	0.05887

[3]FePyNMe3NCSOCOcy23bPAAtrans
Charge: 2+
Energy: -1797715.2384830

Fe	0.72970	0.01975	0.04354
N	-1.17251	0.05431	-0.12423
C	-1.96630	0.15477	0.96669
N	0.57088	-0.64488	-2.11331
N	0.61313	-2.22963	0.28259
N	0.16534	-0.10980	2.22223
C	-3.06720	0.01314	-1.56642
H	-3.50345	-0.02958	-2.55823
C	-1.70750	0.00504	-1.37801
C	-0.69807	0.03339	-2.49711
H	-0.45319	1.08149	-2.69271
H	-1.10855	-0.39440	-3.41985
C	1.70119	-0.12477	-2.92139
H	1.53764	-0.30833	-3.99116
H	2.62111	-0.62170	-2.60901
H	1.79796	0.94601	-2.73735
C	0.47434	-2.13137	-2.18832
H	1.48005	-2.51940	-2.35569
H	-0.12854	-2.43236	-3.05440
C	-0.12005	-2.72727	-0.91375
H	-1.16964	-2.44978	-0.81022
H	-0.07290	-3.82300	-0.96383
C	1.96297	-2.85410	0.35062
H	1.86878	-3.94696	0.36729
H	2.48597	-2.52446	1.24592
H	2.56038	-2.55666	-0.50993
C	-0.13230	-2.48083	1.54842
H	0.00173	-3.52081	1.87137
H	-1.19717	-2.33451	1.35269
C	0.34916	-1.52572	2.63546
H	-0.18065	-1.72632	3.57600
H	1.41312	-1.67372	2.83029
C	1.02491	0.79551	3.02724
H	0.89548	1.81514	2.66392
H	2.06670	0.49402	2.90349
H	0.75964	0.74622	4.09105
C	-3.92391	0.09832	-0.43861
C	-3.34624	0.16347	0.84712
H	-3.95602	0.23610	1.73909
C	-1.26433	0.31191	2.29002
H	-1.79238	-0.23206	3.08261
H	-1.29341	1.37558	2.53292
O	-5.21584	0.10519	-0.69837
C	-6.18462	0.21972	0.37066
H	-7.15386	0.21492	-0.12466
H	-6.04292	1.16108	0.91019
H	-6.10520	-0.63655	1.04762
O	0.89443	1.74674	-0.56129
O	-0.45315	2.79496	0.91203

C	0.28277	2.83964	-0.05477
C	0.63322	4.09121	-0.82377
H	1.70873	4.28234	-0.74429
H	0.40164	3.96408	-1.88612
H	0.07609	4.93526	-0.41530
N	2.64341	-0.04359	0.34837
C	3.77636	0.26890	0.16689
S	5.32495	0.66871	-0.03300

^{3}FePyNMe3OHOCOcy22bCPCAcis
Charge: 2+
Energy: -1587891.3707366

Fe	0.64960	0.10027	-0.17965
N	2.59550	-0.06935	-0.41290
C	3.10742	-1.27287	-0.71169
O	-1.14337	0.24166	0.09671
N	1.17046	2.04632	0.24999
N	0.81850	-0.20730	1.92587
N	0.74935	-1.95293	-0.31056
C	4.71860	0.96976	-0.58850
H	5.32766	1.86756	-0.57926
C	3.34072	1.04739	-0.41679
C	2.50945	2.29840	-0.39323
H	2.31683	2.57173	-1.43547
H	3.00538	3.14440	0.09343
C	0.16507	3.00260	-0.30852
H	0.48924	4.03171	-0.11734
H	-0.79490	2.82108	0.17223
H	0.07120	2.83015	-1.38045
C	1.24468	2.18504	1.75157
H	0.24360	2.44112	2.09847
H	1.90239	3.02166	2.01003
C	1.71731	0.88890	2.39196
H	2.74128	0.65383	2.09819
H	1.69739	0.97698	3.48485
C	-0.46781	-0.15634	2.68726
H	-0.26165	-0.31067	3.75234
H	-1.15272	-0.91940	2.32751
H	-0.95904	0.80139	2.53820
C	1.42087	-1.56655	2.05691
H	1.33352	-1.93863	3.08468
H	2.48371	-1.50594	1.81673
C	0.69203	-2.49286	1.09630
H	1.11020	-3.50499	1.11838
H	-0.36211	-2.56944	1.36302
C	-0.38588	-2.49783	-1.11803
H	-0.37736	-2.02584	-2.10032
H	-1.32185	-2.26684	-0.61238
H	-0.27657	-3.58353	-1.21896
C	-2.14269	0.45570	-0.79324
C	4.47856	-1.42616	-0.89210
H	4.89993	-2.39952	-1.12049
C	2.05077	-2.30473	-0.98581
H	2.35116	-3.32085	-0.71039
H	1.86555	-2.28968	-2.06447
O	-1.94244	0.62182	-1.98965
C	-3.50886	0.41652	-0.15008
H	-3.43797	0.95778	0.80427
C	-4.58462	1.06024	-1.04273
H	-4.58993	0.54590	-2.01119
H	-4.32470	2.10579	-1.24479
C	-3.86499	-1.06036	0.18169
H	-3.10514	-1.48892	0.85063
H	-3.85345	-1.64177	-0.75138
C	-5.96866	0.95854	-0.38287
H	-6.71857	1.39875	-1.04863
H	-5.97971	1.55558	0.54033
C	-5.25767	-1.15142	0.82704
H	-5.49991	-2.20347	1.01577
H	-5.23097	-0.65029	1.80510
C	-6.32948	-0.49772	-0.05699
H	-6.42704	-1.06785	-0.99146
H	-7.30272	-0.54492	0.44301
C	5.29026	-0.29019	-0.80054
H	6.36428	-0.38152	-0.92978
O	0.64857	0.34651	-1.92027
H	-0.30583	0.48823	-2.20065

^{5}FePyNMe3OHOCOcy22bCPCAtrans
Charge: 2+
Energy: -1587890.7328857

Fe	-0.67806	-0.77604	-0.08008
N	-1.00879	1.21025	0.07675
C	-0.68239	1.81448	1.24338
N	-1.68938	-0.32553	-2.05308
N	-2.78156	-1.11345	0.54093
N	-0.49162	-0.47913	2.15710
C	-1.75093	3.27293	-0.84268
H	-2.16235	3.82506	-1.68143
C	-1.50967	1.90554	-0.96337
C	-1.71398	1.15071	-2.25052
H	-0.88630	1.42350	-2.90888
H	-2.64556	1.45810	-2.74071
C	-0.93323	-1.00701	-3.13910
H	-1.42666	-0.85495	-4.10688
H	-0.88613	-2.07351	-2.91540
H	0.07485	-0.59443	-3.17638
C	-3.05411	-0.90032	-1.90786
H	-2.96670	-1.98163	-2.02688
H	-3.71100	-0.53431	-2.70727
C	-3.64226	-0.55681	-0.54544
H	-3.70492	0.52565	-0.41327
H	-4.65893	-0.95829	-0.45861
C	-3.05626	-2.56999	0.72045
H	-4.07885	-2.69963	1.09369
H	-2.34604	-3.00448	1.42002
H	-2.93881	-3.09356	-0.22507
C	-2.96544	-0.38704	1.83143
H	-3.92169	-0.67232	2.28753
H	-3.00929	0.68102	1.61708
C	-1.82226	-0.70342	2.79293
H	-1.92351	-0.09539	3.70008
H	-1.86770	-1.74753	3.10526
C	0.52979	-1.42669	2.67658
H	1.45685	-1.28215	2.12106
H	0.17957	-2.44682	2.51279
H	0.70631	-1.26478	3.74690
C	-0.89660	3.17467	1.41612
H	-0.64179	3.65036	2.35742
C	-0.02240	0.92621	2.26804
H	-0.16923	1.31206	3.28416
H	1.05358	0.92914	2.06589
O	1.23015	1.13194	-1.85450
O	1.09706	-0.51267	-0.31173
C	1.78534	0.38905	-1.07601
C	3.86078	-1.07895	-1.06704
H	3.38397	-1.78637	-0.37426
H	3.62811	-1.40884	-2.08701
C	3.28149	0.33094	-0.81933
H	3.71120	1.03335	-1.54280
C	5.38223	-1.07478	-0.83836
H	5.85788	-0.43499	-1.59390
H	5.77299	-2.08631	-0.99323
C	5.73782	-0.56633	0.56654
H	6.82554	-0.53104	0.68835
H	5.36040	-1.27563	1.31783
C	5.13642	0.82170	0.83030
H	5.59424	1.55910	0.15760
H	5.35371	1.15102	1.85266
C	3.61350	0.81984	0.60966
H	3.19895	1.82346	0.77399
H	3.14572	0.13827	1.33511
C	-1.44195	3.91077	0.35769
H	-1.62143	4.97554	0.47119
O	-0.53908	-2.51941	-0.28397
H	0.37180	-2.79854	-0.50515

^{5}FePyNMe3BrOH
Charge: 2+
Energy: -2937134.8057230

Fe	0.72632	0.00025	0.21983
N	0.36211	2.18438	-0.16835
N	0.98517	0.00161	-1.97961
N	0.36378	-2.18387	-0.17089
C	-3.27036	1.20842	-0.43353
H	-3.78658	2.15898	-0.51981
C	-1.90629	1.18025	-0.16563
C	-1.07915	2.40155	0.13815
H	-1.16380	2.58796	1.21472
H	-1.46267	3.28893	-0.37928
C	1.22692	3.02052	0.71310
H	1.06386	4.08603	0.51158
H	2.27007	2.76563	0.52243
H	0.99512	2.80495	1.75630
C	0.68951	2.43208	-1.60442
H	1.76004	2.63316	-1.66308
H	0.17400	3.33194	-1.96183
C	0.32327	1.24016	-2.48160
H	-0.75518	1.07452	-2.48496
H	0.62956	1.43457	-3.51696
C	2.43635	0.00196	-2.32595
H	2.54718	0.00226	-3.41668
H	2.92448	-0.87364	-1.90440
H	2.92418	0.87753	-1.90397
C	0.32361	-1.23657	-2.48296
H	0.62969	-1.42952	-3.51865
H	-0.75489	-1.07138	-2.48580
C	0.69062	-2.42952	-1.60747
H	0.17515	-3.32902	-1.96585
H	1.76117	-2.63028	-1.66692
C	1.22954	-3.02058	0.70908
H	0.99802	-2.80656	1.75267
H	2.27244	-2.76471	0.51834
H	1.06715	-4.08594	0.50623
C	-3.95586	-0.00121	-0.57629

C	-3.26939	-1.21045	-0.43467
H	-3.78486	-2.16133	-0.52184
C	-1.07719	-2.40233	0.13602
H	-1.46022	-3.28970	-0.38178
H	-1.16124	-2.58939	1.21253
N	-1.25413	-0.00037	-0.06781
C	-1.90536	-1.18146	-0.16672
H	-5.02078	-0.00155	-0.78821
O	2.46071	0.00029	0.41359
H	2.82493	-0.00028	1.32176
Br	0.28078	-0.00146	2.59838

^{5}FePyNMe3ClOH
Charge: 2+
Energy: -1610605.0872927

Fe	0.70530	0.00019	0.54735
N	0.37537	2.18143	0.12538
N	1.14541	0.00061	-1.63345
N	0.37723	-2.18112	0.12535
C	-3.23135	1.20834	-0.40958
H	-3.74190	2.15873	-0.52619
C	-1.88783	1.18002	-0.05224
C	-1.08503	2.39957	0.31755
H	-1.25396	2.58386	1.38443
H	-1.42464	3.28890	-0.22652
C	1.16977	2.99782	1.08732
H	1.01711	4.06755	0.90074
H	2.22519	2.75067	0.96742
H	0.86203	2.75338	2.10445
C	0.81889	2.43142	-1.27753
H	1.89057	2.63263	-1.24914
H	0.33337	3.33115	-1.67491
C	0.52368	1.23987	-2.18314
H	-0.55096	1.07408	-2.27213
H	0.91115	1.43671	-3.19037
C	2.61817	0.00153	-1.87113
H	2.80804	0.00184	-2.95092
H	3.07466	-0.87398	-1.41551
H	3.07361	0.87743	-1.41519
C	0.52523	-1.23944	-2.18313
H	0.91309	-1.43591	-3.19028
H	-0.54960	-1.07492	-2.27231
C	0.82167	-2.43055	-1.27734
H	0.33758	-3.33098	-1.67489
H	1.89363	-2.63026	-1.24847
C	1.17194	-2.99690	1.08757
H	0.86354	-2.75282	2.10458
H	2.22719	-2.74882	0.96815
H	1.02030	-4.06675	0.90081
C	-3.90501	-0.00158	-0.59933
C	-3.23034	-1.21097	-0.40997
H	-3.74008	-2.16176	-0.52687
C	-1.08305	-2.40066	0.31678
H	-1.42165	-3.28996	-0.22796
H	-1.25229	-2.58577	1.38346
N	-1.24304	-0.00056	0.08187
C	-1.88682	-1.18162	-0.05263
H	-4.95348	-0.00197	-0.88161
O	2.42690	0.00065	0.83939
H	2.69690	0.00074	1.78081
Cl	0.13901	0.00015	2.68524

^{3}FePyNMe3FOH
Charge: 2+
Energy: -1384479.7158096

Fe	-0.64555	-0.00001	-0.54558
N	-0.38933	2.03147	-0.34774
N	-1.22686	-0.00001	1.44361
N	-0.38928	-2.03147	-0.34773
C	3.25834	1.21404	0.33932
H	3.78112	2.16142	0.41915
C	1.90959	1.17820	0.00570
C	1.07845	2.33595	-0.46648
H	1.29818	2.47003	-1.53085
H	1.31293	3.27649	0.04259
C	-1.13595	2.76148	-1.41818
H	-0.94804	3.83783	-1.33669
H	-2.19993	2.55775	-1.30293
H	-0.79602	2.38856	-2.38499
C	-0.91554	2.38632	1.01907
H	-1.98677	2.55935	0.91540
H	-0.46608	3.32502	1.35993
C	-0.64686	1.25875	2.00913
H	0.42284	1.11135	2.16593
H	-1.09843	1.48847	2.98066
C	-2.71434	-0.00007	1.64996
H	-2.91744	-0.00009	2.72585
H	-3.16153	-0.87435	1.18519
H	-3.16159	0.87418	1.18521
C	-0.64676	-1.25873	2.00915
H	-1.09829	-1.48845	2.98069
H	0.42293	-1.11124	2.16592
C	-0.91538	-2.38634	1.01913
H	-0.46581	-3.32498	1.35999
H	-1.98660	-2.55948	0.91552
C	-1.13596	-2.76151	-1.41812
H	-0.79610	-2.38860	-2.38495
H	-2.19994	-2.55780	-1.30279
H	-0.94803	-3.83785	-1.33662
C	3.92695	0.00003	0.53689
C	3.25836	-1.21398	0.33926
H	3.78117	-2.16136	0.41906
C	1.07849	-2.33591	-0.46658
H	1.31303	-3.27647	0.04240
H	1.29817	-2.46989	-1.53098
N	1.26229	0.00002	-0.07581
C	1.90962	-1.17816	0.00565
H	4.97868	0.00004	0.80671
O	-2.32644	-0.00001	-0.99512
H	-2.39512	-0.00002	-1.97239
F	-0.13770	-0.00002	-2.23674

^{5}FePyNMe3N$_3$OH
Charge: 2+
Energy: -1424870.7369396

Fe	-0.76273	-0.00005	-0.12158
N	-0.24982	2.19424	0.11113
N	-0.24134	0.00006	2.02132
N	-0.24939	-2.19426	0.11137
C	3.25058	1.20909	-0.91142
H	3.76301	2.15998	-1.01550
C	1.88068	1.17740	-0.67069
C	1.00734	2.40753	-0.65271
H	0.73320	2.62218	-1.69147
H	1.55532	3.28007	-0.27635
C	-1.35598	3.02362	-0.43835
H	-1.14688	4.09279	-0.31195
H	-2.27950	2.76816	0.08337
H	-1.47445	2.80357	-1.50067
C	-0.08439	2.43552	1.57301
H	-1.07571	2.62796	1.98642
H	0.51750	3.33598	1.74924
C	0.55678	1.23946	2.26794
H	1.56988	1.07265	1.89933
H	0.62588	1.42895	3.34608
C	-1.46942	-0.00027	2.87001
H	-1.17646	-0.00019	3.92637
H	-2.07615	-0.87630	2.65383
H	-2.07663	0.87543	2.65381
C	0.55744	-1.23893	2.26791
H	0.62683	-1.42829	3.34606
H	1.57038	-1.07161	1.89909
C	-0.08322	-2.43540	1.57321
H	0.51932	-3.33545	1.74924
H	-1.07427	-2.62849	1.98699
C	-1.35558	-3.02396	-0.43756
H	-1.47462	-2.80395	-1.49983
H	-2.27895	-2.76877	0.08459
H	-1.14610	-4.09306	-0.31124
C	3.94240	0.00024	-1.02388
C	3.25066	-1.20869	-0.91154
H	3.76319	-2.15952	-1.01569
C	1.00743	-2.40725	-0.65309
H	1.55552	-3.28002	-0.27739
H	0.73281	-2.62135	-1.69183
N	1.23745	0.00011	-0.52576
C	1.88078	-1.17714	-0.67085
H	5.01275	0.00028	-1.20626
O	-2.45416	-0.00008	0.34375
H	-3.19030	0.00049	-0.29759
N	-1.03563	-0.00039	-1.95196
N	-2.13573	-0.00036	-2.51422
N	-3.11473	-0.00039	-3.10180

^{3}FePyNMe3NCSOH
Charge: 2+
Energy: -1629977.3672629

Fe	-0.11237	-0.69700	-0.00002
N	-0.27511	-0.38129	-2.04431
N	-2.17841	-0.69779	0.00010
N	-0.27489	-0.38136	2.04430
C	0.05639	3.31810	-1.21313
H	0.08952	3.84459	-2.16127
C	0.04524	1.92719	-1.17450
C	0.23367	1.00276	-2.34795
H	1.31073	0.92241	-2.52890
H	-0.22107	1.38413	-3.26835
C	0.49394	-1.38758	-2.83678
H	0.33935	-1.22237	-3.90907
H	0.15057	-2.38289	-2.55630
H	1.55451	-1.29645	-2.60245
C	-1.73761	-0.50153	-2.38399
H	-1.94186	-1.55842	-2.55548
H	-1.95000	0.02779	-3.31919

C	-2.58567	0.02637	-1.24149
H	-2.42668	1.09573	-1.09217
H	-3.65131	-0.12514	-1.44885
C	-2.80447	-2.06101	0.00015
H	-3.89412	-1.94969	0.00022
H	-2.48472	-2.62477	0.87152
H	-2.48485	-2.62477	-0.87128
C	-2.58553	0.02639	1.24172
H	-3.65115	-0.12510	1.44920
H	-2.42653	1.09574	1.09237
C	-1.73736	-0.50152	2.38414
H	-1.94962	0.02784	3.31935
H	-1.94164	-1.55839	2.55569
C	0.49419	-1.38772	2.83666
H	1.55474	-1.29664	2.60221
H	0.15073	-2.38300	2.55620
H	0.33974	-1.22252	3.90897
C	0.03944	4.01531	0.00006
C	0.05657	3.31805	1.21323
H	0.08985	3.84450	2.16138
C	0.23401	1.00265	2.34791
H	-0.22055	1.38401	3.26841
H	1.31110	0.92224	2.52867
N	-0.01167	1.27868	0.00001
C	0.04541	1.92714	1.17454
H	0.03720	5.10095	0.00009
O	-0.18632	-2.46839	-0.00009
H	0.70961	-2.85361	-0.00000
N	1.78403	-0.71272	-0.00011
C	2.97349	-0.73391	-0.00016
S	4.58629	-0.76499	-0.00013

[5]FePyNMe3OHBr
Charge: 2+
Energy: -2937129.4012349

Fe	-0.41990	-0.00013	-0.43685
N	0.01113	2.18303	-0.10338
N	-0.44651	-0.00014	1.77863
N	0.01188	-2.18298	-0.10317
C	3.67030	1.20947	-0.28113
H	4.19304	2.16054	-0.28186
C	2.28045	1.17521	-0.33660
C	1.42119	2.39784	-0.53093
H	1.41012	2.61179	-1.60502
H	1.84891	3.27459	-0.02974
C	-0.89820	3.03611	-0.92187
H	-0.63356	4.09454	-0.81059
H	-1.92737	2.88164	-0.59945
H	-0.80715	2.74313	-1.96891
C	-0.19009	2.42995	1.35388
H	-1.25647	2.60014	1.51220
H	0.33223	3.34311	1.66595
C	0.28843	1.24526	2.18156
H	1.35620	1.07537	2.04368
H	0.12025	1.43927	3.24728
C	-1.79625	-0.00106	2.43098
H	-1.66027	-0.00141	3.51841
H	-2.36210	-0.88165	2.13596
H	-2.36294	0.87922	2.13666
C	0.29012	-1.24456	2.18152
H	0.12260	-1.43854	3.24735
H	1.35760	-1.07337	2.04317
C	-0.18730	-2.43006	1.35436
H	0.33690	-3.34231	1.66595
H	-1.25320	-2.60208	1.51390
C	-0.89813	-3.03643	-0.92050
H	-0.80848	-2.74348	-1.96766
H	-1.92696	-2.88231	-0.59683
H	-0.63296	-4.09477	-0.80953
C	4.37005	0.00046	-0.24048
C	3.67049	-1.20866	-0.28197
H	4.19339	-2.15965	-0.28337
C	1.42143	-2.39705	-0.53269
H	1.84980	-3.27459	-0.03344
H	1.40900	-2.60914	-1.60714
N	1.62357	0.00028	-0.31877
C	2.28068	-1.17458	-0.33743
H	5.45476	0.00053	-0.19184
O	-0.19274	-0.00059	-2.18597
H	-0.99495	-0.00121	-2.74505
Br	-2.78967	-0.00011	-0.62399

[5]FePyNMe3OHCl
Charge: 2+
Energy: -1610601.1452280

Fe	0.64063	-0.00014	-0.57154
N	0.25125	-2.18380	-0.19138
N	0.90978	-0.00029	1.61726
N	0.25213	2.18377	-0.19143
C	-3.40146	-1.20852	0.03213
H	-3.92132	-2.15950	0.08865
C	-2.02639	-1.17532	-0.17701
C	-1.19489	-2.39928	-0.46577
H	-1.29982	-2.61133	-1.53511
H	-1.56758	-3.27582	0.07786
C	1.08079	-3.01417	-1.11054
H	0.86162	-4.07926	-0.96847
H	2.13564	-2.82677	-0.91132
H	0.85896	-2.72776	-2.13966
C	0.61133	-2.43168	1.23438
H	1.68765	-2.60688	1.27368
H	0.12264	-3.34249	1.60250
C	0.23117	-1.24470	2.10926
H	-0.84587	-1.07654	2.09736
H	0.52499	-1.43362	3.14842
C	2.33658	-0.00125	2.07712
H	2.35103	-0.00169	3.17284
H	2.85693	0.87828	1.70568
H	2.85600	-0.88101	1.70496
C	0.23280	1.24502	2.10927
H	0.52729	1.43385	3.14827
H	-0.84445	1.07808	2.09790
C	0.61390	2.43134	1.23392
H	0.12693	3.34295	1.60235
H	1.69053	2.60489	1.27215
C	1.08112	3.01374	-1.11145
H	0.85831	2.72718	-2.14033
H	2.13609	2.82612	-0.91311
H	0.86235	4.07891	-0.96940
C	-4.09207	0.00066	0.15061
C	-3.40107	1.20966	0.03290
H	-3.92060	2.16079	0.09003
C	-1.19420	2.40009	-0.46423
H	-1.56605	3.27608	0.08086
H	-1.30009	2.61361	-1.53318
N	-1.37161	0.00034	-0.23105
C	-2.02598	1.17613	-0.17627
H	-5.16478	0.00078	0.31875
O	0.20312	-0.00044	-2.27910
H	0.96131	-0.00043	-2.89825
Cl	2.78414	-0.00011	-0.95591

[5]FePyNMe3OHF
Charge: 2+
Energy: -1384478.5231713

Fe	0.71535	0.00023	-0.67990
N	0.36298	-2.20059	-0.25476
N	1.17321	0.00007	1.44053
N	0.36189	2.20093	-0.25466
C	-3.24785	-1.21025	0.27929
H	-3.75885	-2.16113	0.39101
C	-1.89982	-1.17911	-0.06276
C	-1.09903	-2.41058	-0.41452
H	-1.29027	-2.62699	-1.47097
H	-1.43489	-3.28074	0.16225
C	1.14380	-2.98330	-1.25248
H	1.02817	-4.06000	-1.07996
H	2.19654	-2.70761	-1.17106
H	0.78986	-2.73071	-2.25300
C	0.84479	-2.44423	1.13491
H	1.91508	-2.64962	1.08102
H	0.36808	-3.33754	1.55724
C	0.57210	-1.24013	2.02917
H	-0.50021	-1.07469	2.14217
H	0.98911	-1.41034	3.02899
C	2.65865	0.00017	1.62916
H	2.88098	-0.00000	2.70193
H	3.09733	0.87683	1.15890
H	3.09747	-0.87627	1.15859
C	0.57185	1.24019	2.02912
H	0.98889	1.41050	3.02891
H	-0.50041	1.07449	2.14222
C	0.84416	2.44440	1.13487
H	0.36751	3.33763	1.55744
H	1.91440	2.64991	1.08064
C	1.14195	2.98428	-1.25249
H	0.78775	2.73176	-2.25293
H	2.19485	2.70909	-1.17153
H	1.02585	4.06089	-1.07966
C	-3.92459	-0.00102	0.46091
C	-3.24846	1.20860	0.27964
H	-3.75994	2.15919	0.39166
C	-1.10028	2.41031	-0.41373
H	-1.43632	3.27994	0.16374
H	-1.29205	2.62736	-1.46996
N	-1.25639	-0.00024	-0.18883
C	-1.90040	1.17827	-0.06241
H	-4.97604	-0.00132	0.73185
O	0.19311	-0.00001	-2.35659
H	0.95680	0.00028	-2.97209
F	2.39704	0.00071	-1.03728

[6]FePyNMe3OHMeCN2cis
Charge: 2+

Energy: -1405177.8637999

Fe	-0.47105	0.00045	-0.51928
N	-0.00848	2.15055	-0.15301
N	-0.46142	0.00037	1.78530
N	-0.01052	-2.15028	-0.15311
C	3.66099	1.21024	-0.31019
H	4.18617	2.15918	-0.27684
C	2.27430	1.17260	-0.42263
C	1.39535	2.38677	-0.60905
H	1.35916	2.59735	-1.68318
H	1.81813	3.27161	-0.11823
C	-0.94982	2.98344	-0.95091
H	-0.75169	4.05283	-0.80951
H	-1.97077	2.76148	-0.63383
H	-0.84461	2.72078	-2.00432
C	-0.18249	2.41414	1.30781
H	-1.24531	2.59929	1.47817
H	0.35116	3.32796	1.59800
C	0.28619	1.23714	2.15773
H	1.35108	1.05744	2.00203
H	0.14839	1.47142	3.22118
C	-1.79356	0.00167	2.44675
H	-1.68198	0.00252	3.53824
H	-2.36191	-0.87829	2.14622
H	-2.36097	0.88174	2.14473
C	0.28378	-1.23783	2.15786
H	0.14510	-1.47204	3.22120
H	1.34909	-1.06008	2.00264
C	-0.18673	-2.41370	1.30744
H	0.34448	-3.32880	1.59811
H	-1.25018	-2.59632	1.47661
C	-0.95163	-2.98229	-0.95225
H	-0.84487	-2.71962	-2.00550
H	-1.97277	-2.75942	-0.63644
H	-0.75463	-4.05185	-0.81067
C	4.35611	-0.00156	-0.24710
C	3.66009	-1.21286	-0.30918
H	4.18454	-2.16218	-0.27505
C	1.39372	-2.38807	-0.60714
H	1.81535	-3.27239	-0.11438
H	1.35876	-2.60051	-1.68094
N	-2.69538	0.00044	-0.39880
C	-3.84537	0.00031	-0.54440
C	-5.29047	0.00011	-0.72229
H	-5.78800	0.00182	0.25350
H	-5.59537	-0.89249	-1.27959
H	-5.59523	0.89082	-1.28267
O	-0.58978	0.00106	-2.31120
N	1.62078	-0.00063	-0.45463
C	2.27339	-1.17426	-0.42167
H	5.43773	-0.00192	-0.15318
H	-1.28335	0.00121	-2.99041

[6]FePyNMe3OHMeCN2trans

Charge: 2+

Energy: -1405180.9209319

Fe	0.14508	-0.85523	0.00002
N	-0.15151	-0.35627	-2.15805
N	-2.05706	-0.84294	0.00220
N	-0.14751	-0.35445	2.15831
C	-0.15438	3.30246	-1.21177
H	-0.23719	3.82099	-2.16144
C	0.05435	1.92653	-1.17223
C	0.26075	1.05897	-2.39273
H	1.33252	1.05600	-2.61912
H	-0.24976	1.47328	-3.27049
C	0.66438	-1.28049	-2.99359
H	0.51462	-1.08613	-4.06250
H	0.38031	-2.30707	-2.75970
H	1.71836	-1.14576	-2.74278
C	-1.61037	-0.57222	-2.41804
H	-1.74917	-1.63869	-2.60312
H	-1.91730	-0.04493	-3.32993
C	-2.47259	-0.12803	-1.23916
H	-2.36493	0.94487	-1.06833
H	-3.52986	-0.32179	-1.45989
C	-2.57680	-2.24198	0.00427
H	-3.67326	-2.23426	0.00595
H	-2.20590	-2.77446	0.87779
H	-2.20862	-2.77603	-0.86944
C	-2.47001	-0.12535	1.24284
H	-3.52705	-0.31794	1.46570
H	-2.36187	0.94713	1.06975
C	-1.60624	-0.56790	2.42122
H	-1.91094	-0.03805	3.33237
H	-1.74616	-1.63373	2.60911
C	0.66853	-1.27899	2.99334
H	1.72227	-1.14597	2.74062
H	0.38267	-2.30541	2.76092
H	0.52087	-1.08342	4.06232
C	-0.25918	3.99433	-0.00119
C	-0.15103	3.30324	1.20959
H	-0.23120	3.82241	2.15914
C	0.26738	1.06038	2.39070
H	-0.23932	1.47585	3.27011
H	1.34000	1.05605	2.61302
N	0.14749	1.27388	-0.00087
C	0.05759	1.92732	1.17036
N	2.41088	-0.59913	-0.00121
C	3.56990	-0.57352	-0.00219
C	5.02658	-0.54533	-0.00343
H	5.40818	-1.05622	0.88725
H	5.40662	-1.05593	-0.89496
H	5.38211	0.49039	-0.00362
O	0.32561	-2.63670	0.00016
H	-0.42996	5.06656	-0.00130
H	1.06772	-3.26219	0.00020

[5]FePyNMe3OHN$_3$

Charge: 2+

Energy: -1424869.2980290

Fe	-0.63287	0.00068	-0.34679
N	-0.16412	2.19129	-0.03419
N	-0.41819	0.00131	1.86095
N	-0.16779	-2.19044	-0.03226
C	3.44534	1.20607	-0.58872
H	3.96757	2.15636	-0.63146
C	2.05597	1.17470	-0.52082
C	1.18524	2.40217	-0.62306
H	1.05167	2.61049	-1.69010
H	1.67434	3.27818	-0.17974
C	-1.17642	3.02055	-0.74191
H	-0.94365	4.08849	-0.65177
H	-2.15921	2.82861	-0.30877
H	-1.18830	2.73853	-1.79631
C	-0.19720	2.43696	1.43525
H	-1.23501	2.63000	1.71198
H	0.37576	3.33743	1.69039
C	0.34496	1.24077	2.20920
H	1.39658	1.07135	1.97468
H	0.27398	1.43005	3.28713
C	-1.73601	0.00212	2.56360
H	-1.56801	0.00216	3.64663
H	-2.31445	-0.87557	2.28308
H	-2.31350	0.88036	2.28288
C	0.34394	-1.23853	2.21008
H	0.27310	-1.42679	3.28819
H	1.39562	-1.07024	1.97511
C	-0.19945	-2.43503	1.43741
H	0.37350	-3.33548	1.69262
H	-1.23701	-2.62762	1.71537
C	-1.18228	-3.01850	-0.73826
H	-1.19510	-2.73691	-1.79276
H	-2.16422	-2.82485	-0.30392
H	-0.95102	-4.08674	-0.64784
C	4.14437	-0.00372	-0.61241
C	3.44301	-1.21219	-0.58858
H	3.96342	-2.16348	-0.63121
C	1.18045	-2.40380	-0.62277
H	1.66820	-3.28113	-0.18059
H	1.04515	-2.61100	-1.68980
N	1.40079	-0.00106	-0.45303
C	2.05373	-1.17815	-0.52068
H	5.22910	-0.00477	-0.65982
O	-0.62672	-0.00097	-2.11392
H	-1.44971	0.00447	-2.63954
N	-2.45427	0.00242	-0.14418
N	-3.30410	0.00055	-1.03950
N	-4.14011	-0.00154	-1.81586

[3]FePyNMe3OHNCS

Charge: 2+

Energy: -1629976.9322168

Fe	-0.23601	-0.00002	-0.31097
N	0.04086	2.04463	-0.11875
N	-0.24248	-0.00002	1.81270
N	0.04096	-2.04462	-0.11872
C	3.72940	1.21190	-0.49363
H	4.25286	2.16073	-0.54552
C	2.33936	1.17335	-0.45861
C	1.41497	2.33880	-0.65881
H	1.31216	2.47759	-1.73957
H	1.79889	3.27286	-0.23533
C	-0.95350	2.84375	-0.89414
H	-0.71803	3.91185	-0.82446
H	-1.94950	2.66539	-0.49000
H	-0.92093	2.52294	-1.93541
C	-0.05084	2.38696	1.34466
H	-1.10253	2.56990	1.56827
H	0.48758	3.31948	1.54639
C	0.48557	1.24646	2.19650
H	1.55197	1.09493	2.02346
H	0.35039	1.46818	3.26193
C	-1.59118	-0.00007	2.45711
H	-1.47958	-0.00011	3.54726

H	-2.15750	-0.87811	2.15365
H	-2.15752	0.87800	2.15373
C	0.48572	-1.24641	2.19651
H	0.35059	-1.46812	3.26195
H	1.55209	-1.09475	2.02345
C	-0.05055	-2.38699	1.34470
H	0.48805	-3.31941	1.54637
H	-1.10218	-2.57013	1.56839
C	-0.95346	-2.84376	-0.89402
H	-0.92102	-2.52290	-1.93528
H	-1.94942	-2.66543	-0.48976
H	-0.71796	-3.91185	-0.82439
C	4.42791	0.00007	-0.48614
C	3.72944	-1.21179	-0.49373
H	4.25293	-2.16060	-0.54568
C	1.41502	-2.33873	-0.65895
H	1.79899	-3.27284	-0.23560
H	1.31210	-2.47740	-1.73971
N	1.69120	0.00002	-0.37797
C	2.33940	-1.17329	-0.45870
H	5.51332	0.00009	-0.50524
O	-0.11929	-0.00015	-2.08530
H	-1.00658	0.00032	-2.49012
N	-2.12422	0.00001	-0.37324
C	-3.30181	-0.00004	-0.54684
S	-4.89909	-0.00003	-0.75592

^{4}FeTpMePhBrSOCH2CHNH2CO2EtC
Charge: 0
Energy: -3907887.2598739

Fe	-0.51156	0.04393	-0.13465
O	-0.20100	1.63535	1.31119
S	0.83946	2.72628	0.96892
N	-0.59050	-1.97394	-1.13083
N	-1.66834	-2.73559	-0.78008
C	-1.44710	-4.04258	-1.07139
C	-0.18150	-4.13501	-1.63197
C	0.31854	-2.82027	-1.65536
C	-2.44435	-5.12692	-0.80449
H	-3.39660	-4.93364	-1.31042
H	-2.65884	-5.22286	0.26590
H	-2.05281	-6.08336	-1.16204
H	0.30293	-5.02416	-2.00915
N	-2.64975	0.34094	-0.43763
N	-3.33757	-0.82542	-0.62931
C	-4.47563	-0.59468	-1.32871
C	-4.53371	0.76720	-1.59158
C	-3.38128	1.32012	-1.00329
C	-5.44535	-1.67678	-1.68830
H	-4.96275	-2.47178	-2.26786
H	-6.25827	-1.26055	-2.28958
H	-5.88087	-2.14286	-0.79673
H	-5.32559	1.30021	-2.09764
N	-1.13632	-1.22141	1.66261
N	-2.35302	-1.80507	1.45706
C	-3.03865	-1.90052	2.62233
C	-2.23095	-1.37755	3.62670
C	-1.04878	-0.97520	2.98183
C	-4.41565	-2.48050	2.71250
H	-4.75914	-2.46340	3.75049
H	-4.44195	-3.51672	2.35710
H	-5.12880	-1.91027	2.10611
H	-2.44897	-1.33497	4.68425
B	-2.83982	-2.12975	0.02105
H	-3.73768	-2.92088	0.07099
C	1.65003	-2.37996	-2.10965
C	2.79485	-3.08584	-1.69697
C	4.06873	-2.63644	-2.04722
C	4.21547	-1.47766	-2.81507
C	3.08182	-0.78031	-3.24196
C	1.80684	-1.23276	-2.90201
H	2.67912	-3.96670	-1.07127
H	4.94428	-3.18071	-1.70432
H	5.20761	-1.11970	-3.07825
H	3.18252	0.12564	-3.83254
H	0.93122	-0.67924	-3.21610
C	-3.01966	2.74157	-0.91209
C	-3.18555	3.58919	-2.01599
C	-2.86165	4.94152	-1.92210
C	-2.37295	5.46458	-0.72236
C	-2.21965	4.62777	0.38605
C	-2.54734	3.27556	0.29508
H	-3.53565	3.17378	-2.95655
H	-2.97827	5.58537	-2.78984
H	-2.11659	6.51851	-0.65119
H	-1.85211	5.03046	1.32690
H	-2.42222	2.61886	1.14740
C	0.18671	-0.43537	3.58379
C	0.18729	0.78725	4.26939
C	1.36939	1.29139	4.81215
C	2.56881	0.58359	4.67377
C	2.57749	-0.64164	4.00268
C	1.38925	-1.15179	3.47345
H	-0.73748	1.35083	4.34356
H	1.35866	2.24526	5.33298
H	3.48926	0.98388	5.09051
H	3.50313	-1.19472	3.87656
H	1.38426	-2.11694	2.97291
C	2.45638	1.86803	1.08567
C	2.62910	0.68302	0.11675
N	1.61899	-0.35385	0.35403
C	4.03499	0.11081	0.30886
O	4.29015	-0.87199	0.97337
O	4.94562	0.84535	-0.34891
C	6.31161	0.36815	-0.28831
C	7.12934	1.23916	-1.22202
H	3.21696	2.62898	0.87925
H	2.56328	1.52916	2.12299
H	2.52124	1.03189	-0.91216
H	1.65754	-0.63553	1.33408
H	1.87979	-1.18124	-0.18114
H	6.32130	-0.68453	-0.58750
H	6.65953	0.42498	0.74884
H	7.08628	2.28894	-0.91476
H	6.74987	1.16519	-2.24633
H	8.17620	0.91706	-1.21362
Br	0.11211	1.71199	-2.11047

^{4}FeTpMePhBrSOCH2CHNH2CO2EtD
Charge: 0
Energy: -3907909.2253408

Fe	0.57490	0.01278	-0.25479
O	-0.39394	1.98085	-0.35929
S	-1.37267	2.30959	-1.50613
N	0.73145	0.05473	2.05916
N	1.81603	-0.64531	2.49520
C	1.60138	-1.13758	3.74047
C	0.33261	-0.73049	4.13602
C	-0.16721	0.02665	3.05960
C	2.61419	-1.95471	4.48014
H	3.54519	-1.39820	4.63607
H	2.86992	-2.86789	3.93094
H	2.21741	-2.24227	5.45771
H	-0.14103	-0.90633	5.09131
N	2.49882	1.01106	-0.07090
N	3.34798	0.49843	0.87228
C	4.27242	1.42472	1.23035
C	4.02252	2.57075	0.49049
C	2.90750	2.27100	-0.31377
C	5.33871	1.17081	2.25023
H	4.91140	0.98537	3.24251
H	5.99679	2.04146	2.31950
H	5.94759	0.29802	1.99037
H	4.59244	3.48864	0.49465
N	1.43246	-2.02204	0.03493
N	2.69935	-1.94014	0.54155
C	3.46140	-2.96482	0.08920
C	2.65865	-3.75042	-0.72960
C	1.39516	-3.13519	-0.72264
C	4.89675	-3.14194	0.47434
H	5.31723	-4.00682	-0.04598
H	5.00902	-3.30067	1.55325
H	5.49233	-2.26053	0.21125
H	2.93532	-4.66850	-1.22763
B	3.04313	-0.84277	1.56670
H	3.99025	-1.18157	2.21771
C	-1.43222	0.77374	2.98044
C	-2.64373	0.18263	3.37402
C	-3.84154	0.89406	3.28329
C	-3.84337	2.20751	2.80576
C	-2.63942	2.80765	2.42355
C	-1.44108	2.09743	2.50861
H	-2.64394	-0.84494	3.72752
H	-4.77374	0.41867	3.57707
H	-4.77679	2.75848	2.72917
H	-2.63303	3.82760	2.04895
H	-0.50854	2.54636	2.18568
C	2.26132	3.16557	-1.28821
C	1.95854	4.48690	-0.92260
C	1.34404	5.34828	-1.83047
C	1.02916	4.90053	-3.11739
C	1.34019	3.59060	-3.48981
C	1.95958	2.72893	-2.58409
H	2.18674	4.82434	0.08505
H	1.10511	6.36620	-1.53288
H	0.54669	5.57044	-3.82465
H	1.09697	3.22981	-4.48531
H	2.18543	1.70903	-2.86913
C	0.14908	-3.61269	-1.34301
C	0.11009	-3.98589	-2.69358
C	-1.08180	-4.42336	-3.26822
C	-2.25265	-4.48465	-2.50630
C	-2.22189	-4.12980	-1.15581
C	-1.02139	-3.71389	-0.57634
H	1.00759	-3.88616	-3.29547
H	-1.10338	-4.69347	-4.32056

H	-3.18355	-4.81043	-2.96310
H	-3.12462	-4.16406	-0.55317
H	-0.98037	-3.46564	0.48053
C	-2.65245	0.97010	-1.47521
C	-2.65414	0.22396	-0.13725
N	-1.52191	-0.70128	-0.02386
C	-3.97652	-0.49810	0.13353
O	-4.06352	-1.66199	0.46325
O	-5.01945	0.34232	0.03051
C	-6.30915	-0.19007	0.41803
C	-7.29746	0.95865	0.36446
H	-3.61423	1.46486	-1.63825
H	-2.43144	0.29569	-2.30850
H	-2.56097	0.96122	0.66030
H	-1.59580	-1.42792	-0.73908
H	-1.59868	-1.19311	0.86601
H	-6.21987	-0.61433	1.42339
H	-6.57479	-1.00308	-0.26556
H	-7.35718	1.37459	-0.64636
H	-6.99447	1.75761	1.04913
H	-8.29390	0.60946	0.65540
Br	0.33368	-0.38350	-2.85693

[4]FeTpMePhClSOCH2CHNH2CO2EtC
Charge: 0
Energy: -2581381.4630333

Fe	-0.50052	0.01881	-0.38056
O	-0.32966	2.12459	-0.01281
S	0.82357	2.92736	-0.65578
N	-0.52859	-2.19597	-0.52026
N	-1.80179	-2.68078	-0.46588
C	-1.91461	-3.80406	-1.21412
C	-0.66305	-4.06524	-1.76503
C	0.17522	-3.04182	-1.29393
C	-3.19632	-4.56501	-1.34787
H	-3.99705	-3.93048	-1.74432
H	-3.53754	-4.95409	-0.38143
H	-3.05947	-5.40891	-2.02953
H	-0.38798	-4.90183	-2.39111
N	-2.65277	0.24017	-0.70495
N	-3.44716	-0.75105	-0.19506
C	-4.73767	-0.33414	-0.12289
C	-4.78316	0.96328	-0.60674
C	-3.45878	1.28764	-0.96060
C	-5.85199	-1.18776	0.39825
H	-5.91742	-2.14071	-0.13808
H	-6.80355	-0.66147	0.28163
H	-5.71922	-1.42149	1.46101
H	-5.65886	1.58422	-0.72904
N	-1.26801	-0.47114	1.74265
N	-2.09214	-1.55619	1.75736
C	-2.07401	-2.15236	2.97634
C	-1.21368	-1.42087	3.78630
C	-0.74298	-0.37002	2.97585
C	-2.87894	-3.37222	3.30041
H	-2.70268	-3.66833	4.33825
H	-2.60985	-4.21422	2.65259
H	-3.95231	-3.19365	3.17082
H	-0.99789	-1.59242	4.83121
B	-2.82948	-1.99889	0.46419
H	-3.69649	-2.77791	0.74082
C	1.63629	-2.88188	-1.46191
C	2.47584	-3.04593	-0.34792
C	3.85529	-2.84951	-0.45770
C	4.40991	-2.50088	-1.69099
C	3.58353	-2.36328	-2.81045
C	2.20559	-2.55161	-2.69891
H	2.03829	-3.33020	0.60638
H	4.48644	-2.95620	0.41946
H	5.48163	-2.34220	-1.78175
H	4.01052	-2.08668	-3.77055
H	1.55690	-2.39420	-3.55282
C	-2.99412	2.56986	-1.51524
C	-2.08847	2.62263	-2.58311
C	-1.65850	3.85308	-3.07976
C	-2.13694	5.04501	-2.52831
C	-3.05479	4.99925	-1.47547
C	-3.48190	3.76991	-0.97398
H	-1.70146	1.70090	-2.99936
H	-0.94683	3.87567	-3.90082
H	-1.80084	6.00257	-2.91815
H	-3.43313	5.92080	-1.04018
H	-4.18001	3.73272	-0.14172
C	0.15783	0.73801	3.33445
C	-0.14259	2.05144	2.93685
C	0.72228	3.09828	3.25385
C	1.90009	2.84977	3.96679
C	2.20567	1.54634	4.36781
C	1.33693	0.49829	4.06045
H	-1.04623	2.23489	2.36775
H	0.47670	4.10972	2.94059
H	2.57440	3.66685	4.20948
H	3.12377	1.34270	4.91147
H	1.58143	-0.51859	4.35511
C	2.35907	2.25942	0.09480
C	2.58708	0.75494	-0.14649
N	1.54576	-0.04581	0.49981
C	3.97053	0.38804	0.39486
O	4.16837	-0.16483	1.45614
O	4.93356	0.76814	-0.46065
C	6.28990	0.42583	-0.08769
C	7.17808	0.78034	-1.26445
H	3.17515	2.83635	-0.35444
H	2.32444	2.46767	1.17091
H	2.55560	0.54283	-1.21799
H	1.54347	0.14373	1.50275
H	1.79392	-1.03022	0.40124
H	6.32413	-0.64210	0.14964
H	6.55654	0.97831	0.81988
H	7.11297	1.84850	-1.49494
H	6.87711	0.21755	-2.15395
H	8.22085	0.53756	-1.03327
Cl	0.35256	0.20724	-2.62524

[6]FeTpMePhClSOCH2CHNH2CO2EtD
Charge: 0
Energy: -2581377.4548103

Fe	0.55512	-0.02162	-0.57308
O	-0.02027	1.93431	0.39798
S	-1.10498	2.88814	-0.14646
N	0.96115	-0.71722	1.60445
N	2.28382	-0.96801	1.82633
C	2.59825	-0.74401	3.12587
C	1.43388	-0.35100	3.77762
C	0.43507	-0.36379	2.78841
C	3.98084	-0.91663	3.67330
H	4.69039	-0.23838	3.18527
H	4.35133	-1.93697	3.52478
H	3.98581	-0.70088	4.74537
H	1.31462	-0.13642	4.83003
N	2.58437	0.77336	-0.44855
N	3.58654	-0.09352	-0.12223
C	4.79312	0.52436	-0.21203
C	4.55903	1.83330	-0.60969
C	3.16175	1.94898	-0.73798
C	6.09084	-0.15906	0.08950
H	6.18207	-0.41154	1.15261
H	6.92413	0.49718	-0.17698
H	6.19400	-1.09213	-0.47472
H	5.29477	2.60352	-0.79103
N	1.32064	-2.08120	-0.85484
N	2.47935	-2.41456	-0.21169
C	2.61056	-3.76701	-0.14743
C	1.50441	-4.32418	-0.77078
C	0.72214	-3.23363	-1.19548
C	3.77153	-4.45395	0.50240
H	3.70594	-5.53163	0.32767
H	3.78774	-4.28432	1.58539
H	4.72705	-4.09736	0.10333
H	1.30195	-5.37378	-0.92874
B	3.22540	-1.37705	0.64935
H	4.22253	-1.86862	1.09219
C	-1.01729	-0.16636	2.95438
C	-1.89651	-1.22301	2.66450
C	-3.27476	-1.06708	2.82237
C	-3.79171	0.14945	3.27800
C	-2.92373	1.20292	3.58016
C	-1.54460	1.04594	3.42284
H	-1.48426	-2.16634	2.31654
H	-3.94278	-1.88763	2.57734
H	-4.86456	0.27654	3.39514
H	-3.32160	2.15214	3.92876
H	-0.86798	1.86813	3.63587
C	2.39628	3.17961	-1.04921
C	2.23972	4.15003	-0.04736
C	1.53200	5.32499	-0.30101
C	0.97468	5.54407	-1.56427
C	1.13660	4.58647	-2.56833
C	1.84927	3.41227	-2.31575
H	2.66230	3.96570	0.93634
H	1.41264	6.06583	0.48553
H	0.42024	6.45757	-1.76470
H	0.70637	4.74934	-3.55291
H	1.95710	2.66075	-3.08753
C	-0.60254	-3.26684	-1.84241
C	-0.85060	-2.57821	-3.03779
C	-2.13626	-2.56095	-3.58359
C	-3.18163	-3.23687	-2.94974
C	-2.93608	-3.94480	-1.77057
C	-1.65379	-3.96335	-1.22261
H	-0.04706	-2.02722	-3.51026
H	-2.31764	-2.00729	-4.50074
H	-4.18447	-3.20716	-3.36661
H	-3.74758	-4.46295	-1.26753
H	-1.46044	-4.49559	-0.29446
C	-2.37286	1.81477	-0.93244

C	-2.58717	0.52287	-0.12182
N	-1.63944	-0.52679	-0.51169
C	-4.03331	0.02244	-0.18179
O	-4.35402	-1.12020	-0.42494
O	-4.89903	0.99902	0.14831
C	-6.28671	0.60424	0.26575
C	-7.05544	1.81808	0.75066
H	-3.28186	2.42283	-0.95357
H	-2.04271	1.58742	-1.95180
H	-2.41418	0.74614	0.93285
H	-1.81330	-0.80469	-1.47981
H	-1.82749	-1.36220	0.04040
H	-6.35053	-0.23469	0.96669
H	-6.63665	0.25005	-0.70941
H	-6.96483	2.64572	0.03986
H	-6.67385	2.15345	1.72062
H	-8.11655	1.57011	0.86066
Cl	0.17178	0.61168	-2.86594

^{6}FeTpMePhFSOCH2CHNH2CO2EtC
Charge: 0
Energy: -2355260.2731729

Fe	-0.51374	0.47069	0.10749
O	-0.00981	1.72122	1.44440
S	1.28830	2.71729	1.35935
N	-0.82867	-1.49785	-1.28976
N	-1.98951	-2.18204	-1.08459
C	-1.99822	-3.34170	-1.79473
C	-0.79701	-3.41303	-2.48101
C	-0.09387	-2.23786	-2.14171
C	-3.14206	-4.30806	-1.79040
H	-4.08000	-3.82930	-2.09266
H	-3.30568	-4.74262	-0.79757
H	-2.93511	-5.12485	-2.48752
H	-0.48368	-4.18574	-3.16814
N	-2.59958	0.81239	-0.30142
N	-3.45898	-0.24459	-0.40890
C	-4.59378	0.14150	-1.04422
C	-4.46728	1.48936	-1.34700
C	-3.20425	1.87675	-0.86550
C	-5.73468	-0.78480	-1.32884
H	-5.43758	-1.59278	-2.00739
H	-6.55059	-0.22877	-1.79865
H	-6.11630	-1.25086	-0.41405
H	-5.20473	2.12333	-1.81714
N	-1.27035	-0.97969	1.63677
N	-2.37860	-1.72389	1.35284
C	-2.63852	-2.58903	2.36532
C	-1.66482	-2.39802	3.33648
C	-0.83202	-1.37889	2.84459
C	-3.79069	-3.54504	2.36394
H	-3.83265	-4.06998	3.32229
H	-3.69660	-4.29404	1.56950
H	-4.74388	-3.02783	2.21205
H	-1.57994	-2.90445	4.28694
B	-3.02433	-1.67757	-0.05027
H	-3.97939	-2.39533	-0.06568
C	1.24967	-1.85744	-2.61815
C	2.23094	-2.85228	-2.77854
C	3.50657	-2.52682	-3.23759
C	3.82332	-1.20092	-3.54386
C	2.85616	-0.20554	-3.38163
C	1.57524	-0.52662	-2.92974
H	1.99323	-3.88063	-2.52070
H	4.25516	-3.30703	-3.34594
H	4.81693	-0.94501	-3.90333
H	3.09703	0.83027	-3.60556
H	0.83949	0.25172	-2.76382
C	-2.61142	3.22159	-0.92091
C	-2.77136	4.00193	-2.07644
C	-2.24242	5.29031	-2.13740
C	-1.55093	5.81636	-1.04310
C	-1.39641	5.04746	0.11265
C	-1.92928	3.76117	0.17815
H	-3.29249	3.58397	-2.93352
H	-2.36364	5.88085	-3.04181
H	-1.13476	6.81925	-1.09206
H	-0.85999	5.44875	0.96829
H	-1.79804	3.15845	1.06827
C	0.36413	-0.81990	3.51325
C	0.38542	0.49838	3.98912
C	1.51544	0.99194	4.64014
C	2.63936	0.17874	4.81758
C	2.62675	-1.13693	4.34819
C	1.48997	-1.63690	3.70852
H	-0.47324	1.13564	3.81962
H	1.52290	2.01827	4.99491
H	3.52108	0.56978	5.31842
H	3.49712	-1.77404	4.47800
H	1.47216	-2.66114	3.34490
C	2.68308	1.53924	1.26373
C	2.56310	0.52478	0.11399
N	1.47999	-0.43650	0.37727
C	3.88224	-0.21787	-0.08423
O	4.06981	-1.37771	0.21659
O	4.80417	0.58591	-0.64057
C	6.07879	-0.02818	-0.94616
C	6.86160	0.96493	-1.78313
H	3.56673	2.16655	1.10164
H	2.80186	1.01237	2.21735
H	2.31507	1.05655	-0.80608
H	1.57431	-0.81649	1.32017
H	1.56924	-1.22726	-0.26002
H	5.89129	-0.96376	-1.48098
H	6.58601	-0.27229	-0.00622
H	7.01104	1.90329	-1.23949
H	6.32644	1.18730	-2.71219
H	7.84310	0.54993	-2.03690
F	0.04493	1.41882	-1.33165

^{6}FeTpMePhFSOCH2CHNH2CO2EtD
Charge: 0
Energy: -2355260.9116198

Fe	0.51155	0.25773	-0.31785
O	0.09417	2.08492	0.28268
S	-1.16975	2.95086	-0.14894
N	1.04075	-0.53669	1.74796
N	2.09992	-1.39092	1.82299
C	2.08982	-2.05709	3.00532
C	0.98695	-1.61469	3.72399
C	0.36361	-0.65640	2.90428
C	3.12290	-3.06991	3.39017
H	4.13481	-2.65348	3.34394
H	3.09915	-3.94232	2.72717
H	2.93867	-3.41449	4.41155
H	0.69715	-1.90723	4.72294
N	2.64270	0.66892	-0.41693
N	3.51267	-0.27784	0.04667
C	4.77939	0.21078	0.05478
C	4.72557	1.51124	-0.41800
C	3.36916	1.76752	-0.70290
C	5.96981	-0.57977	0.50138
H	5.89710	-0.86072	1.55823
H	6.87632	0.01739	0.36896
H	6.08129	-1.50523	-0.07427
H	5.56016	2.17872	-0.57450
N	0.99551	-1.92892	-0.89431
N	2.20080	-2.40498	-0.46411
C	2.39127	-3.68217	-0.88881
C	1.26797	-4.04788	-1.61123
C	0.41640	-2.92409	-1.59269
C	3.62565	-4.47764	-0.59546
H	3.58496	-5.42906	-1.13322
H	3.72893	-4.69570	0.47381
H	4.53161	-3.94628	-0.90646
H	1.09331	-4.98627	-2.11740
B	3.01695	-1.62690	0.59044
H	3.95559	-2.28565	0.92523
C	-0.83715	0.14132	3.21396
C	-2.00758	-0.49637	3.65903
C	-3.15091	0.24717	3.95742
C	-3.13383	1.63887	3.82788
C	-1.96974	2.28030	3.39446
C	-0.82806	1.53838	3.08767
H	-2.01764	-1.57908	3.75600
H	-4.05298	-0.25997	4.28921
H	-4.02304	2.21905	4.05901
H	-1.95075	3.36037	3.28315
H	0.06638	2.02954	2.72383
C	2.82107	3.02971	-1.22823
C	3.42095	4.24017	-0.83865
C	2.95901	5.45729	-1.33640
C	1.88965	5.48409	-2.23512
C	1.28938	4.28495	-2.62538
C	1.74971	3.06376	-2.13357
H	4.24001	4.22474	-0.12470
H	3.42975	6.38393	-1.01782
H	1.52610	6.43201	-2.62383
H	0.45274	4.29543	-3.31923
H	1.25460	2.14275	-2.41859
C	-0.92931	-2.85859	-2.19721
C	-1.36742	-1.75024	-2.94110
C	-2.65329	-1.73697	-3.48528
C	-3.50981	-2.82613	-3.31588
C	-3.07415	-3.93835	-2.59224
C	-1.79533	-3.95500	-2.03805
H	-0.71530	-0.89035	-3.03673
H	-2.98206	-0.86793	-4.05024
H	-4.51087	-2.80821	-3.73852
H	-3.73561	-4.78831	-2.44684
H	-1.46464	-4.81247	-1.45800
C	-2.38420	1.74170	-0.80716
C	-2.64278	0.57905	0.17427
N	-1.57952	-0.43411	0.08848
C	-4.01305	-0.06370	-0.05968
O	-4.19049	-1.24184	-0.27979

O	-4.99941	0.84653	0.03918
C	-6.34560	0.34265	-0.14007
C	-7.28674	1.52428	-0.00630
H	-3.29684	2.32548	-0.96044
H	-2.00741	1.35387	-1.75587
H	-2.65980	0.97530	1.19200
H	-1.78768	-1.06453	-0.68958
H	-1.59560	-1.01402	0.92557
H	-6.53420	-0.42691	0.61585
H	-6.41309	-0.13501	-1.12303
H	-7.07044	2.28093	-0.76740
H	-7.18809	1.98891	0.98002
H	-8.32298	1.19245	-0.13202
F	0.00352	0.62417	-2.07507

^{6}FeTpMePhN$_3$SOCH2CHNH2CO2EtC
Charge: 0
Energy: -2395646.8018685

Fe	-0.55272	0.30762	0.22149
O	0.01723	1.05025	1.87277
S	1.31780	2.03918	2.05621
N	-0.90069	-1.05502	-1.70412
N	-1.99721	-1.86316	-1.69139
C	-1.96297	-2.73462	-2.73348
C	-0.79797	-2.48389	-3.44462
C	-0.16569	-1.42165	-2.77073
C	-3.03413	-3.74602	-3.00161
H	-4.02016	-3.27750	-3.09268
H	-3.10174	-4.49046	-2.20009
H	-2.81735	-4.27244	-3.93529
H	-0.46484	-2.97346	-4.34847
N	-2.69860	0.63137	0.08640
N	-3.51662	-0.38773	-0.31224
C	-4.73119	0.10061	-0.67123
C	-4.69913	1.47511	-0.49098
C	-3.40909	1.77224	-0.01484
C	-5.85297	-0.76000	-1.16304
H	-5.59268	-1.26561	-2.10014
H	-6.73709	-0.14248	-1.34369
H	-6.11725	-1.53608	-0.43655
H	-5.51046	2.17140	-0.64514
N	-1.16073	-1.60331	1.24684
N	-2.23966	-2.29110	0.77035
C	-2.40011	-3.45401	1.45100
C	-1.38951	-3.52252	2.39962
C	-0.64071	-2.34343	2.24384
C	-3.49892	-4.43285	1.17514
H	-3.45534	-5.24719	1.90365
H	-3.41477	-4.86816	0.17299
H	-4.48543	-3.96223	1.24327
H	-1.22786	-4.30228	3.12963
B	-2.98464	-1.81879	-0.49733
H	-3.89741	-2.55801	-0.71608
C	1.12817	-0.79058	-3.10541
C	2.27690	-1.58726	-3.24347
C	3.51836	-1.00329	-3.50474
C	3.62638	0.38314	-3.63300
C	2.48385	1.18183	-3.52061
C	1.24223	0.59905	-3.26734
H	2.19640	-2.66321	-3.11467
H	4.39983	-1.63249	-3.59122
H	4.59407	0.83999	-3.82239
H	2.55727	2.26072	-3.62555
H	0.35446	1.21061	-3.17252
C	-2.87425	3.09852	0.32727
C	-3.18956	4.20078	-0.48310
C	-2.68689	5.46595	-0.18248
C	-1.86351	5.64616	0.93110
C	-1.55373	4.55539	1.74684
C	-2.06255	3.29112	1.45472
H	-3.80774	4.05412	-1.36473
H	-2.92493	6.30787	-0.82698
H	-1.45856	6.62890	1.15627
H	-0.90999	4.68582	2.61237
H	-1.80789	2.44228	2.07714
C	0.54943	-1.95876	3.03521
C	0.52069	-0.86583	3.91299
C	1.64090	-0.55301	4.68167
C	2.80486	-1.32194	4.57880
C	2.84309	-2.41218	3.70658
C	1.71631	-2.73536	2.94677
H	-0.37034	-0.25301	3.96484
H	1.60918	0.30158	5.35092
H	3.67847	-1.06957	5.17407
H	3.74507	-3.01072	3.61489
H	1.73897	-3.58597	2.27043
C	2.70941	0.95367	1.58589
C	2.60051	0.34202	0.17715
N	1.47406	-0.59959	0.10152
C	3.90813	-0.37352	-0.16107
O	4.05743	-1.57732	-0.14826
O	4.87171	0.51256	-0.46160
C	6.15173	-0.04407	-0.84230
C	7.03015	1.11432	-1.27362
H	3.59413	1.59870	1.63118
H	2.82757	0.15324	2.32404
H	2.43607	1.12949	-0.56165
H	1.56013	-1.28457	0.85368
H	1.53951	-1.12548	-0.76826
H	5.98865	-0.76412	-1.65039
H	6.56818	-0.58887	0.01183
H	7.16174	1.82957	-0.45551
H	6.58054	1.64159	-2.12134
H	8.01631	0.74522	-1.57531
N	-0.16555	1.83641	-0.89521
N	0.25511	2.96164	-0.97472
N	0.66190	4.03436	-1.11012

^{6}FeTpMePhN$_3$SOCH2CHNH2CO2EtD
Charge: 0
Energy: -2395645.9800382

Fe	0.51571	0.10060	-0.25673
O	-0.21679	1.89003	-0.33022
S	-1.55164	2.47470	-0.97598
N	0.90315	-0.02133	2.02193
N	1.99771	-0.74870	2.38349
C	1.87315	-1.20454	3.65476
C	0.65559	-0.74777	4.14240
C	0.08934	0.00134	3.09366
C	2.91910	-2.03405	4.33177
H	3.87251	-1.49907	4.40608
H	3.11017	-2.96370	3.78416
H	2.59029	-2.29237	5.34214
H	0.25701	-0.88669	5.13709
N	2.55292	0.86724	-0.22680
N	3.45262	0.34257	0.65603
C	4.47419	1.21139	0.85729
C	4.23071	2.33195	0.07428
C	3.01935	2.07670	-0.59431
C	5.62394	0.92398	1.77185
H	5.29185	0.79757	2.80867
H	6.33702	1.75231	1.74010
H	6.14894	0.00615	1.48470
H	4.86368	3.20058	-0.03562
N	1.42700	-2.02633	-0.13656
N	2.69917	-2.04916	0.35872
C	3.42128	-3.04032	-0.22024
C	2.58378	-3.69485	-1.11486
C	1.34570	-3.03378	-1.02428
C	4.85521	-3.30629	0.11696
H	5.22440	-4.15077	-0.47139
H	4.98400	-3.54381	1.17918
H	5.48594	-2.43653	-0.10058
H	2.82123	-4.55770	-1.72043
B	3.14952	-0.98717	1.37779
H	4.12683	-1.36215	1.95985
C	-1.16500	0.76976	3.11288
C	-2.33025	0.21449	3.66813
C	-3.52279	0.93976	3.68354
C	-3.56309	2.23328	3.15493
C	-2.40481	2.79589	2.60994
C	-1.21256	2.07079	2.58681
H	-2.29872	-0.79529	4.06917
H	-4.42042	0.49307	4.10286
H	-4.49221	2.79646	3.16192
H	-2.43035	3.79577	2.18726
H	-0.32130	2.48904	2.13318
C	2.31904	2.93753	-1.55997
C	2.16783	4.30748	-1.30081
C	1.46990	5.11967	-2.19476
C	0.91700	4.57178	-3.35561
C	1.07943	3.21071	-3.62853
C	1.78673	2.40169	-2.74096
H	2.57384	4.72423	-0.38276
H	1.34810	6.17827	-1.97966
H	0.36209	5.20306	-4.04472
H	0.64483	2.77036	-4.52054
H	1.91525	1.34464	-2.93915
C	0.09043	-3.34953	-1.72968
C	0.04810	-3.37797	-3.13098
C	-1.15210	-3.62237	-3.79579
C	-2.32669	-3.84539	-3.07004
C	-2.29143	-3.84437	-1.67436
C	-1.08458	-3.60904	-1.00961
H	0.95269	-3.16087	-3.69088
H	-1.17664	-3.61524	-4.88192
H	-3.26383	-4.02052	-3.59161
H	-3.19683	-4.00585	-1.09800
H	-1.04713	-3.62609	0.07652
C	-2.69142	1.03928	-1.13728
C	-2.70469	0.15735	0.12189
N	-1.51985	-0.70879	0.19384
C	-3.98472	-0.67505	0.23044
O	-4.01183	-1.88216	0.34989
O	-5.07319	0.11146	0.22460
C	-6.34737	-0.55787	0.39120

C	-7.41488	0.51877	0.41617
H	-3.67381	1.50277	-1.27233
H	-2.46168	0.45662	-2.03347
H	-2.70273	0.81324	0.99135
H	-1.61673	-1.46918	-0.48274
H	-1.49078	-1.15979	1.10778
H	-6.31772	-1.13643	1.32032
H	-6.48423	-1.26226	-0.43585
H	-7.41529	1.08728	-0.51929
H	-7.24149	1.21472	1.24331
H	-8.40233	0.06301	0.54569
N	0.22209	-0.34173	-2.18365
N	-0.37064	0.02141	-3.16229
N	-0.93735	0.33385	-4.12671

^{6}FeTpMePhNCSSOCH2CHNH2CO2EtC
Charge: 0
Energy: -2600756.8161809

Fe	-0.59055	0.16834	0.26202
O	-0.00375	0.88211	1.99022
S	1.34330	1.62798	2.37363
N	-0.96690	-0.89609	-1.80696
N	-2.15517	-1.55891	-1.91556
C	-2.15524	-2.36836	-3.00674
C	-0.92176	-2.22903	-3.62587
C	-0.21181	-1.29496	-2.84795
C	-3.32157	-3.21848	-3.40585
H	-4.23553	-2.62541	-3.51943
H	-3.53059	-3.99792	-2.66410
H	-3.10977	-3.70821	-4.36036
H	-0.58927	-2.70387	-4.53772
N	-2.63681	0.82299	0.13659
N	-3.53403	0.00955	-0.49645
C	-4.59087	0.73715	-0.93643
C	-4.37601	2.05773	-0.56337
C	-3.14400	2.07052	0.11270
C	-5.74265	0.13939	-1.68230
H	-5.41899	-0.30498	-2.63069
H	-6.48079	0.91487	-1.90393
H	-6.23430	-0.64983	-1.10296
H	-5.03862	2.89604	-0.72189
N	-1.47207	-1.68729	1.05206
N	-2.62089	-2.15040	0.47754
C	-2.99322	-3.32314	1.04934
C	-2.05223	-3.63031	2.02412
C	-1.12299	-2.57722	1.99762
C	-4.21788	-4.08689	0.65142
H	-4.34206	-4.95054	1.31046
H	-4.15262	-4.45198	-0.37964
H	-5.11856	-3.46796	0.72058
H	-2.05204	-4.48308	2.68731
B	-3.20726	-1.46635	-0.78315
H	-4.20085	-2.04095	-1.11677
C	1.16659	-0.81308	-3.06998
C	2.21901	-1.73682	-3.18751
C	3.53301	-1.29458	-3.35459
C	3.80921	0.07396	-3.40613
C	2.76544	0.99960	-3.31097
C	1.45193	0.55767	-3.15393
H	2.00445	-2.80015	-3.12095
H	4.33819	-2.02041	-3.42771
H	4.83317	0.41897	-3.52409
H	2.96142	2.06706	-3.34552
H	0.64210	1.27149	-3.08580
C	-2.46570	3.21337	0.74448
C	-2.31311	4.41650	0.04104
C	-1.65752	5.49745	0.62840
C	-1.15850	5.39146	1.92836
C	-1.32085	4.20008	2.63994
C	-1.97337	3.11693	2.05357
H	-2.67331	4.48534	-0.98137
H	-1.51698	6.41356	0.06243
H	-0.64002	6.23172	2.38225
H	-0.93812	4.11330	3.65368
H	-2.08701	2.18476	2.59425
C	0.07371	-2.42024	2.85299
C	0.15057	-1.39513	3.80632
C	1.27464	-1.27708	4.62358
C	2.33965	-2.17400	4.49118
C	2.27330	-3.19661	3.54153
C	1.14096	-3.32551	2.73404
H	-0.66380	-0.68483	3.88552
H	1.32354	-0.47665	5.35620
H	3.21684	-2.07545	5.12509
H	3.09936	-3.89263	3.42704
H	1.08206	-4.12218	1.99711
C	2.67066	0.49714	1.81084
C	2.55811	0.00409	0.35802
N	1.38163	-0.86091	0.17944
C	3.83582	-0.76210	0.00958
O	3.91290	-1.97078	-0.05609
O	4.85598	0.08399	-0.19578
C	6.11461	-0.51560	-0.58633
C	7.06627	0.61984	-0.90881
H	3.59433	1.07472	1.92760
H	2.71072	-0.36261	2.48965
H	2.46014	0.85306	-0.32081
H	1.40932	-1.61745	0.86537
H	1.44764	-1.30992	-0.73391
H	5.93308	-1.16291	-1.44974
H	6.47539	-1.14437	0.23485
H	7.21541	1.26391	-0.03639
H	6.66863	1.23312	-1.72380
H	8.03816	0.21823	-1.21521
N	0.14788	1.83963	-0.61459
C	0.61370	2.84811	-1.03605
S	1.27707	4.18235	-1.67377

^{6}FeTpMePhNCSSOCH2CHNH2CO2EtD
Charge: 0
Energy: -2600757.0332992

Fe	0.54560	0.07500	0.12817
O	-0.23276	-0.63221	1.83499
S	-1.56580	-0.28923	2.59062
N	1.04934	-1.89606	-0.87336
N	2.17405	-1.87377	-1.64381
C	2.11672	-2.83247	-2.60073
C	0.91428	-3.51021	-2.44035
C	0.28552	-2.90172	-1.33840
C	3.20884	-3.05446	-3.59983
H	4.15456	-3.31503	-3.11162
H	3.39002	-2.15647	-4.20093
H	2.93401	-3.86972	-4.27466
H	0.56582	-4.36345	-3.00431
N	2.55598	-0.16012	0.93361
N	3.51409	-0.71097	0.13081
C	4.52031	-1.22144	0.88258
C	4.20681	-0.98757	2.21531
C	2.97071	-0.31588	2.20612
C	5.72231	-1.89041	0.29219
H	5.44672	-2.78961	-0.27061
H	6.41093	-2.18381	1.08922
H	6.25580	-1.22641	-0.39702
H	4.81001	-1.22806	3.07879
N	1.49446	0.91861	-1.77874
N	2.79623	0.53777	-1.94091
C	3.50586	1.51397	-2.56004
C	2.63055	2.55988	-2.82385
C	1.38225	2.14117	-2.32851
C	4.96512	1.38689	-2.86791
H	5.31996	2.29348	-3.36558
H	5.16758	0.53214	-3.52350
H	5.55577	1.24444	-1.95552
H	2.85160	3.48147	-3.34277
B	3.27926	-0.81653	-1.39024
H	4.29243	-1.14887	-1.93571
C	-0.98069	-3.28408	-0.69371
C	-2.11796	-3.56851	-1.46787
C	-3.32039	-3.92712	-0.85571
C	-3.39840	-4.01760	0.53704
C	-2.26760	-3.74576	1.31372
C	-1.06630	-3.37963	0.70492
H	-2.05778	-3.48836	-2.55015
H	-4.19621	-4.13082	-1.46595
H	-4.33491	-4.29283	1.01406
H	-2.32205	-3.80700	2.39675
H	-0.19552	-3.13807	1.30398
C	2.19589	0.17956	3.35439
C	1.99259	-0.64075	4.47437
C	1.21880	-0.19084	5.54390
C	0.64228	1.08269	5.50586
C	0.85658	1.91164	4.40135
C	1.63875	1.46533	3.33728
H	2.41853	-1.64067	4.48688
H	1.05718	-0.83738	6.40276
H	0.02995	1.42756	6.33505
H	0.40682	2.89898	4.35278
H	1.80018	2.09864	2.47426
C	0.08628	2.83743	-2.40587
C	-0.06168	4.13831	-1.90647
C	-1.30399	4.76973	-1.94123
C	-2.41296	4.11291	-2.48165
C	-2.27256	2.82506	-3.00380
C	-1.02530	2.19655	-2.97482
H	0.78850	4.62936	-1.44309
H	-1.41235	5.76225	-1.51485
H	-3.38313	4.60224	-2.49189
H	-3.12819	2.29921	-3.41591
H	-0.90259	1.20259	-3.39724
C	-2.71324	0.40891	1.33130
C	-2.66895	-0.37688	0.01085
N	-1.49018	-0.03262	-0.79534
C	-3.94989	-0.20444	-0.81119
O	-3.97424	0.13449	-1.97547
O	-5.03490	-0.53263	-0.09192
C	-6.30434	-0.48116	-0.78998

C	-7.36989	-0.92932	0.19120
H	-3.70048	0.30479	1.79181
H	-2.50458	1.47041	1.17634
H	-2.61754	-1.43873	0.25032
H	-1.61090	0.90463	-1.18689
H	-1.44942	-0.65725	-1.60029
H	-6.24460	-1.13372	-1.66720
H	-6.46718	0.54151	-1.14512
H	-7.40000	-0.26624	1.06165
H	-7.17093	-1.94813	0.53917
H	-8.35273	-0.91236	-0.29172
N	0.03041	1.99388	0.65635
C	-0.46826	2.94812	1.15535
S	-1.17612	4.23361	1.85074

^{6}FeTpMePhOHSOCH2CHNH2CO2EtC
Charge: 0
Energy: -2340164.0813663

Fe	-0.48620	0.20133	-0.16220
O	0.80683	3.58081	0.80575
S	1.97452	3.24975	-0.12435
N	-0.69792	-1.90573	-0.82814
N	-1.86610	-2.53620	-0.51306
C	-1.80023	-3.85254	-0.84300
C	-0.54837	-4.08047	-1.39251
C	0.11077	-2.83474	-1.37105
C	-2.92555	-4.81732	-0.63076
H	-3.84256	-4.48739	-1.13116
H	-3.16250	-4.93932	0.43236
H	-2.64982	-5.79680	-1.03149
H	-0.17563	-5.00979	-1.79821
N	-2.63329	0.51996	-0.72149
N	-3.45619	-0.55375	-0.56219
C	-4.63816	-0.34712	-1.20319
C	-4.57433	0.90465	-1.79348
C	-3.30305	1.41904	-1.46088
C	-5.75667	-1.34216	-1.21102
H	-5.44776	-2.29507	-1.65608
H	-6.59433	-0.94975	-1.79439
H	-6.11566	-1.55798	-0.19832
H	-5.35544	1.39789	-2.35362
N	-1.43032	-0.48568	1.76705
N	-2.47275	-1.35853	1.63020
C	-2.84125	-1.84947	2.84169
C	-2.01263	-1.27693	3.79463
C	-1.14915	-0.42463	3.08192
C	-3.96024	-2.82493	3.03718
H	-4.09534	-3.01783	4.10511
H	-3.75755	-3.78087	2.54128
H	-4.90439	-2.44351	2.63407
H	-2.05533	-1.41824	4.86478
B	-2.99686	-1.78627	0.23458
H	-3.92103	-2.52933	0.37963
C	1.45762	-2.54518	-1.89149
C	2.47016	-3.51260	-1.76963
C	3.73740	-3.28798	-2.30495
C	4.01421	-2.09037	-2.97003
C	3.01656	-1.11930	-3.08530
C	1.74339	-1.34191	-2.55785
H	2.26210	-4.43693	-1.23796
H	4.50950	-4.04537	-2.19740
H	5.00048	-1.91473	-3.39239
H	3.22555	-0.17937	-3.58949
H	0.98603	-0.56603	-2.62414
C	-2.74293	2.73148	-1.81609
C	-3.10209	3.34470	-3.02850
C	-2.58735	4.59353	-3.37381
C	-1.69973	5.24939	-2.51621
C	-1.33464	4.64935	-1.30882
C	-1.85768	3.40489	-0.95788
H	-3.77280	2.82653	-3.70843
H	-2.87162	5.05012	-4.31840
H	-1.29457	6.22041	-2.78858
H	-0.64071	5.13348	-0.62975
H	-1.57079	2.95169	-0.01535
C	-0.10602	0.44569	3.64298
C	0.12307	1.73055	3.12916
C	1.10120	2.55310	3.69037
C	1.86358	2.10389	4.77122
C	1.64698	0.82208	5.28690
C	0.67004	-0.00024	4.72842
H	-0.45577	2.08635	2.28420
H	1.26080	3.53773	3.26438
H	2.62270	2.74665	5.20910
H	2.24313	0.46086	6.12065
H	0.51117	-1.00194	5.11819
C	2.95840	1.88141	0.63845
C	2.66623	0.45872	0.12550
N	1.51599	-0.17246	0.79006
C	3.90409	-0.43632	0.24898
O	3.92999	-1.49281	0.84401
O	4.94480	0.07611	-0.42984
C	6.13687	-0.74472	-0.47944
C	7.08570	-0.08962	-1.46402
H	3.99379	2.13585	0.39094
H	2.82843	1.95758	1.72322
H	2.43004	0.52652	-0.93832
H	1.53405	0.02097	1.79103
H	1.62471	-1.18524	0.70889
H	5.84740	-1.75202	-0.79069
H	6.56060	-0.80888	0.52868
H	7.33878	0.92756	-1.14783
H	6.62859	-0.03803	-2.45757
H	8.01122	-0.67114	-1.53581
O	0.34090	1.23899	-1.50280
H	-0.19572	1.92460	-1.92625

^{6}FeTpMePhOHSOCH2CHNH2CO2EtD
Charge: 0
Energy: -2340168.5906054

Fe	-0.53774	0.46454	-0.05117
O	-0.50490	1.66541	1.37280
O	0.17169	1.68428	-1.34252
S	1.36658	2.76661	-1.04333
N	-0.73343	-1.18420	-1.66183
N	-1.83600	-1.98694	-1.62851
C	-1.73205	-2.98077	-2.54837
C	-0.51793	-2.81715	-3.19887
C	0.07263	-1.68002	-2.61819
C	-2.78252	-4.02542	-2.76564
H	-3.76137	-3.57830	-2.96863
H	-2.89735	-4.67586	-1.89106
H	-2.50637	-4.65067	-3.61935
H	-0.12160	-3.41472	-4.00704
N	-2.70328	0.66576	-0.34959
N	-3.48657	-0.44676	-0.45786
C	-4.79434	-0.12100	-0.29297
C	-4.85798	1.24644	-0.07616
C	-3.52828	1.70466	-0.11571
C	-5.90935	-1.11842	-0.34959
H	-5.90845	-1.67514	-1.29287
H	-6.86842	-0.60132	-0.25626
H	-5.83757	-1.85196	0.46178
H	-5.74727	1.84506	0.05726
N	-1.14243	-1.36484	1.30086
N	-2.16604	-2.15112	0.85508
C	-2.32982	-3.22884	1.66645
C	-1.37714	-3.14150	2.66834
C	-0.65506	-1.95962	2.40744
C	-3.38072	-4.27477	1.45603
H	-3.35046	-4.99477	2.27867
H	-3.23001	-4.82298	0.51906
H	-4.38536	-3.83949	1.41846
H	-1.24155	-3.81638	3.50110
B	-2.87204	-1.85551	-0.49238
H	-3.74024	-2.65813	-0.66183
C	1.39278	-1.11169	-2.96288
C	2.54190	-1.90573	-2.80940
C	3.80328	-1.40030	-3.13141
C	3.92762	-0.09929	-3.62594
C	2.78665	0.69052	-3.79509
C	1.52574	0.18951	-3.46675
H	2.43945	-2.91716	-2.42412
H	4.68508	-2.02046	-2.99375
H	4.90827	0.29946	-3.87116
H	2.87683	1.70664	-4.16681
H	0.64509	0.81239	-3.55806
C	-3.07924	3.09346	0.07167
C	-2.08860	3.66309	-0.74165
C	-1.68374	4.98297	-0.53903
C	-2.27603	5.75735	0.46157
C	-3.27686	5.20222	1.26359
C	-3.67587	3.88030	1.07046
H	-1.62121	3.05565	-1.50674
H	-0.90284	5.40324	-1.16637
H	-1.95965	6.78547	0.61684
H	-3.73985	5.79580	2.04760
H	-4.43594	3.44024	1.71002
C	0.48750	-1.45057	3.18942
C	0.64218	-0.08432	3.47858
C	1.75558	0.35613	4.19692
C	2.71378	-0.55202	4.65182
C	2.55693	-1.91352	4.38198
C	1.45396	-2.35926	3.65666
H	-0.08105	0.62823	3.09767
H	1.86692	1.41758	4.40440
H	3.57976	-0.20282	5.20817
H	3.30348	-2.62688	4.72027
H	1.34746	-3.41505	3.42251
C	2.39626	1.93593	0.23296
C	2.64981	0.45727	-0.11189
N	1.49872	-0.37348	0.27700
C	3.92889	-0.07237	0.53587
O	3.97878	-1.01000	1.30277
O	5.00213	0.62426	0.11895
C	6.28140	0.18755	0.63573

C	7.34000	1.07930	0.01568
H	3.33750	2.49409	0.23882
H	1.91011	2.00400	1.21003
H	2.79038	0.37292	-1.18913
H	1.56928	-0.58921	1.27356
H	1.54442	-1.27003	-0.20527
H	6.42257	-0.86689	0.37592
H	6.26315	0.25979	1.72834
H	7.17037	2.12718	0.28345
H	7.32396	0.99585	-1.07582
H	8.33306	0.78594	0.37284
H	-0.57084	2.59097	1.08134

^{5}FeBPMENCNBrOH
Charge: 0
Energy: -3100391.6870458

Fe	0.00906	-0.12103	-0.37506
N	-2.42329	-0.24958	0.10539
N	2.31833	-0.13738	-0.03616
N	-0.40862	-2.03436	0.87930
N	0.38904	0.60115	1.83754
C	-3.39993	0.64193	-0.16680
C	-2.72276	-1.55287	0.02863
C	-4.68466	0.27449	-0.57750
C	-3.99747	-2.00785	-0.33983
C	-4.98121	-1.08489	-0.66981
C	3.25561	-0.69222	-0.83082
C	2.72702	0.64596	0.97425
C	4.62852	-0.48152	-0.65458
C	4.08083	0.88690	1.23353
C	5.04425	0.32382	0.40288
C	1.65716	1.34405	1.78226
C	-1.63177	-2.57437	0.28017
C	0.49005	-0.60693	2.68282
C	-0.55767	-1.65458	2.29203
C	-0.68241	1.50359	2.29915
C	0.70233	-2.97342	0.65335
H	-5.42211	1.03826	-0.79713
H	-5.96852	-1.41245	-0.98122
H	-4.19502	-3.07500	-0.37992
H	-2.04151	-3.41149	0.87274
H	-1.34613	-2.95152	-0.70609
H	5.33594	-0.94745	-1.33129
H	6.10086	0.50482	0.57469
H	4.36303	1.51837	2.07043
H	2.03442	1.57730	2.79170
H	1.44538	2.28731	1.26469
H	-1.55875	-1.23873	2.42910
H	-0.47208	-2.52957	2.95815
H	0.38462	-0.35140	3.74950
H	1.49055	-1.02797	2.55197
H	-0.46025	1.90978	3.29929
H	-0.79075	2.31568	1.57905
H	-1.62644	0.95964	2.33666
H	0.84948	-3.06323	-0.42433
H	0.50046	-3.96116	1.10070
H	1.61931	-2.57155	1.08798
C	-3.14264	2.04155	0.06054
N	-3.07484	3.17291	0.31516
C	2.85014	-1.55859	-1.90982
N	2.68489	-2.29353	-2.79432
O	-0.16493	-1.29940	-1.81703
H	0.02374	-0.90618	-2.68137
Br	0.18876	2.30325	-1.27053

^{5}FeBPMENCNClOH
Charge: 0
Energy: -1773861.8301493

Fe	0.02232	-0.07969	-0.50711
N	-2.39906	-0.08732	0.00138
N	2.33680	0.04058	-0.19627
N	-0.36559	-1.49916	1.31553
N	0.39902	1.30590	1.38100
C	-3.38826	0.66326	-0.52661
C	-2.69330	-1.33535	0.38957
C	-4.68665	0.18760	-0.73530
C	-3.97895	-1.87844	0.24930
C	-4.97987	-1.11691	-0.34015
C	3.28317	-0.73010	-0.76768
C	2.73337	1.09449	0.53476
C	4.65507	-0.48200	-0.63455
C	4.08478	1.39870	0.73479
C	5.05851	0.60488	0.13689
C	1.65413	2.00622	1.07400
C	-1.58423	-2.21518	0.93085
C	0.51911	0.43638	2.56739
C	-0.51460	-0.69412	2.53631
C	-0.68670	2.29194	1.52823
C	0.75788	-2.44687	1.38914
H	-5.43589	0.83452	-1.17760
H	-5.97734	-1.52270	-0.47995
H	-4.17294	-2.89191	0.58792
H	-1.97553	-2.83188	1.75942
H	-1.30012	-2.87553	0.10599
H	5.37040	-1.13365	-1.12362
H	6.11346	0.82504	0.26885
H	4.35758	2.25420	1.34508
H	2.03175	2.56495	1.94664
H	1.42495	2.72072	0.27528
H	-1.52098	-0.26802	2.54248
H	-0.41572	-1.31220	3.44477
H	0.41151	1.01723	3.49799
H	1.52518	0.00798	2.57262
H	-0.47185	3.00780	2.33865
H	-0.80922	2.81888	0.58117
H	-1.62125	1.77521	1.74904
H	0.89999	-2.87174	0.39387
H	0.57415	-3.24363	2.12976
H	1.67077	-1.91549	1.66449
C	-3.12899	2.05127	-0.81663
N	-3.06522	3.19835	-0.98831
C	2.88969	-1.87424	-1.55273
N	2.73620	-2.82940	-2.19612
O	-0.12333	-1.68678	-1.46489
H	0.08322	-1.62469	-2.40834
Cl	0.12848	1.85644	-1.91274

^{5}FeBPMENCNFOH
Charge: 0
Energy: -1547732.3414009

Fe	-0.02119	-0.08506	-0.72267
N	-2.32212	-0.26768	-0.25134
N	2.34508	0.25513	-0.51451
N	-0.24992	-1.18480	1.45123
N	0.30690	1.59959	1.04768
C	-3.34923	0.40619	-0.80196
C	-2.59667	-1.24397	0.63165
C	-4.69139	0.12844	-0.50766
C	-3.90967	-1.57204	0.98918
C	-4.97026	-0.88384	0.40613
C	3.32422	-0.61523	-0.81531
C	2.63897	1.29315	0.28925
C	4.62667	-0.51315	-0.30474
C	3.91182	1.46863	0.84077
C	4.91796	0.54892	0.54563
C	1.51183	2.27089	0.54115
C	-1.42423	-2.02426	1.18826
C	0.47756	0.98938	2.37089
C	-0.46057	-0.21266	2.53062
C	-0.84411	2.51031	0.98262
C	0.93640	-2.02542	1.66178
H	-5.47782	0.70191	-0.98543
H	-5.99724	-1.12465	0.66412
H	-4.08672	-2.35925	1.71553
H	-1.74256	-2.58627	2.08374
H	-1.11667	-2.72741	0.40614
H	5.37530	-1.24739	-0.58124
H	5.91277	0.66023	0.96644
H	4.10234	2.31518	1.49317
H	1.85323	3.07875	1.21093
H	1.22657	2.69531	-0.42603
H	-1.49766	0.13202	2.48197
H	-0.32000	-0.66883	3.52599
H	0.30024	1.71328	3.18461
H	1.51456	0.65459	2.46720
H	-0.68679	3.41838	1.59012
H	-1.00177	2.76422	-0.06609
H	-1.73684	1.99698	1.34780
H	1.10198	-2.59124	0.74311
H	0.81630	-2.70085	2.52697
H	1.81006	-1.39169	1.83401
C	-3.08529	1.47955	-1.72934
N	-3.05709	2.37619	-2.46713
C	3.04658	-1.68187	-1.74639
N	2.98444	-2.54602	-2.52077
O	0.14718	-1.92142	-1.21822
H	0.39944	-2.11752	-2.13063
F	-0.19890	1.48915	-1.68537

^{5}FeBPMENCNN$_3$OH
Charge: 0
Energy: -1588121.8349972

Fe	-0.05971	-0.11667	-0.49414
N	-2.45806	0.04011	-0.16838
N	2.24931	-0.20000	-0.02928
N	-0.69079	-1.79565	1.01144
N	0.30501	0.85634	1.67985
C	-3.32841	0.99109	-0.56386
C	-2.93104	-1.19210	0.07037
C	-4.69008	0.74767	-0.77370
C	-4.28753	-1.51172	-0.08498
C	-5.17268	-0.53687	-0.52940
C	3.18281	-0.84836	-0.75874
C	2.66952	0.69789	0.87286

C	4.55603	-0.62531	-0.61847
C	4.02712	0.96601	1.08881
C	4.98233	0.30300	0.32949
C	1.62233	1.50060	1.61770
C	-1.94823	-2.28484	0.44003
C	0.27964	-0.23947	2.66608
C	-0.83995	-1.23969	2.36355
C	-0.72584	1.87276	1.94785
C	0.33507	-2.84901	0.93702
H	-5.33928	1.55082	-1.10391
H	-6.22432	-0.76577	-0.67345
H	-4.62908	-2.51940	0.13190
H	-2.44272	-3.01944	1.09945
H	-1.68042	-2.77638	-0.50097
H	5.25699	-1.17172	-1.23938
H	6.04021	0.50394	0.46691
H	4.31569	1.70173	1.83306
H	1.99570	1.74836	2.62608
H	1.51499	2.44738	1.07987
H	-1.80729	-0.73308	2.41985
H	-0.84515	-2.03283	3.13027
H	0.16706	0.14959	3.69207
H	1.24490	-0.75145	2.62094
H	-0.53154	2.41174	2.88989
H	-0.74694	2.57289	1.11122
H	-1.70500	1.39616	2.00971
H	0.49010	-3.08640	-0.11684
H	0.04008	-3.74871	1.50328
H	1.27688	-2.47096	1.33950
C	-2.85595	2.34390	-0.72209
N	-2.60168	3.47413	-0.80491
C	2.76417	-1.83357	-1.72488
N	2.57564	-2.66075	-2.51877
O	-0.26038	-1.51602	-1.73804
H	0.03896	-1.34430	-2.64166
N	0.20083	1.75230	-1.29408
N	1.23919	2.35880	-1.36473
N	2.23336	2.96437	-1.40710

^{5}FeBPMENCNNCSOH
Charge: 0
Energy: -1793233.9939299

Fe	-0.18376	-0.25373	-0.47985
N	-2.50322	0.21027	-0.22337
N	2.10843	-0.73381	0.08462
N	-1.07412	-1.98579	0.76875
N	0.24414	0.41956	1.78928
C	-3.20430	1.32749	-0.50376
C	-3.17112	-0.94775	-0.10852
C	-4.58806	1.33426	-0.70792
C	-4.56137	-1.02249	-0.27055
C	-5.27501	0.12739	-0.58855
C	2.97774	-1.37222	-0.72847
C	2.60051	0.13552	0.97427
C	4.35634	-1.14561	-0.70469
C	3.97073	0.41738	1.06963
C	4.85668	-0.22290	0.21365
C	1.63297	0.89572	1.85779
C	-2.37085	-2.21302	0.12313
C	0.04778	-0.78757	2.61658
C	-1.18637	-1.58082	2.17878
C	-0.66347	1.51289	2.17972
C	-0.20973	-3.16420	0.58258
H	-5.09653	2.26311	-0.94061
H	-6.35059	0.09082	-0.73257
H	-5.06390	-1.97811	-0.15606
H	-2.98431	-2.94570	0.67506
H	-2.14737	-2.61667	-0.87008
H	5.00486	-1.68009	-1.38973
H	5.91977	-0.00731	0.25312
H	4.31812	1.14753	1.79333
H	2.00230	0.88546	2.89764
H	1.66101	1.93856	1.52749
H	-2.07915	-0.95872	2.28669
H	-1.31918	-2.45358	2.83942
H	-0.03700	-0.52556	3.68450
H	0.93745	-1.41277	2.50620
H	-0.44605	1.87866	3.19637
H	-0.55743	2.32903	1.46339
H	-1.69697	1.16516	2.14431
H	-0.05768	-3.30279	-0.48860
H	-0.65050	-4.06736	1.03669
H	0.76446	-2.97605	1.03680
C	-2.50348	2.58539	-0.54902
N	-2.04002	3.65042	-0.54547
C	2.46442	-2.35651	-1.64819
N	2.16351	-3.19911	-2.38948
O	-0.48018	-1.40672	-1.92740
H	-0.09209	-1.16612	-2.78019
N	0.54948	1.60230	-1.02112
C	1.38950	2.43645	-0.93624
S	2.56720	3.54624	-0.72697

^{5}FeBPMENFBrOH
Charge: 0
Energy: -3109195.9783984

Fe	-0.02178	0.03070	-0.54013
N	2.27381	-0.29193	-0.16506
N	-2.38768	-0.01200	-0.03571
N	0.39306	0.07176	1.81777
N	-0.59439	-2.12260	0.17100
C	3.15152	-0.71255	-1.05878
C	2.73966	0.16800	1.01351
C	4.53336	-0.70997	-0.88169
C	4.10153	0.19540	1.30668
C	5.00948	-0.24044	0.33822
C	-3.24738	0.98224	0.10355
C	-2.87850	-1.24301	-0.28809
C	-4.63110	0.86633	-0.01785
C	-4.24815	-1.47906	-0.40141
C	-5.13237	-0.40429	-0.27941
C	-1.87423	-2.35246	-0.51106
C	1.70795	0.71611	1.97051
C	-0.69578	-2.16368	1.63768
C	0.41154	-1.32801	2.28903
C	0.42950	-3.03358	-0.36235
C	-0.62942	0.87907	2.50608
H	5.18187	-1.06754	-1.67250
H	6.07724	-0.21925	0.53526
H	4.44164	0.56210	2.26974
H	2.07498	0.64829	3.00828
H	1.57043	1.77386	1.71674
H	-5.26070	1.74001	0.10060
H	-6.20302	-0.55869	-0.37716
H	-4.61107	-2.48395	-0.59193
H	-2.32006	-3.32351	-0.23481
H	-1.64644	-2.35370	-1.58248
H	1.38423	-1.75510	2.03104
H	0.31866	-1.37816	3.38655
H	-0.64820	-3.19762	2.01913
H	-1.67128	-1.76233	1.92373
H	0.13577	-4.09101	-0.24897
H	0.58338	-2.78582	-1.41442
H	1.37208	-2.87243	0.16410
H	-0.72096	1.83618	1.98846
H	-0.36962	1.03870	3.56554
H	-1.59309	0.37207	2.45185
F	-2.73352	2.17154	0.40935
F	2.65305	-1.18338	-2.20200
O	-0.30294	-0.65607	-2.26283
H	-0.15458	0.01560	-2.94498
Br	0.44267	2.60177	-0.70051

^{5}FeBPMENFClOH
Charge: 0
Energy: -1782665.9236606

Fe	-0.00834	-0.05469	-0.67909
N	-2.32176	0.06632	-0.24108
N	2.35414	-0.11164	-0.17365
N	-0.42740	-0.87354	1.54461
N	0.50320	1.75941	0.73311
C	-3.21380	0.73926	-0.94502
C	-2.76861	-0.75990	0.72595
C	-4.59401	0.65852	-0.77076
C	-4.12744	-0.90289	1.00100
C	-5.05118	-0.18952	0.23269
C	3.23831	-1.07572	-0.35840
C	2.81338	1.13737	0.04775
C	4.62162	-0.90133	-0.36520
C	4.17818	1.42112	0.08796
C	5.09125	0.38743	-0.13595
C	1.78008	2.23414	0.18570
C	-1.71979	-1.57048	1.45066
C	0.59633	1.31728	2.13211
C	-0.48856	0.28439	2.45640
C	-0.54450	2.76777	0.51625
C	0.62132	-1.83415	1.92675
H	-5.25530	1.24361	-1.39865
H	-6.11645	-0.28979	0.41878
H	-4.45295	-1.56758	1.79465
H	-2.09181	-1.87314	2.44406
H	-1.54544	-2.47101	0.85120
H	5.27445	-1.74920	-0.53480
H	6.15938	0.58408	-0.12176
H	4.51578	2.43409	0.28219
H	2.19648	3.07014	0.77391
H	1.55915	2.58263	-0.82910
H	-1.47267	0.74766	2.34523
H	-0.39893	-0.03113	3.50944
H	0.51814	2.16592	2.83280
H	1.58197	0.86921	2.28320
H	-0.28561	3.73468	0.98099
H	-0.68264	2.87993	-0.56087
H	-1.48514	2.41402	0.94273
H	0.74600	-2.54997	1.11173

H	0.36757	-2.35725	2.86384
H	1.56688	-1.30828	2.06343
F	2.75140	-2.30340	-0.52446
F	-2.73397	1.56235	-1.87808
O	0.24387	1.21103	-2.04862
H	0.10350	0.83255	-2.92893
Cl	-0.35566	-2.30127	-1.50730

^{5}FeBPMENFFOH
Charge: 0
Energy: -1556535.9038760

Fe	-0.06515	-0.01253	-0.91546
N	2.36687	0.08295	-0.56379
N	-2.34300	-0.08981	-0.40110
N	0.41040	1.46972	1.02483
N	-0.35959	-1.28747	1.20599
C	3.27591	-0.81114	-0.88757
C	2.73085	1.08717	0.26430
C	4.59746	-0.81782	-0.44119
C	4.02478	1.17959	0.77493
C	4.96994	0.21326	0.41368
C	-3.28458	0.71543	-0.85516
C	-2.70281	-1.08901	0.43370
C	-4.64022	0.61545	-0.54257
C	-4.02907	-1.27317	0.82073
C	-5.00976	-0.41212	0.31814
C	-1.59363	-2.01306	0.88421
C	1.65764	2.10484	0.57784
C	-0.48136	-0.40308	2.36836
C	0.53535	0.74417	2.29303
C	0.76820	-2.22002	1.29814
C	-0.68544	2.44652	1.02539
H	5.27792	-1.59807	-0.76097
H	5.98415	0.26324	0.79912
H	4.28452	1.99230	1.44532
H	2.03774	2.84115	1.30710
H	1.40617	2.60971	-0.35998
H	-5.34795	1.31980	-0.96330
H	-6.05062	-0.53790	0.60208
H	-4.28652	-2.07723	1.50236
H	-1.94355	-2.63908	1.72395
H	-1.34459	-2.65353	0.03024
H	1.54784	0.33454	2.35589
H	0.40870	1.41035	3.16435
H	-0.35466	-0.94930	3.32000
H	-1.49373	0.01198	2.37481
H	0.60515	-2.99710	2.06601
H	0.89451	-2.66593	0.30869
H	1.68038	-1.67279	1.54817
H	-0.83446	2.76941	-0.00617
H	-0.47336	3.30801	1.68317
H	-1.60377	1.96482	1.36937
F	-2.88453	1.69667	-1.66299
F	2.88409	-1.79045	-1.71491
O	-0.10788	-1.79757	-1.60851
H	0.62073	-1.98492	-2.21529
F	0.02489	1.65236	-1.72899

^{5}FeBPMENFN$_3$OH
Charge: 0
Energy: -1596926.0271154

Fe	-0.07347	0.05837	-0.66385
N	2.21894	-0.24057	-0.17336
N	-2.41398	0.24593	-0.25399
N	0.31529	0.49678	1.70533
N	-0.77878	-1.89481	0.46721
C	3.10259	-0.80519	-0.97749
C	2.67816	0.37414	0.93505
C	4.47844	-0.82646	-0.76479
C	4.03298	0.39662	1.25828
C	4.94489	-0.20554	0.38926
C	-3.19596	1.30802	-0.31379
C	-2.99493	-0.96924	-0.16773
C	-4.58972	1.27642	-0.30835
C	-4.38115	-1.11640	-0.13337
C	-5.18596	0.02322	-0.21650
C	-2.07092	-2.16774	-0.17491
C	1.65350	1.09865	1.77998
C	-0.88940	-1.66806	1.91511
C	0.25511	-0.78709	2.42575
C	0.19555	-2.94046	0.12183
C	-0.68803	1.46233	2.17892
H	5.13049	-1.31017	-1.48209
H	6.00814	-0.19061	0.60934
H	4.36591	0.89444	2.16307
H	2.00874	1.16635	2.82249
H	1.58181	2.12086	1.39699
H	-5.15445	2.19918	-0.36736
H	-6.26837	-0.06549	-0.20087
H	-4.81909	-2.10577	-0.04983
H	-2.58087	-3.03869	0.27158
H	-1.84393	-2.38060	-1.22531
H	1.20642	-1.30265	2.26696
H	0.14963	-0.63347	3.51344
H	-0.90080	-2.61833	2.47563
H	-1.84479	-1.17343	2.11100
H	-0.14328	-3.94054	0.44303
H	0.34747	-2.90893	-0.95886
H	1.15070	-2.72013	0.60312
H	-0.72845	2.28988	1.46719
H	-0.45149	1.83508	3.18967
H	-1.67100	0.99011	2.20258
F	-2.58424	2.49084	-0.36239
F	2.61337	-1.40655	-2.06332
O	-0.35092	-1.00736	-2.19887
H	-0.11994	-0.56156	-3.02653
N	0.31405	2.06390	-0.98853
N	1.42397	2.53456	-1.03203
N	2.48645	3.01105	-1.04267

^{5}FeBPMENFNCSOH
Charge: 0
Energy: -1802038.6479515

Fe	-0.07768	-0.26449	-0.68780
N	2.20638	-0.59818	-0.18633
N	-2.36537	0.08073	-0.26209
N	0.36366	0.35122	1.63755
N	-0.83688	-2.08879	0.55550
C	3.05795	-1.23842	-0.96933
C	2.70771	0.14509	0.82035
C	4.44383	-1.19707	-0.84630
C	4.08034	0.24491	1.04633
C	4.95747	-0.42675	0.19299
C	-3.08282	1.18459	-0.37033
C	-3.01451	-1.09068	-0.09467
C	-4.47538	1.23624	-0.33928
C	-4.40537	-1.15215	-0.02921
C	-5.14217	0.02813	-0.16514
C	-2.15703	-2.33685	-0.04154
C	1.72218	0.91348	1.67260
C	-0.90435	-1.76479	1.98955
C	0.28498	-0.90028	2.41607
C	0.07613	-3.20499	0.26324
C	-0.59586	1.36183	2.11533
H	5.06759	-1.74847	-1.53954
H	6.03108	-0.35516	0.33970
H	4.45040	0.84887	1.86840
H	2.10069	0.97520	2.70734
H	1.67691	1.93943	1.29176
H	-4.98567	2.18649	-0.44112
H	-6.22733	0.00604	-0.12606
H	-4.89978	-2.10662	0.11948
H	-2.69968	-3.14691	0.47440
H	-1.96713	-2.63435	-1.07850
H	1.21166	-1.45575	2.24851
H	0.22382	-0.69204	3.49777
H	-0.93769	-2.67740	2.60768
H	-1.83536	-1.22220	2.17437
H	-0.30726	-4.16152	0.65702
H	0.20811	-3.25361	-0.81915
H	1.05052	-3.00241	0.71231
H	-0.60428	2.20359	1.42104
H	-0.33716	1.71907	3.12557
H	-1.59816	0.93251	2.14206
F	-2.40193	2.32168	-0.49711
F	2.52205	-1.98165	-1.93981
O	-0.39427	-1.38321	-2.16844
H	-0.14736	-0.99318	-3.01940
N	0.45138	1.67604	-1.17925
C	0.77982	2.77380	-0.87463
S	1.24295	4.25729	-0.36717

^{5}FeBPMENHBrOH
Charge: 0
Energy: -2984598.1705162

Fe	-0.00168	0.10276	-0.63226
N	-2.23719	0.16788	-0.23936
N	2.17636	-0.19979	-0.38038
N	-0.63414	-2.10667	-0.11943
N	0.46118	-0.14746	1.76222
C	-2.97460	1.25235	0.03883
C	-2.84259	-1.02600	-0.37872
C	-4.35812	1.19180	0.20295
C	-4.22135	-1.17156	-0.21807
C	-4.99030	-0.04469	0.07552
C	2.93847	-0.52874	-1.43309
C	2.74322	-0.01062	0.82128
C	4.31849	-0.68743	-1.32708
C	4.11674	-0.16535	1.01368
C	4.91598	-0.50416	-0.07865
C	1.80541	0.43478	1.92143
C	-1.94752	-2.18047	-0.77576
C	0.45583	-1.59492	2.04251
C	-0.70314	-2.30373	1.33635

C	-0.51256	0.58280	2.58597
C	0.32400	-3.00672	-0.77480
H	-4.91831	2.09394	0.42678
H	-6.06567	-0.13337	0.20413
H	-4.67868	-2.15097	-0.32368
H	-2.45367	-3.14295	-0.58945
H	-1.74974	-2.08199	-1.84914
H	4.90588	-0.95121	-2.20082
H	5.98870	-0.62541	0.04442
H	4.54694	-0.01766	2.00007
H	2.23371	0.21087	2.91310
H	1.69135	1.52090	1.82931
H	-1.65224	-1.89283	1.69159
H	-0.69821	-3.37493	1.59987
H	0.40688	-1.79122	3.12704
H	1.40255	-2.00942	1.68557
H	-0.25462	0.54269	3.65792
H	-0.54172	1.62047	2.24567
H	-1.50737	0.15532	2.44607
H	0.42598	-2.68755	-1.81363
H	0.00135	-4.06069	-0.72122
H	1.30113	-2.91049	-0.29678
H	-2.41080	2.17805	0.11892
H	2.38053	-0.65796	-2.35667
O	-0.00574	-0.46745	-2.44943
H	-0.10569	0.27665	-3.06252
Br	0.25915	2.72960	-0.34909

^{5}FeBPMENHClOH
Charge: 0
Energy: -1658067.9579159

Fe	-0.01651	-0.20176	-0.74875
N	2.21625	-0.29543	-0.37686
N	-2.20298	-0.01566	-0.44523
N	0.56087	1.83741	0.31324
N	-0.48515	-0.55201	1.63722
C	2.97167	-1.40227	-0.37400
C	2.79464	0.90481	-0.19134
C	4.35136	-1.36102	-0.17398
C	4.16751	1.02902	0.02753
C	4.95699	-0.12191	0.03417
C	-2.97383	0.56054	-1.37802
C	-2.76075	-0.50741	0.67214
C	-4.35517	0.67150	-1.23197
C	-4.13488	-0.42224	0.90069
C	-4.94387	0.17155	-0.06902
C	-1.80929	-1.19691	1.62542
C	1.87422	2.10290	-0.29172
C	-0.52126	0.77693	2.27108
C	0.61985	1.66881	1.77264
C	0.50995	-1.43968	2.25327
C	-0.41778	2.84832	-0.10705
H	4.92943	-2.27955	-0.17934
H	6.02824	-0.05020	0.20200
H	4.60458	2.01026	0.18805
H	2.35790	2.99808	0.13532
H	1.68138	2.27390	-1.35681
H	-4.95003	1.14158	-2.00870
H	-6.01711	0.24576	0.08375
H	-4.55804	-0.81740	1.81975
H	-2.24674	-1.25511	2.63674
H	-1.65728	-2.21533	1.25145
H	1.57865	1.20669	2.02392
H	0.58577	2.64065	2.29390
H	-0.47857	0.69847	3.37098
H	-1.47853	1.24297	2.02158
H	0.24891	-1.68813	3.29636
H	0.57407	-2.34990	1.65326
H	1.49049	-0.95939	2.24091
H	-0.50799	2.79506	-1.19354
H	-0.12360	3.86376	0.21032
H	-1.39366	2.61226	0.32262
H	2.42263	-2.32499	-0.54228
H	-2.42115	0.92847	-2.23854
O	-0.03081	0.82756	-2.35778
H	0.10605	0.27925	-3.14505
Cl	-0.15874	-2.64057	-1.00557

^{5}FeBPMENHFOH
Charge: 0
Energy: -1431936.3774148

Fe	0.01180	-0.08190	-0.94781
N	-2.20092	0.00905	-0.63067
N	2.21505	-0.05046	-0.64315
N	-0.47018	-1.32418	1.11691
N	0.46523	1.42435	0.97837
C	-2.96399	0.96883	-1.16670
C	-2.73205	-0.87602	0.22896
C	-4.32436	1.07743	-0.87979
C	-4.08258	-0.82610	0.57825
C	-4.89027	0.16087	0.00834
C	3.00121	-1.04539	-1.07371
C	2.72777	0.92529	0.12630
C	4.35943	-1.10346	-0.76147
C	4.07403	0.93285	0.49180
C	4.90311	-0.09450	0.03484
C	1.74271	2.00015	0.53313
C	-1.76696	-1.91881	0.75436
C	0.55714	0.64666	2.21730
C	-0.54187	-0.42399	2.27451
C	-0.57646	2.45456	1.01072
C	0.55380	-2.36418	1.26300
H	-4.91881	1.86411	-1.33384
H	-5.94498	0.21872	0.26372
H	-4.48832	-1.54367	1.28563
H	-2.22040	-2.48085	1.58936
H	-1.55012	-2.60578	-0.07111
H	4.96962	-1.92281	-1.12864
H	5.95548	-0.10991	0.30545
H	4.46050	1.72672	1.12449
H	2.18928	2.67098	1.28776
H	1.50417	2.57937	-0.36481
H	-1.52081	0.06432	2.26615
H	-0.47020	-0.97796	3.22694
H	0.49434	1.28883	3.11374
H	1.53712	0.16078	2.24337
H	-0.32391	3.28403	1.69495
H	-0.70265	2.81291	-0.01195
H	-1.52282	2.01329	1.33228
H	0.64931	-2.87261	0.30163
H	0.30473	-3.08327	2.06383
H	1.51555	-1.90069	1.49635
H	-2.41972	1.64927	-1.81591
H	2.47476	-1.79619	-1.65818
O	0.10147	-1.87967	-1.68536
H	-0.24552	-1.94243	-2.58739
F	-0.12813	1.61925	-1.78747

^{5}FeBPMENHN$_3$OH
Charge: 0
Energy: -1472326.9313453

Fe	-0.05790	0.12629	-0.74691
N	-2.26481	0.40740	-0.40260
N	2.11006	-0.20973	-0.41649
N	-0.83511	-1.88713	0.24299
N	0.41965	0.33810	1.68477
C	-2.90117	1.58546	-0.37230
C	-2.96196	-0.73360	-0.26348
C	-4.28082	1.67941	-0.19220
C	-4.34395	-0.72401	-0.06746
C	-5.01175	0.50125	-0.03401
C	2.84659	-0.76628	-1.39078
C	2.69884	0.16700	0.72913
C	4.21805	-0.96794	-1.26051
C	4.06653	-0.01322	0.94225
C	4.83790	-0.58253	-0.07005
C	1.80208	0.83865	1.74865
C	-2.15781	-2.01116	-0.38770
C	0.30637	-1.01204	2.26047
C	-0.90485	-1.76782	1.70652
C	-0.50714	1.29557	2.29869
C	0.05660	-2.96626	-0.20196
H	-4.76397	2.65109	-0.17372
H	-6.08734	0.53409	0.11704
H	-4.88153	-1.65963	0.05596
H	-2.73066	-2.86857	0.00509
H	-1.96414	-2.16862	-1.45473
H	4.78253	-1.41776	-2.07111
H	5.90573	-0.72623	0.06988
H	4.51388	0.29568	1.88250
H	2.22749	0.72812	2.76106
H	1.79055	1.90909	1.52035
H	-1.81998	-1.22552	1.96100
H	-0.97485	-2.75726	2.19002
H	0.24860	-0.97602	3.36242
H	1.21898	-1.55898	2.00696
H	-0.25466	1.50222	3.35286
H	-0.48014	2.21951	1.71687
H	-1.52589	0.90556	2.25131
H	0.16683	-2.88309	-1.28472
H	-0.32989	-3.96212	0.07620
H	1.04345	-2.83194	0.24641
H	-2.25401	2.44948	-0.49947
H	2.27235	-1.04524	-2.27043
O	-0.09990	-0.85878	-2.38877
H	-0.22416	-0.29248	-3.16508
N	0.11720	2.21287	-0.85066
N	1.15157	2.81591	-0.69949
N	2.13633	3.41264	-0.52971

^{5}FeBPMENHNCSOH
Charge: 0
Energy: -1677439.3367951

Fe	-0.03096	-0.23946	-0.80641

N	-2.22714	0.10747	-0.45455
N	2.14085	-0.51084	-0.43280
N	-0.78308	-2.10175	0.41874
N	0.44991	0.31026	1.57378
C	-2.86445	1.28329	-0.53196
C	-2.92042	-1.00785	-0.16286
C	-4.23627	1.40300	-0.31387
C	-4.29442	-0.97080	0.07838
C	-4.96122	0.25292	-0.00093
C	2.88570	-1.18836	-1.31957
C	2.72661	0.06168	0.63075
C	4.26499	-1.32222	-1.18154
C	4.10272	-0.03748	0.84649
C	4.88287	-0.73371	-0.07625
C	1.81975	0.85094	1.55223
C	-2.12148	-2.29468	-0.16139
C	0.39321	-0.97923	2.28619
C	-0.81902	-1.81111	1.86132
C	-0.47992	1.29397	2.14773
C	0.09551	-3.23300	0.08903
H	-4.71576	2.37388	-0.38395
H	-6.03059	0.30657	0.18370
H	-4.82691	-1.88479	0.32438
H	-2.68392	-3.09786	0.34385
H	-1.95616	-2.57898	-1.20665
H	4.83638	-1.87482	-1.92054
H	5.95637	-0.81882	0.06810
H	4.54893	0.42790	1.72054
H	2.25456	0.89243	2.56565
H	1.76612	1.88058	1.18233
H	-1.73618	-1.25595	2.07657
H	-0.85928	-2.73878	2.45637
H	0.37571	-0.82949	3.37950
H	1.30741	-1.53229	2.05389
H	-0.23656	1.52020	3.19978
H	-0.43588	2.21710	1.56733
H	-1.50061	0.90978	2.09788
H	0.18364	-3.28375	-0.99760
H	-0.28913	-4.18422	0.49488
H	1.09150	-3.05009	0.49824
H	-2.23443	2.13332	-0.77469
H	2.31437	-1.61391	-2.14045
O	-0.06674	-1.39457	-2.32332
H	-0.15230	-0.92164	-3.16465
N	0.25185	1.80534	-1.20009
C	0.46197	2.90534	-0.80695
S	0.74487	4.39228	-0.18922

^{5}FeBPMENMeBrOH
Charge: 0
Energy: -3033963.1990403

Fe	-0.02696	0.07991	-0.50419
N	-2.51332	0.00334	-0.09192
N	2.34106	-0.29505	-0.16555
N	-0.60735	-2.08316	0.11376
N	0.39156	0.05068	1.80765
C	-3.43898	0.97365	0.06414
C	-2.92808	-1.26153	-0.30391
C	-4.81178	0.69146	0.00392
C	-4.27764	-1.61485	-0.34422
C	-5.23716	-0.61621	-0.19584
C	3.24569	-0.71805	-1.07106
C	2.76336	0.08195	1.05718
C	4.61225	-0.77734	-0.75555
C	4.10104	0.02499	1.44199
C	5.04500	-0.40918	0.51173
C	1.72307	0.65604	1.99146
C	-1.87664	-2.31059	-0.58974
C	0.37682	-1.35719	2.25832
C	-0.73517	-2.15684	1.57738
C	-0.61943	0.86469	2.50229
C	0.41845	-2.99434	-0.41241
H	-5.52680	1.49977	0.12219
H	-6.29647	-0.85560	-0.23440
H	-4.56248	-2.65070	-0.50230
H	-2.28160	-3.31448	-0.37501
H	-1.64277	-2.23956	-1.65734
H	5.31571	-1.11679	-1.51008
H	6.09832	-0.45787	0.77436
H	4.39262	0.32607	2.44375
H	2.05722	0.56695	3.03845
H	1.62244	1.71946	1.74819
H	-1.70751	-1.74259	1.85457
H	-0.71309	-3.20031	1.93440
H	0.26675	-1.41812	3.35329
H	1.34595	-1.79598	2.00852
H	-0.41329	0.93008	3.58339
H	-0.61290	1.86354	2.06120
H	-1.60814	0.43083	2.34883
H	0.53234	-2.79554	-1.47911
H	0.14606	-4.05177	-0.25270
H	1.37593	-2.79428	0.07047
C	-2.96473	2.37445	0.33066
H	-1.99260	2.55802	-0.13347
H	-3.68977	3.10795	-0.03620
H	-2.85147	2.53879	1.41045
C	2.76378	-1.13415	-2.43553
H	3.32871	-0.60275	-3.21089
H	2.94001	-2.20763	-2.58897
H	1.69493	-0.92601	-2.55681
O	-0.30190	-0.48980	-2.28898
H	-0.32586	0.27773	-2.88184
Br	0.57089	2.64455	-0.66698

^{5}FeBPMENMeClOH
Charge: 0
Energy: -1707433.5352975

Fe	-0.00025	0.14718	-0.65411
N	-2.46123	0.07716	-0.19042
N	2.40177	0.01673	-0.29617
N	-0.46183	-1.74945	0.63751
N	0.44859	0.83483	1.56206
C	-3.42675	1.01034	-0.32653
C	-2.81962	-1.20294	0.03380
C	-4.78606	0.67267	-0.24510
C	-4.15194	-1.60022	0.15505
C	-5.15370	-0.64398	0.00406
C	3.31383	-0.65036	-1.02974
C	2.80581	0.69449	0.79630
C	4.66607	-0.68145	-0.65101
C	4.12954	0.69926	1.23120
C	5.07809	-0.00689	0.49082
C	1.75464	1.51597	1.50712
C	-1.72327	-2.24475	0.07174
C	0.49832	-0.35556	2.43418
C	-0.57764	-1.37360	2.05423
C	-0.59148	1.78747	1.98138
C	0.60961	-2.72492	0.39456
H	-5.53546	1.44819	-0.37068
H	-6.20132	-0.92254	0.08115
H	-4.39170	-2.64094	0.35145
H	-2.07923	-3.14359	0.60437
H	-1.50132	-2.50693	-0.96797
H	5.37486	-1.23451	-1.26023
H	6.11918	-0.02688	0.80180
H	4.40633	1.24682	2.12710
H	2.10161	1.79167	2.51686
H	1.60645	2.43132	0.92480
H	-1.56697	-0.93574	2.20879
H	-0.50595	-2.25416	2.71521
H	0.39174	-0.07407	3.49471
H	1.48592	-0.81033	2.32234
H	-0.37990	2.20571	2.97966
H	-0.63459	2.58896	1.24143
H	-1.56085	1.28737	1.99885
H	0.70208	-2.86294	-0.68381
H	0.40092	-3.69254	0.88301
H	1.55853	-2.33472	0.76575
C	-3.01079	2.43816	-0.54503
H	-3.76170	2.97678	-1.13227
H	-2.91677	2.95664	0.41867
H	-2.04003	2.49549	-1.04367
C	2.85856	-1.33671	-2.28917
H	3.18968	-0.75289	-3.15867
H	3.30984	-2.33251	-2.37618
H	1.76532	-1.40428	-2.32781
O	-0.24320	-1.02248	-2.13438
H	-0.32120	-0.51641	-2.95803
Cl	0.38861	2.41962	-1.43958

^{5}FeBPMENMeFOH
Charge: 0
Energy: -1481304.9768946

Fe	0.00953	-0.07186	-0.84318
N	-2.40131	-0.14084	-0.47519
N	2.41671	0.12744	-0.52531
N	-0.37683	-1.32559	1.18482
N	0.37503	1.43474	1.03364
C	-3.34970	0.69235	-0.94380
C	-2.72933	-1.06647	0.44999
C	-4.66518	0.64344	-0.45315
C	-4.01663	-1.16955	0.97560
C	-5.00091	-0.29224	0.51719
C	3.37501	-0.74464	-0.89507
C	2.72497	1.12609	0.32638
C	4.67239	-0.66433	-0.36192
C	3.99446	1.26831	0.88435
C	4.98428	0.34689	0.53828
C	1.61502	2.11048	0.62192
C	-1.63205	-2.02332	0.86433
C	0.51183	0.69622	2.29462
C	-0.49990	-0.45049	2.35875
C	-0.74050	2.38795	1.04616
C	0.72789	-2.28497	1.30870
H	-5.40510	1.33703	-0.84163

H	-6.01197	-0.34136	0.91305
H	-4.23681	-1.91848	1.73035
H	-1.97532	-2.65297	1.70346
H	-1.40415	-2.65331	-0.00162
H	5.41937	-1.39101	-0.66688
H	5.98197	0.42213	0.96289
H	4.19610	2.07992	1.57687
H	1.94891	2.84771	1.37236
H	1.37344	2.62613	-0.31174
H	-1.51327	-0.03973	2.37076
H	-0.37149	-1.01232	3.30006
H	0.38781	1.35509	3.17164
H	1.52619	0.29041	2.34289
H	-0.57140	3.21407	1.75909
H	-0.85021	2.77275	0.03181
H	-1.66537	1.87304	1.31463
H	0.81796	-2.81706	0.36045
H	0.56341	-2.99897	2.13514
H	1.66284	-1.74819	1.48593
C	-2.96502	1.64979	-2.03971
H	-3.25202	1.22324	-3.01117
H	-3.49778	2.60193	-1.93476
H	-1.88141	1.81091	-2.05083
C	3.01742	-1.77407	-1.92969
H	3.15448	-1.33927	-2.92985
H	3.66722	-2.65292	-1.85737
H	1.95705	-2.05240	-1.84159
O	-0.03072	-1.85562	-1.60416
H	-0.28980	-1.85010	-2.53815
F	0.00312	1.59421	-1.74368

^{5}FeBPMENMeN$_{3}$OH
Charge: 0
Energy: -1521693.3556011

Fe	-0.08293	0.33805	-0.48647
N	-2.49235	0.26283	-0.17655
N	2.31542	0.01816	-0.17654
N	-0.69000	-1.91711	-0.21395
N	0.30438	-0.13970	1.82637
C	-3.36691	1.24762	0.11496
C	-2.96360	-0.95274	-0.52412
C	-4.75207	1.02971	0.06581
C	-4.32776	-1.24093	-0.56681
C	-5.23807	-0.22753	-0.27162
C	3.23319	-0.22018	-1.13332
C	2.67902	-0.04884	1.11719
C	4.53458	-0.62748	-0.79896
C	3.95287	-0.44383	1.52033
C	4.89431	-0.75254	0.53736
C	1.64045	0.40539	2.11847
C	-1.95508	-1.99623	-0.95535
C	0.25729	-1.59710	2.04248
C	-0.84789	-2.24639	1.20940
C	-0.71136	0.57737	2.60974
C	0.34252	-2.72539	-0.87715
H	-5.42818	1.84686	0.29850
H	-6.30750	-0.41788	-0.30489
H	-4.66302	-2.23777	-0.83684
H	-2.40349	-3.00261	-0.88948
H	-1.70440	-1.77927	-1.99877
H	5.24985	-0.82727	-1.59071
H	5.89588	-1.07153	0.81314
H	4.19889	-0.50011	2.57638
H	1.95960	0.15650	3.14434
H	1.55713	1.49408	2.03965
H	-1.82129	-1.87154	1.53732
H	-0.84877	-3.33702	1.37698
H	0.11625	-1.83876	3.10930
H	1.22601	-2.00904	1.74712
H	-0.53390	0.48260	3.69440
H	-0.68288	1.62924	2.31835
H	-1.70261	0.18675	2.37426
H	0.47018	-2.33900	-1.88962
H	0.07181	-3.79516	-0.90719
H	1.29357	-2.61289	-0.35258
C	-2.82098	2.59038	0.51898
H	-3.46970	3.39522	0.15686
H	-2.78894	2.66972	1.61425
H	-1.80331	2.73600	0.14646
C	2.83033	0.03763	-2.55571
H	2.90649	1.11905	-2.73527
H	3.48916	-0.47780	-3.26185
H	1.78065	-0.23589	-2.71701
O	-0.27775	-0.06805	-2.34743
H	-0.32934	0.73214	-2.89228
N	0.31547	2.33767	-0.07380
N	1.36319	2.82283	-0.43625
N	2.36461	3.30205	-0.77403

^{5}FeBPMENMeNCCH3
Charge: 0
Energy: -1537623.0857805

Fe	0.01927	0.28572	0.25756
N	2.30960	0.10852	-0.11082
N	-2.35841	-0.05294	0.17623
N	0.48184	-2.05947	-0.04012
N	-0.56809	-0.17115	-2.02408
C	3.19944	1.06432	-0.53340
C	2.78473	-1.18059	-0.02929
C	4.50131	0.76472	-0.90314
C	4.06891	-1.54443	-0.40240
C	4.96999	-0.56685	-0.85338
C	-3.22511	-0.39715	1.17396
C	-2.85108	-0.04941	-1.10091
C	-4.54166	-0.76687	0.92710
C	-4.15018	-0.42430	-1.41647
C	-5.03266	-0.79463	-0.39257
C	-1.90235	0.43717	-2.16829
C	1.82807	-2.19216	0.54691
C	-0.62778	-1.62988	-2.21572
C	0.50468	-2.34209	-1.48398
C	0.41018	0.46258	-2.90937
C	-0.49721	-2.88257	0.66846
H	5.15737	1.56801	-1.22877
H	5.98173	-0.82200	-1.15125
H	4.36834	-2.58759	-0.32798
H	2.22900	-3.21359	0.41728
H	1.70882	-2.01760	1.62395
H	-5.18541	-1.03044	1.76209
H	-6.05426	-1.09167	-0.60751
H	-4.47117	-0.41542	-2.45543
H	-2.32875	0.25115	-3.17040
H	-1.75960	1.51998	-2.06419
H	1.47052	-2.00239	-1.86919
H	0.44571	-3.42739	-1.68082
H	-0.59910	-1.89272	-3.28801
H	-1.59307	-1.97273	-1.83159
H	0.17406	0.29869	-3.97694
H	0.42125	1.53708	-2.70963
H	1.40948	0.07846	-2.69579
H	-0.48168	-2.61391	1.72782
H	-0.28498	-3.96355	0.57028
H	-1.50143	-2.67727	0.29189
C	1.67642	0.23692	4.59950
C	0.97641	0.20256	3.32104
N	0.44434	0.17359	2.28297
H	2.75969	0.21773	4.43228
H	1.42840	1.14536	5.16151
H	1.40542	-0.63172	5.21073
C	-1.30617	4.72405	-0.13714
C	-0.81304	3.35624	-0.02832
N	-0.42974	2.25637	0.06960
H	-0.61422	5.33911	-0.72464
H	-2.28517	4.73944	-0.63098
H	-1.41580	5.18177	0.85388
C	2.69441	2.48129	-0.56102
H	2.31395	2.77365	0.42525
H	3.48260	3.18045	-0.85934
H	1.85000	2.58449	-1.25173
C	-2.68452	-0.34228	2.57673
H	-2.27001	0.65034	2.78707
H	-3.46012	-0.57086	3.31491
H	-1.85601	-1.04784	2.70241

^{5}FeBPMENMeNCSOH
Charge: 0
Energy: -1726806.0296500

Fe	-0.04846	-0.25004	-0.67503
N	-2.44944	0.00276	-0.36756
N	2.32132	-0.55332	-0.16625
N	-0.75400	-2.10677	0.51192
N	0.37037	0.33997	1.62099
C	-3.25395	1.08051	-0.48558
C	-2.99304	-1.19091	-0.05634
C	-4.63360	0.98575	-0.25139
C	-4.35486	-1.34988	0.20275
C	-5.18872	-0.23774	0.10631
C	3.23498	-1.16643	-0.95044
C	2.74635	0.22052	0.84940
C	4.60890	-0.98736	-0.73979
C	4.09890	0.41748	1.13038
C	5.04695	-0.18803	0.31028
C	1.70891	0.94926	1.67833
C	-2.07146	-2.39100	-0.07547
C	0.34003	-0.92518	2.38239
C	-0.82636	-1.81298	1.95249
C	-0.62824	1.30073	2.12040
C	0.18418	-3.19705	0.20639
H	-5.25335	1.87099	-0.35276
H	-6.25413	-0.32638	0.30084
H	-4.74675	-2.32752	0.46609
H	-2.55793	-3.25058	0.41545
H	-1.88439	-2.63577	-1.12637
H	5.31665	-1.48246	-1.39770
H	6.10848	-0.04166	0.49037

H	4.39353	1.04629	1.96529
H	2.05888	1.02308	2.72232
H	1.63099	1.97288	1.30017
H	-1.77158	-1.30011	2.14895
H	-0.83205	-2.73838	2.55188
H	0.28345	-0.73064	3.46662
H	1.28162	-1.44742	2.19612
H	-0.45726	1.54737	3.18142
H	-0.56364	2.21691	1.53117
H	-1.63136	0.88751	2.00650
H	0.26060	-3.28130	-0.87830
H	-0.14712	-4.15485	0.64246
H	1.17293	-2.94699	0.59506
C	-2.63087	2.38665	-0.89004
H	-3.39598	3.11057	-1.18446
H	-2.04751	2.82466	-0.07360
H	-1.93002	2.23597	-1.71338
C	2.74332	-2.07791	-2.04277
H	3.39966	-2.02093	-2.91799
H	2.75975	-3.11992	-1.69300
H	1.71164	-1.83575	-2.32318
O	-0.28171	-1.32479	-2.22968
H	-0.32872	-0.79122	-3.03779
N	0.49157	1.69625	-1.18571
C	0.67521	2.81573	-0.83878
S	0.88992	4.33436	-0.27743

^{5}FeBPMENOHBrOH
Charge: 0
Energy: -3079059.9639106

Fe	-0.04065	0.00068	-0.60083
N	-2.35721	0.05049	-0.26133
N	2.28890	-0.27370	-0.12644
N	-0.63774	-2.16437	-0.00287
N	0.28519	-0.07914	1.79050
C	-3.18343	1.08221	-0.03068
C	-2.88504	-1.19225	-0.36944
C	-4.57473	0.91275	0.13687
C	-4.24034	-1.44435	-0.20865
C	-5.09674	-0.36288	0.04808
C	3.23150	-0.60223	-1.01184
C	2.67188	0.09006	1.11231
C	4.60234	-0.59558	-0.70907
C	4.00723	0.10706	1.51019
C	4.98571	-0.23560	0.57574
C	1.58277	0.56228	2.04837
C	-1.91650	-2.30169	-0.71803
C	0.31154	-1.50543	2.17602
C	-0.77235	-2.30748	1.45360
C	-0.77911	0.66108	2.48981
C	0.37726	-3.05619	-0.57983
H	-5.18670	1.78711	0.32526
H	-6.16339	-0.52682	0.17549
H	-4.61998	-2.45769	-0.28703
H	-2.38389	-3.28376	-0.53540
H	-1.67641	-2.21146	-1.78268
H	5.33568	-0.86922	-1.46256
H	6.03736	-0.22460	0.84731
H	4.27094	0.39465	2.52255
H	1.89856	0.42430	3.09619
H	1.45093	1.63494	1.86819
H	-1.75965	-1.93870	1.74409
H	-0.72046	-3.36389	1.76552
H	0.20226	-1.62114	3.26727
H	1.29338	-1.90402	1.90728
H	-0.58278	0.72541	3.57279
H	-0.84549	1.66525	2.06600
H	-1.73740	0.16551	2.33239
H	0.53289	-2.74769	-1.61537
H	0.07247	-4.11521	-0.52248
H	1.32091	-2.92844	-0.04464
O	-2.70402	2.31749	0.07130
H	-1.73981	2.36343	-0.17791
O	2.76775	-0.95510	-2.23328
H	3.51751	-1.13468	-2.82186
O	-0.17571	-0.56633	-2.37737
H	0.50404	-0.19163	-2.95500
Br	0.45560	2.63911	-0.53397

^{5}FeBPMENOHClOH
Charge: 0
Energy: -1752511.9273493

Fe	0.05013	-0.13839	-0.66653
N	2.38052	-0.08964	-0.17391
N	-2.34066	0.13438	-0.22730
N	0.49881	1.71604	0.78436
N	-0.45240	-0.89751	1.55710
C	3.28273	-1.05097	-0.38321
C	2.81338	1.16327	0.06135
C	4.66608	-0.80731	-0.40679
C	4.16780	1.49198	0.09231
C	5.10330	0.48803	-0.16501
C	-3.22923	0.80575	-0.95852
C	-2.79180	-0.71301	0.71590
C	-4.61672	0.67716	-0.79199
C	-4.15170	-0.88870	0.97211
C	-5.07375	-0.18618	0.19545
C	-1.76077	-1.55028	1.44117
C	1.75043	2.22421	0.20955
C	-0.48211	0.23864	2.49573
C	0.61267	1.26283	2.17523
C	0.57311	-1.88888	1.91781
C	-0.56313	2.71010	0.58273
H	5.36566	-1.61758	-0.59161
H	6.16651	0.71181	-0.16524
H	4.47664	2.51188	0.29623
H	2.14539	3.08524	0.77587
H	1.48847	2.53169	-0.81096
H	-5.30556	1.24195	-1.41413
H	-6.14066	-0.30781	0.36006
H	-4.47604	-1.57171	1.75033
H	-2.15322	-1.85894	2.42582
H	-1.60960	-2.44865	0.83190
H	1.59501	0.80038	2.30306
H	0.55418	2.10245	2.88934
H	-0.38099	-0.10307	3.53979
H	-1.46102	0.71871	2.41242
H	0.32698	-2.40208	2.86372
H	0.66000	-2.60937	1.10258
H	1.53775	-1.39109	2.02400
H	-0.70202	2.81759	-0.49468
H	-0.30785	3.67905	1.04583
H	-1.49892	2.34994	1.01293
O	2.75961	-2.28341	-0.53663
H	3.44328	-2.90340	-0.83324
O	-2.69055	1.64490	-1.87725
H	-3.39960	2.04460	-2.40453
O	0.32611	1.19251	-2.04534
H	-0.48741	1.32429	-2.55211
Cl	-0.39455	-2.32015	-1.52168

^{3}FeBPMENOHFOH
Charge: 0
Energy: -1526386.7295107

Fe	-0.00847	-0.02284	-0.54551
N	2.04759	-0.03868	-0.42473
N	-2.09002	-0.07381	-0.43175
N	0.40434	1.67335	1.03541
N	-0.26312	-1.10913	1.35511
C	2.84291	-1.03766	-0.88237
C	2.61496	1.06457	0.11847
C	4.25406	-0.94676	-0.76514
C	3.98419	1.20143	0.28188
C	4.81612	0.16758	-0.17940
C	-3.02159	0.67713	-1.04273
C	-2.53957	-1.02087	0.43777
C	-4.39949	0.52809	-0.83265
C	-3.88663	-1.21995	0.71645
C	-4.83827	-0.43717	0.06126
C	-1.48121	-1.88772	1.06510
C	1.66311	2.18288	0.48218
C	-0.46630	-0.13339	2.44887
C	0.52967	1.02686	2.34303
C	0.85343	-2.02901	1.63986
C	-0.66561	2.66463	0.95744
H	4.84768	-1.77156	-1.14257
H	5.89546	0.24574	-0.07558
H	4.39256	2.09662	0.73930
H	2.15517	2.90562	1.15531
H	1.39788	2.68369	-0.45371
H	-5.09973	1.16732	-1.36343
H	-5.89909	-0.57246	0.24894
H	-4.17967	-1.98208	1.43042
H	-1.87177	-2.39326	1.96255
H	-1.18638	-2.63023	0.31877
H	1.55061	0.64663	2.43928
H	0.36870	1.73171	3.17637
H	-0.38738	-0.62354	3.43237
H	-1.48446	0.25711	2.36190
H	0.62269	-2.68397	2.49514
H	1.03645	-2.62279	0.74530
H	1.75493	-1.45648	1.85926
H	-0.82095	2.90355	-0.09733
H	-0.43565	3.58131	1.52910
H	-1.59444	2.23660	1.34572
O	2.32577	-2.11300	-1.41777
H	1.23813	-2.08602	-1.45001
O	-2.54859	1.62397	-1.88767
H	-3.29190	2.07413	-2.31803
O	0.21766	1.20024	-1.90514
H	-0.61374	1.32942	-2.37960
F	-0.04263	-2.01097	-1.32555

^{5}FeBPMENOHN$_3$OH

Charge: 0
Energy: -1566774.0752425

Fe	0.00355	-0.11933	-0.73125
N	-2.32281	0.01281	-0.30279
N	2.36358	-0.23290	-0.15815
N	-0.57909	-1.94831	0.64393
N	0.36899	0.65908	1.56371
C	-3.13542	1.05856	-0.46196
C	-2.85110	-1.19013	-0.01434
C	-4.53247	0.96057	-0.35143
C	-4.22441	-1.37898	0.13578
C	-5.07163	-0.28286	-0.04729
C	3.30559	-0.83167	-0.88728
C	2.74007	0.66510	0.76833
C	4.67545	-0.56239	-0.73939
C	4.07833	0.98007	1.00481
C	5.05615	0.36161	0.22532
C	1.64844	1.38039	1.53917
C	-1.87748	-2.34605	0.08311
C	0.44585	-0.54896	2.40673
C	-0.65516	-1.55413	2.05749
C	-0.69681	1.57014	2.01663
C	0.42985	-2.98717	0.39309
H	-5.16202	1.83406	-0.49448
H	-6.14738	-0.39673	0.05450
H	-4.61770	-2.35937	0.38351
H	-2.33443	-3.17801	0.64636
H	-1.67319	-2.67499	-0.94144
H	5.40996	-1.06759	-1.36062
H	6.10736	0.59308	0.37228
H	4.34207	1.70185	1.77106
H	2.00582	1.58848	2.56352
H	1.47420	2.35041	1.06285
H	-1.63434	-1.10152	2.23583
H	-0.58115	-2.42843	2.72651
H	0.38633	-0.28878	3.47798
H	1.42136	-1.01292	2.24125
H	-0.49032	1.95621	3.02993
H	-0.78366	2.40542	1.32012
H	-1.64979	1.04052	2.03083
H	0.54697	-3.07805	-0.68807
H	0.14593	-3.95264	0.84760
H	1.38871	-2.66733	0.80582
O	-2.48977	2.21031	-0.71636
H	-3.10350	2.95445	-0.80909
O	2.83906	-1.73463	-1.78076
H	3.58183	-2.09093	-2.29257
O	-0.23883	-1.37495	-2.12298
H	0.14638	-1.07920	-2.96013
N	0.53863	1.77451	-1.39734
N	0.24424	2.86750	-1.00497
N	-0.00879	3.93648	-0.60478

^{5}FeBPMENOHNCSOH
Charge: 0
Energy: -1771887.4621924

Fe	-0.01585	-0.25163	-0.69457
N	-2.33952	-0.13638	-0.23695
N	2.33310	-0.39064	-0.22917
N	-0.59486	-2.15878	0.54955
N	0.39355	0.36319	1.62985
C	-3.16106	0.91299	-0.33215
C	-2.86593	-1.36535	-0.08139
C	-4.56033	0.78724	-0.30274
C	-4.24111	-1.58215	-0.01439
C	-5.09517	-0.48379	-0.14188
C	3.24803	-0.95323	-1.01970
C	2.75236	0.34292	0.81886
C	4.62904	-0.82414	-0.80784
C	4.10370	0.51262	1.11894
C	5.05290	-0.07629	0.28318
C	1.69431	1.04638	1.64181
C	-1.88795	-2.52170	-0.04543
C	0.43977	-0.89384	2.40121
C	-0.67694	-1.85498	1.98496
C	-0.64380	1.27772	2.13830
C	0.41509	-3.17939	0.23655
H	-5.19500	1.66402	-0.39264
H	-6.17273	-0.61795	-0.10552
H	-4.63045	-2.58528	0.12458
H	-2.34742	-3.38782	0.46104
H	-1.67369	-2.78904	-1.08580
H	5.33926	-1.29833	-1.47958
H	6.11407	0.04374	0.48164
H	4.40027	1.10341	1.97926
H	2.06254	1.18714	2.67260
H	1.54774	2.04273	1.21240
H	-1.64888	-1.39558	2.18315
H	-0.62372	-2.77090	2.59763
H	0.37815	-0.69642	3.48506
H	1.40850	-1.36558	2.21587
H	-0.41409	1.61359	3.16361
H	-0.71969	2.14238	1.47784
H	-1.60896	0.77032	2.14050
H	0.53117	-3.19999	-0.84857
H	0.13066	-4.17220	0.62627
H	1.37361	-2.88860	0.67158
O	-2.53068	2.09512	-0.42994
H	-3.15644	2.82725	-0.53959
O	2.74195	-1.67252	-2.05076
H	3.47160	-2.01393	-2.59096
O	-0.25261	-1.38064	-2.18434
H	0.40301	-1.23019	-2.87966
N	0.38589	1.74101	-1.16711
C	0.31679	2.88557	-0.87000
S	0.21301	4.44449	-0.37905

^{5}FeBPMENSiH3BrOH
Charge: 0
Energy: -3349459.7808881

Fe	0.07541	0.01788	-0.25059
N	-2.32827	-0.44111	-0.23618
N	2.24315	0.04210	0.03649
N	-0.15548	-2.14466	0.51906
N	0.34344	0.26814	2.05306
C	-3.43203	0.35509	-0.26138
C	-2.49407	-1.78035	-0.25952
C	-4.71917	-0.20867	-0.30246
C	-3.75128	-2.39024	-0.29226
C	-4.88598	-1.59079	-0.31823
C	3.10895	-0.35797	-0.92436
C	2.67695	0.47709	1.23100
C	4.48655	-0.33643	-0.64647
C	4.03069	0.49726	1.56124
C	4.95021	0.08025	0.60025
C	1.61308	1.01790	2.16478
C	-1.25738	-2.64954	-0.30964
C	0.45025	-1.07869	2.65437
C	-0.48049	-2.07008	1.95396
C	-0.77125	1.03730	2.63106
C	1.04862	-2.95336	0.27115
H	-5.58661	0.44226	-0.31851
H	-5.87863	-2.03207	-0.34441
H	-3.82401	-3.47360	-0.29745
H	-1.52232	-3.68628	-0.04266
H	-0.88478	-2.63946	-1.34036
H	5.18311	-0.65118	-1.41573
H	6.01473	0.08556	0.81996
H	4.34990	0.84003	2.54140
H	1.97551	1.03674	3.20487
H	1.39875	2.04551	1.85265
H	-1.51491	-1.73135	2.05391
H	-0.41009	-3.05938	2.43580
H	0.22608	-1.04695	3.73177
H	1.48567	-1.41276	2.55315
H	-0.62199	1.22357	3.70681
H	-0.85249	1.98363	2.09453
H	-1.70458	0.48678	2.48957
H	1.27849	-2.92620	-0.79385
H	0.90060	-3.99863	0.58975
H	1.90141	-2.53389	0.80505
Si	-3.36863	2.26883	-0.27449
H	-2.88618	2.79338	-1.56489
H	-4.81611	2.62078	-0.14304
H	-2.67824	2.81147	0.91114
Si	2.51200	-0.94641	-2.67530
H	2.09347	-2.37538	-2.78220
H	2.06677	0.06213	-3.68069
H	3.93639	-1.12783	-3.20128
O	0.49046	-0.70696	-2.03082
H	0.12746	-0.09071	-2.68785
Br	0.06255	2.59048	-0.63561

^{5}FeBPMENSiH3ClOH
Charge: 0
Energy: -2022931.2482123

Fe	-0.07361	-0.11870	-0.36453
N	2.28863	0.33043	-0.25981
N	-2.23674	-0.27243	-0.10267
N	0.13457	1.74465	0.99772
N	-0.32650	-1.00894	1.78926
C	3.37555	-0.44775	-0.51058
C	2.47529	1.59495	0.17415
C	4.67248	0.05409	-0.30006
C	3.74161	2.13715	0.40637
C	4.86217	1.35209	0.16612
C	-3.11675	0.36813	-0.90751
C	-2.65294	-1.03690	0.92090
C	-4.49182	0.24232	-0.64433
C	-4.00384	-1.17522	1.23444
C	-4.93813	-0.51971	0.43393
C	-1.57245	-1.79426	1.66803
C	1.24850	2.46021	0.36135
C	-0.47522	0.11238	2.73899
C	0.44156	1.27632	2.35974

C	0.81019	-1.87667	2.13771
C	-1.07281	2.58399	0.96310
H	5.52902	-0.57906	-0.50424
H	5.86216	1.74123	0.33780
H	3.83328	3.15663	0.76867
H	1.51740	3.37267	0.91939
H	0.88758	2.75124	-0.63145
H	-5.19941	0.74888	-1.29149
H	-6.00060	-0.60682	0.64644
H	-4.30968	-1.78701	2.07842
H	-1.93704	-2.12181	2.65495
H	-1.32602	-2.68160	1.07650
H	1.48218	0.94148	2.37983
H	0.34516	2.09006	3.09768
H	-0.26622	-0.21246	3.77040
H	-1.51668	0.44245	2.71251
H	0.66167	-2.37201	3.11109
H	0.92987	-2.62216	1.35040
H	1.72450	-1.27930	2.17868
H	-1.28649	2.84911	-0.07211
H	-0.94116	3.50135	1.56095
H	-1.92837	2.02716	1.34645
Si	3.27690	-2.23466	-1.20012
H	2.69821	-2.28059	-2.55505
H	4.72989	-2.57462	-1.32225
H	2.70603	-3.18438	-0.22441
Si	-2.54133	1.44111	-2.42008
H	-2.19567	2.86465	-2.12817
H	-2.05355	0.77157	-3.66269
H	-3.97380	1.70147	-2.89172
O	-0.52789	1.12672	-1.83354
H	-0.10775	0.80478	-2.64722
Cl	0.06673	-2.34255	-1.25976

^{5}FeBPMENSiH3N$_3$OH
Charge: 0
Energy: -1837193.2340009

Fe	0.00950	-0.03347	-0.35624
N	-2.23752	-0.29122	-0.37728
N	2.15748	0.14520	-0.01287
N	-0.30692	-2.09510	0.65090
N	0.21154	0.45993	1.95754
C	-3.18099	0.67547	-0.51046
C	-2.59895	-1.56637	-0.13032
C	-4.53859	0.33798	-0.35946
C	-3.93011	-1.94671	0.03630
C	-4.91725	-0.97209	-0.07571
C	3.06779	-0.31495	-0.90780
C	2.54580	0.70928	1.14484
C	4.43509	-0.20265	-0.60405
C	3.88904	0.82483	1.49675
C	4.85002	0.36033	0.60124
C	1.44498	1.26664	2.02745
C	-1.48097	-2.58909	-0.08549
C	0.36822	-0.82904	2.65936
C	-0.57358	-1.88824	2.08492
C	-0.94360	1.22177	2.45442
C	0.85196	-2.97077	0.42084
H	-5.29171	1.11026	-0.46828
H	-5.96535	-1.22918	0.05260
H	-4.17736	-2.98252	0.24894
H	-1.85339	-3.54237	0.32457
H	-1.14115	-2.76420	-1.11223
H	5.16255	-0.56267	-1.32309
H	5.90745	0.43868	0.84004
H	4.16790	1.27507	2.44509
H	1.80123	1.36162	3.06637
H	1.20588	2.27559	1.67685
H	-1.60951	-1.55589	2.19561
H	-0.47288	-2.82841	2.65145
H	0.19416	-0.71598	3.74182
H	1.40359	-1.15569	2.53200
H	-0.81584	1.52043	3.50763
H	-1.07715	2.10740	1.83206
H	-1.84880	0.61715	2.36451
H	1.04640	-3.01789	-0.65063
H	0.67940	-3.98515	0.81720
H	1.73621	-2.54575	0.89923
Si	-2.80415	2.51786	-0.96738
H	-2.26785	2.74808	-2.32789
H	-4.24310	2.95688	-1.11068
H	-2.34531	3.40087	0.13572
Si	2.55220	-1.12534	-2.59789
H	2.27446	-2.59307	-2.56469
H	2.06080	-0.26861	-3.72234
H	4.00073	-1.22948	-3.08091
O	0.54910	-0.98111	-2.01128
H	0.10719	-0.58945	-2.78082
N	-0.43066	1.94255	-0.72729
N	0.29535	2.89995	-0.57327
N	0.95587	3.83579	-0.40930

^{5}FeBPMENSiH3NCSOH
Charge: 0
Energy: -2042303.4681173

Fe	-0.01154	-0.16806	-0.34600
N	-2.35740	-0.36876	-0.33979
N	2.16111	-0.20819	-0.05337
N	-0.42576	-2.15234	0.76663
N	0.29794	0.42022	1.92505
C	-3.32292	0.57061	-0.52042
C	-2.71585	-1.63379	-0.03725
C	-4.67848	0.23360	-0.36629
C	-4.04717	-2.01797	0.13628
C	-5.04711	-1.06604	-0.02714
C	3.00073	-0.78379	-0.94876
C	2.62940	0.38636	1.05748
C	4.38218	-0.76725	-0.69363
C	3.98995	0.41157	1.36199
C	4.87999	-0.17675	0.46677
C	1.61408	1.09071	1.93858
C	-1.60828	-2.66076	0.05763
C	0.33067	-0.83320	2.70630
C	-0.69259	-1.83956	2.18127
C	-0.76130	1.32832	2.39410
C	0.69324	-3.09499	0.60894
H	-5.43856	0.99318	-0.51572
H	-6.09284	-1.33098	0.10320
H	-4.28311	-3.04607	0.39379
H	-1.99216	-3.58775	0.51488
H	-1.27299	-2.88721	-0.96047
H	5.05537	-1.22054	-1.41277
H	5.94777	-0.17123	0.66962
H	4.33601	0.88994	2.27371
H	2.00029	1.18145	2.96664
H	1.47728	2.10658	1.55560
H	-1.69607	-1.41078	2.25251
H	-0.68153	-2.74982	2.80328
H	0.15232	-0.63685	3.77550
H	1.33489	-1.25610	2.62209
H	-0.59628	1.64484	3.43657
H	-0.78997	2.20544	1.74729
H	-1.72937	0.82544	2.32495
H	0.88312	-3.23617	-0.45488
H	0.47102	-4.06626	1.08114
H	1.59732	-2.67838	1.05432
Si	-2.93242	2.37072	-1.04402
H	-2.18434	2.41962	-2.31469
H	-4.29812	2.92628	-1.28206
H	-2.32706	3.15073	0.05466
Si	2.36939	-1.62028	-2.58278
H	1.93650	-3.04492	-2.47299
H	1.91313	-0.76945	-3.72353
H	3.78108	-1.88984	-3.10129
O	0.37000	-1.25861	-1.94788
H	-0.04623	-0.87105	-2.73363
N	0.01802	1.84613	-0.77341
C	0.43975	2.94324	-0.59147
S	0.96187	4.44630	-0.27036

^{5}FeBPMENtBuBrOH
Charge: 0
Energy: -3182037.9000618

Fe	-0.17136	-0.10999	-0.22383
N	-2.69701	-0.00062	0.41073
N	2.81387	0.56846	-0.56952
N	-0.28868	0.69278	1.93224
N	0.27149	2.21406	-0.42390
C	-3.84941	0.01828	-0.30279
C	-2.74063	0.30143	1.72485
C	-5.04313	0.46758	0.28883
C	-3.89792	0.73990	2.36884
C	-5.06702	0.84853	1.62473
C	4.01869	0.02200	-0.31300
C	2.73246	1.87886	-0.85279
C	5.17139	0.82216	-0.23384
C	3.83690	2.73341	-0.78950
C	5.07472	2.19223	-0.45307
C	1.40346	2.40059	-1.35389
C	-1.48450	0.07077	2.53439
C	0.52194	2.79406	0.90227
C	-0.41290	2.16710	1.93017
C	-0.94295	2.77131	-1.04165
C	0.91976	0.26283	2.66448
H	-5.95499	0.51022	-0.29077
H	-5.98747	1.20284	2.08101
H	-3.87353	0.98390	3.42632
H	-1.62930	0.43239	3.56490
H	-1.29860	-1.00791	2.56334
H	6.13443	0.37971	-0.01295
H	5.95644	2.82431	-0.38591
H	3.72488	3.79054	-1.01110
H	1.50925	3.46750	-1.61400
H	1.13930	1.83334	-2.25128
H	-1.44918	2.41554	1.68907

H	-0.20714	2.57521	2.93256
H	0.39371	3.89013	0.90030
H	1.56104	2.59336	1.17327
H	-0.88010	3.86894	-1.13952
H	-1.06303	2.32265	-2.02620
H	-1.82289	2.51031	-0.45078
H	1.81116	0.62231	2.14737
H	0.95001	-0.82681	2.67075
H	0.91457	0.64320	3.69861
C	-3.83957	-0.50529	-1.74872
C	4.07089	-1.50226	-0.14473
C	-3.11002	0.49257	-2.67487
H	-3.51769	1.50582	-2.56392
H	-2.03538	0.49042	-2.47718
H	-3.25483	0.18732	-3.71891
C	-5.27248	-0.70390	-2.28787
H	-5.86773	-1.36562	-1.64746
H	-5.80979	0.24458	-2.40813
H	-5.21441	-1.16779	-3.27803
C	-3.12493	-1.87407	-1.78561
H	-2.10946	-1.81640	-1.39571
H	-3.66675	-2.61637	-1.18803
H	-3.08144	-2.23379	-2.82076
C	3.21987	-2.16042	-1.25382
H	3.20860	-3.24710	-1.11572
H	2.18873	-1.80611	-1.22623
H	3.63981	-1.94035	-2.24352
C	3.49861	-1.87113	1.23933
H	3.57037	-2.95267	1.40043
H	4.04993	-1.36495	2.04277
H	2.44354	-1.60918	1.29675
C	5.51141	-2.04115	-0.24442
H	5.99308	-1.74666	-1.18461
H	6.14135	-1.70533	0.58816
H	5.48793	-3.13556	-0.20990
O	-0.08011	-0.10513	-2.08882
H	-0.04766	-0.99683	-2.46733
Br	-0.13760	-2.58084	0.60719

^{5}FeBPMENtBuClOH
Charge: 0
Energy: -1855508.8008830

Fe	0.12771	0.32263	-0.10915
N	2.69313	0.05817	0.50690
N	-2.76314	-0.19387	-0.62744
N	0.28204	-1.14010	1.69549
N	-0.25833	-1.83323	-1.01940
C	3.84843	0.28303	-0.16132
C	2.72809	-0.66402	1.64456
C	5.04243	-0.33287	0.25393
C	3.88374	-1.28933	2.11410
C	5.05866	-1.13923	1.38537
C	-3.95390	0.26430	-0.19260
C	-2.71053	-1.36135	-1.29213
C	-5.11731	-0.51341	-0.32677
C	-3.82795	-2.18296	-1.46188
C	-5.04906	-1.75568	-0.94758
C	-1.39775	-1.72633	-1.95033
C	1.46289	-0.71565	2.47168
C	-0.49127	-2.81448	0.04855
C	0.43314	-2.53317	1.22764
C	0.96128	-2.13794	-1.78501
C	-0.93538	-0.97943	2.51352
H	5.95845	-0.17430	-0.29894
H	5.97797	-1.62283	1.70491
H	3.85457	-1.87248	3.02935
H	1.61069	-1.37525	3.34222
H	1.25584	0.29784	2.82837
H	-6.06782	-0.14807	0.04046
H	-5.93982	-2.37011	-1.05002
H	-3.73785	-3.12584	-1.99290
H	-1.52227	-2.66649	-2.51437
H	-1.13585	-0.91987	-2.64144
H	1.47332	-2.67458	0.92434
H	0.23521	-3.24483	2.04566
H	-0.34111	-3.84831	-0.30711
H	-1.53354	-2.73360	0.36651
H	0.91465	-3.14343	-2.23814
H	1.07122	-1.38624	-2.56475
H	1.83797	-2.07286	-1.13762
H	-1.81975	-1.16698	1.90162
H	-0.98106	0.05185	2.86233
H	-0.93203	-1.66644	3.37559
C	3.83575	1.25755	-1.34999
C	-3.98754	1.67065	0.42151
C	3.15912	0.59412	-2.57013
H	3.60850	-0.38367	-2.78771
H	2.08355	0.49037	-2.40622
H	3.30143	1.23052	-3.45292
C	5.26641	1.67240	-1.75508
H	5.82897	2.09227	-0.91261
H	5.83979	0.83885	-2.17824
H	5.20409	2.44441	-2.52927
C	3.06504	2.53552	-0.95085
H	2.05303	2.31585	-0.61183
H	3.57805	3.06395	-0.13858
H	3.00755	3.20989	-1.81393
C	-3.11026	2.61776	-0.42665
H	-3.10765	3.61722	0.02235
H	-2.07861	2.26866	-0.47552
H	-3.50350	2.69736	-1.44793
C	-3.44034	1.60296	1.86277
H	-3.51739	2.58738	2.33871
H	-4.00819	0.88349	2.46726
H	-2.38612	1.33073	1.85843
C	-5.42072	2.23859	0.46385
H	-5.89075	2.23452	-0.52698
H	-6.06837	1.68872	1.15718
H	-5.38443	3.27612	0.81264
O	0.10361	0.85271	-1.90871
H	0.06931	1.81468	-2.02097
Cl	0.09111	2.18639	1.39799

^{5}FeBPMENtBuFOH
Charge: 0
Energy: -1629381.1973487

Fe	-0.09769	0.31616	0.07755
N	-2.48562	0.01146	-0.64601
N	2.58004	0.20557	0.75345
N	-0.12190	-1.66936	-1.20884
N	0.23542	-1.61655	1.59961
C	-3.66781	0.46746	-0.17000
C	-2.48596	-0.98858	-1.55461
C	-4.86929	-0.17354	-0.52417
C	-3.64707	-1.64855	-1.95438
C	-4.86038	-1.24623	-1.40571
C	3.59207	0.53790	-0.06333
C	2.62190	-0.95765	1.43434
C	4.65032	-0.36276	-0.29628
C	3.67273	-1.86422	1.29808
C	4.69149	-1.56882	0.38951
C	1.44875	-1.23772	2.35143
C	-1.16167	-1.34328	-2.19590
C	0.36858	-2.88728	0.87509
C	-0.46248	-2.85208	-0.40758
C	-0.93716	-1.61224	2.48303
C	1.18272	-1.79184	-1.87704
H	-5.81032	0.17353	-0.11988
H	-5.78709	-1.74575	-1.67581
H	-3.59118	-2.45609	-2.67762
H	-1.30587	-2.16778	-2.91478
H	-0.79980	-0.45944	-2.72790
H	5.43894	-0.10805	-0.99532
H	5.51093	-2.26528	0.23167
H	3.68227	-2.78261	1.87789
H	1.72070	-2.01370	3.08824
H	1.19171	-0.31246	2.87122
H	-1.52422	-2.78880	-0.15263
H	-0.31908	-3.78579	-0.97934
H	0.06272	-3.74556	1.49632
H	1.41913	-3.04253	0.62208
H	-0.85944	-2.37783	3.27539
H	-1.02382	-0.61929	2.92296
H	-1.83957	-1.80275	1.89495
H	1.96905	-1.95860	-1.13866
H	1.38765	-0.84445	-2.37371
H	1.19263	-2.62095	-2.60566
C	-3.68441	1.71152	0.73371
C	3.60068	1.92696	-0.71825
C	-3.27019	1.31563	2.16990
H	-3.87554	0.47642	2.53702
H	-2.20734	1.07211	2.20912
H	-3.43414	2.16758	2.84183
C	-5.09628	2.33731	0.78772
H	-5.48363	2.56749	-0.21224
H	-5.82119	1.69656	1.30346
H	-5.04546	3.27537	1.35001
C	-2.71134	2.77891	0.18345
H	-1.67451	2.45723	0.27709
H	-2.92755	3.00873	-0.86651
H	-2.82282	3.70048	0.76717
C	2.52785	2.85021	-0.11238
H	2.65186	3.85992	-0.52182
H	1.52853	2.50152	-0.37258
H	2.62145	2.91078	0.97789
C	3.32617	1.77325	-2.23302
H	3.42241	2.74827	-2.72690
H	4.03948	1.08634	-2.70574
H	2.30544	1.41073	-2.37880
C	4.98764	2.57861	-0.49857
H	5.22418	2.65905	0.56929
H	5.79774	2.02417	-0.98455
H	4.98658	3.58932	-0.92206
O	-0.19371	1.26555	1.72898
H	0.59427	1.82093	1.81889
F	0.34863	1.04123	-1.59843

^{5}FeBPMENtBuN$_3$OH
Charge: 0
Energy: -1669768.9231065

Fe	-0.10680	0.20496	-0.15839
N	2.64537	0.19031	0.47402
N	-2.69029	-0.32082	-0.58461
N	0.28410	-0.98402	1.97878
N	-0.30939	-2.04493	-0.60852
C	3.64033	0.18409	-0.42866
C	2.70040	-0.64904	1.52578
C	4.66827	-0.77715	-0.35462
C	3.71935	-1.58588	1.69115
C	4.70636	-1.66959	0.70729
C	-3.87121	0.29128	-0.33088
C	-2.70093	-1.54742	-1.14399
C	-5.08760	-0.37345	-0.55675
C	-3.87706	-2.26016	-1.38739
C	-5.09214	-1.66478	-1.07119
C	-1.38332	-2.12410	-1.61155
C	1.57873	-0.52627	2.53380
C	-0.63765	-2.81754	0.59863
C	0.28981	-2.44238	1.74941
C	0.96318	-2.46544	-1.22347
C	-0.81699	-0.59900	2.87531
H	5.43813	-0.80867	-1.11683
H	5.50122	-2.40716	0.78093
H	3.73135	-2.23625	2.56087
H	1.82761	-1.09385	3.44634
H	1.47529	0.52440	2.81170
H	-6.02683	0.11543	-0.33646
H	-6.02946	-2.18929	-1.23701
H	-3.82986	-3.25414	-1.82123
H	-1.53241	-3.16568	-1.94235
H	-1.04402	-1.51856	-2.45767
H	1.30879	-2.75175	1.51038
H	-0.00209	-2.98957	2.66031
H	-0.57998	-3.90361	0.40954
H	-1.67279	-2.58893	0.86764
H	0.92764	-3.52103	-1.54281
H	1.15026	-1.81774	-2.07996
H	1.78569	-2.33222	-0.51970
H	-1.77135	-0.88948	2.42874
H	-0.81671	0.48512	2.98770
H	-0.72261	-1.07556	3.86568
C	3.66413	1.25563	-1.52768
C	-3.84137	1.73960	0.17801
C	3.25072	0.60882	-2.87032
H	3.89553	-0.24387	-3.11953
H	2.20796	0.27919	-2.81955
H	3.34452	1.34526	-3.67870
C	5.09595	1.83229	-1.64980
H	5.44439	2.23608	-0.69210
H	5.82534	1.09155	-1.99530
H	5.09525	2.64878	-2.38059
C	2.71167	2.41801	-1.19727
H	1.67488	2.08577	-1.17551
H	2.94095	2.86414	-0.22507
H	2.80966	3.19193	-1.96832
C	-2.95984	2.58738	-0.76755
H	-2.91148	3.61850	-0.39968
H	-1.94040	2.20634	-0.81698
H	-3.38453	2.60126	-1.77915
C	-3.26978	1.76126	1.61041
H	-3.29814	2.78309	2.00680
H	-3.86041	1.11915	2.27673
H	-2.22874	1.44495	1.61315
C	-5.24827	2.37058	0.20972
H	-5.72867	2.35844	-0.77592
H	-5.91170	1.87393	0.92784
H	-5.16026	3.41669	0.52120
O	0.11295	0.34778	-2.03732
H	0.00190	1.24246	-2.39073
N	-0.12689	1.91511	0.90208
N	0.74427	2.47633	1.51662
N	1.55612	3.03421	2.13049

^{5}FeBPMENtBuNCSOH
Charge: 0
Energy: -1874880.8696523

Fe	-0.13182	-0.06913	-0.29009
N	2.66791	0.21159	0.26500
N	-2.66651	-0.73058	-0.42219
N	0.30384	-0.17738	2.14482
N	-0.27816	-2.27310	0.27290
C	3.67520	-0.17920	-0.53287
C	2.72411	-0.05249	1.58326
C	4.72309	-0.97326	-0.02711
C	3.75945	-0.78786	2.16018
C	4.76198	-1.28466	1.32537
C	-3.84802	-0.06849	-0.47233
C	-2.67610	-2.07857	-0.42010
C	-5.06420	-0.76859	-0.43664
C	-3.85288	-2.82897	-0.37330
C	-5.06904	-2.15714	-0.36812
C	-1.35560	-2.79861	-0.58122
C	1.59292	0.50116	2.42147
C	-0.58949	-2.44107	1.70152
C	0.34336	-1.59484	2.56068
C	0.99762	-2.90842	-0.10854
C	-0.78524	0.53266	2.83870
H	5.50683	-1.32635	-0.68713
H	5.57120	-1.88698	1.72986
H	3.77338	-0.97057	3.23066
H	1.84356	0.42080	3.49227
H	1.46385	1.55907	2.18247
H	-6.00326	-0.23287	-0.46439
H	-6.00721	-2.70404	-0.32636
H	-3.80528	-3.91323	-0.35128
H	-1.49845	-3.87820	-0.40845
H	-1.02432	-2.63888	-1.61191
H	1.36613	-1.96054	2.45603
H	0.07538	-1.70419	3.62348
H	-0.52220	-3.50025	2.00377
H	-1.62465	-2.12244	1.85402
H	0.97542	-3.99618	0.07278
H	1.17006	-2.70605	-1.16549
H	1.82219	-2.46787	0.45273
H	-1.74451	0.07837	2.57853
H	-0.79972	1.57395	2.51731
H	-0.65628	0.49575	3.93316
C	3.67874	0.27963	-1.99743
C	-3.81469	1.46110	-0.59849
C	3.22407	-0.89449	-2.89559
H	3.85129	-1.78161	-2.73854
H	2.17780	-1.14151	-2.68990
H	3.31121	-0.60698	-3.95124
C	5.10783	0.71315	-2.40353
H	5.49609	1.48756	-1.73175
H	5.81803	-0.12096	-2.41178
H	5.08551	1.12616	-3.41815
C	2.73848	1.48210	-2.19848
H	1.70538	1.22364	-1.97444
H	3.01574	2.32027	-1.55084
H	2.79865	1.81562	-3.24163
C	-2.94406	1.84552	-1.81701
H	-2.87624	2.93636	-1.89284
H	-1.93063	1.45567	-1.72774
H	-3.38863	1.46088	-2.74331
C	-3.22784	2.05661	0.69607
H	-3.18079	3.14884	0.62501
H	-3.84674	1.79268	1.56319
H	-2.21409	1.70015	0.85359
C	-5.21902	2.06044	-0.81148
H	-5.70439	1.66593	-1.71208
H	-5.87969	1.88737	0.04634
H	-5.12585	3.14441	-0.93492
O	0.08776	-0.71182	-2.05267
H	0.00257	-0.04531	-2.75001
N	-0.05594	1.93459	-0.05822
C	0.22001	2.98908	0.41226
S	0.58286	4.40743	1.11706

^{6}FeH1CYPBrK
Charge: 0
Energy: -3614500.4622253

Fe	0.67871	-0.34996	-0.28642
N	0.83960	-2.35091	-1.27447
C	2.13218	-2.85644	-0.80101
C	0.81663	-1.96763	-2.69717
C	-0.30633	-3.14219	-0.82584
H	1.74069	-1.41826	-2.88698
H	-1.12387	-3.04718	-1.54441
H	-0.06911	-4.21276	-0.76256
H	1.98881	-3.25305	0.20885
H	2.52494	-3.65992	-1.43787
C	-0.40082	-1.07338	-2.96790
H	-1.28569	-1.67585	-3.19718
H	-0.20372	-0.47203	-3.86547
N	2.61630	-0.47397	-0.66159
N	-0.15736	-1.63564	1.08380
C	-0.41529	-1.38427	2.50801
N	-0.68175	-0.20148	-1.81705
C	-1.99771	0.16181	-1.73574
O	-2.90625	-0.30330	-2.45914
K	-3.53592	-1.42516	0.26836
N	-2.33767	1.03289	-0.68483
H	-1.50598	1.43595	-0.25745
C	-3.05988	2.88236	-2.19027
H	-2.04700	3.29889	-2.15538
H	-3.13674	2.22106	-3.05822
C	-4.78217	1.52402	-0.95032
H	-5.51056	2.33090	-1.08619
H	-4.88076	0.81777	-1.77687
C	-3.35825	2.10552	-0.89469

H	-3.41269	2.48934	1.25442
H	-2.24399	3.49086	0.37990
H	-3.98004	3.84283	0.25154
H	0.80281	-2.85303	-3.35105
H	-5.03818	1.02780	-0.00099
H	-3.76758	3.70939	-2.31898
C	-3.23972	3.03882	0.32100
C	3.16442	-1.72922	-0.72954
O	4.36193	-2.00560	-0.74163
C	3.58214	0.62461	-0.79382
C	3.05461	1.84068	-1.60814
H	1.96165	1.84034	-1.65411
H	3.41931	1.78500	-2.64058
C	4.09747	1.20364	0.53922
H	3.26413	1.31884	1.23910
H	4.84488	0.54612	0.99486
H	4.44998	0.20828	-1.31566
C	4.64026	2.57882	0.12428
C	3.58126	3.10035	-0.87220
H	5.60996	2.45923	-0.37872
H	4.79315	3.25479	0.97286
H	3.98294	3.85385	-1.55852
H	2.75980	3.56438	-0.31644
C	-0.80599	-2.68306	0.54490
O	-1.78723	-3.28715	1.03606
C	-1.51770	-0.32904	2.83514
H	-1.70645	0.30658	1.96448
H	-2.45382	-0.83812	3.10838
C	0.83839	-0.90312	3.26042
H	1.53521	-1.72572	3.45550
H	1.36333	-0.15125	2.66291
H	-0.73187	-2.33839	2.94425
C	-0.96940	0.51419	4.01603
C	0.26143	-0.26358	4.53048
H	0.97962	0.37910	5.05005
H	-0.04975	-1.04675	5.23575
H	-0.64978	1.49057	3.63937
H	-1.71712	0.68628	4.79780
Br	0.50957	1.92075	0.88204

^{6}FeH1CYPClK
Charge: 0
Energy: -2287974.2118767

Fe	0.72288	-0.18399	-0.26082
N	1.00127	-1.94877	-1.61793
C	2.34099	-2.43453	-1.26957
C	0.91322	-1.30293	-2.94060
C	-0.07148	-2.90048	-1.32029
H	1.78545	-0.65173	-3.02795
H	-0.88617	-2.78044	-2.03815
H	0.26751	-3.94117	-1.41087
H	2.25416	-3.02855	-0.35437
H	2.77291	-3.06771	-2.05583
C	-0.37356	-0.47587	-3.02496
H	-1.22538	-1.10507	-3.30795
H	-0.26890	0.26105	-3.83258
N	2.65796	-0.10538	-0.64658
N	-0.03404	-1.75265	0.82685
C	-0.33901	-1.75372	2.26321
N	-0.64584	0.19020	-1.74416
C	-1.95452	0.56366	-1.60998
O	-2.85742	0.26235	-2.42251
K	-3.39355	-1.47869	-0.03601
N	-2.29019	1.21539	-0.41351
H	-1.46185	1.52309	0.09315
C	-3.10990	3.29526	-1.51392
H	-2.10973	3.73473	-1.42763
H	-3.19528	2.80898	-2.48972
C	-4.74840	1.66652	-0.50635
H	-5.50579	2.45652	-0.45641
H	-4.85743	1.13511	-1.45403
C	-3.33971	2.27475	-0.38385
H	-3.32654	2.23727	1.79960
H	-2.21238	3.42142	1.09819
H	-3.95885	3.74210	1.09505
H	0.95387	-2.04427	-3.75344
H	-4.94965	0.98260	0.33291
H	-3.84664	4.10518	-1.46133
C	-3.19974	2.96050	0.98493
C	3.29323	-1.26972	-0.98722
O	4.50675	-1.44649	-1.07426
C	3.53068	1.06577	-0.50370
C	2.90993	2.38860	-1.04251
H	1.82592	2.29757	-1.15848
H	3.32086	2.61595	-2.03316
C	3.96642	1.36869	0.94518
H	3.11368	1.23724	1.61891
H	4.76990	0.69881	1.26847
H	4.43836	0.84640	-1.07499
C	4.36960	2.84872	0.88093
C	3.27168	3.47974	-0.00229
H	5.35117	2.94690	0.39650
H	4.44343	3.31845	1.86813
H	3.58974	4.41952	-0.46699
H	2.39318	3.69592	0.61484
C	-0.63083	-2.70558	0.09073
O	-1.60314	-3.41692	0.43404
C	-1.49102	-0.80510	2.72557
H	-1.70624	-0.06143	1.95247
H	-2.40272	-1.39024	2.91644
C	0.87759	-1.35515	3.11948
H	1.59626	-2.17688	3.21127
H	1.39155	-0.50780	2.65473
H	-0.62690	-2.77808	2.52528
C	-0.98773	-0.11265	4.01820
C	0.24934	-0.92690	4.45226
H	0.93439	-0.35127	5.08342
H	-0.05900	-1.81333	5.02408
H	-0.68153	0.91015	3.77824
H	-1.75511	-0.05851	4.79808
Cl	0.43894	1.62587	1.20925

^{6}FeH1CYPFK
Charge: 0
Energy: -2061854.2897799

Fe	0.75826	-0.29762	-0.09354
N	1.18434	-2.35002	-0.93737
C	2.59278	-2.59186	-0.59150
C	0.96742	-2.10171	-2.37758
C	0.22961	-3.29025	-0.33097
H	1.76479	-1.42729	-2.70101
H	-0.49190	-3.63893	-1.07500
H	0.73887	-4.18871	0.03900
H	2.62706	-2.97494	0.43332
H	3.06214	-3.33354	-1.25144
C	-0.38715	-1.42897	-2.59973
H	-1.19948	-2.16723	-2.51314
H	-0.44073	-1.06442	-3.63443
N	2.68866	-0.16689	-0.44332
N	-0.03244	-1.53335	1.32800
C	-0.57346	-1.03041	2.59500
N	-0.55137	-0.33715	-1.64304
C	-1.78952	0.25429	-1.67266
O	-2.76042	-0.21883	-2.31833
K	-3.30201	-1.68949	-0.03702
N	-1.94315	1.35151	-0.85781
H	-1.10332	1.65901	-0.36953
C	-3.21410	2.87323	-2.34436
H	-2.29024	3.37727	-2.64914
H	-3.41975	2.06538	-3.05110
C	-4.38261	1.64243	-0.47716
H	-5.19797	2.37428	-0.46770
H	-4.65034	0.84242	-1.17306
C	-3.06297	2.30714	-0.91995
H	-2.58083	3.04315	1.08010
H	-1.78098	3.93352	-0.22979
H	-3.50880	4.18480	0.08205
H	1.04355	-3.03290	-2.96050
H	-4.28423	1.24540	0.54306
H	-4.03388	3.60017	-2.38665
C	-2.71159	3.43449	0.06446
C	3.42535	-1.30186	-0.61918
O	4.64549	-1.38290	-0.75574
C	3.41401	1.10383	-0.44825
C	2.76049	2.19694	-1.31258
H	1.69941	2.26150	-1.04790
H	2.83515	1.98782	-2.38571
C	3.50497	1.78646	0.93073
H	2.50736	1.76365	1.38057
H	4.20137	1.27390	1.60266
H	4.42677	0.90651	-0.81832
C	3.91339	3.24315	0.60759
C	3.49797	3.48024	-0.88082
H	4.99347	3.38279	0.72832
H	3.42615	3.95224	1.28550
H	4.38997	3.62794	-1.50107
H	2.87540	4.37288	-1.00407
C	-0.54129	-2.67544	0.84553
O	-1.57018	-3.27021	1.24674
C	-1.74400	0.00504	2.46866
H	-1.90993	0.28486	1.42433
H	-2.67003	-0.42986	2.87231
C	0.51201	-0.30343	3.41939
H	1.12553	-1.00322	3.99657
H	1.17313	0.24022	2.73631
H	-0.94030	-1.89543	3.15822
C	-1.31527	1.24405	3.28699
C	-0.27033	0.69956	4.27729
H	0.36451	1.48398	4.70318
H	-0.76574	0.18485	5.11281
H	-0.82791	1.95073	2.60912
H	-2.15607	1.75047	3.77398
F	0.34728	1.35449	0.64017

^{6}FeH1CYPN$_3$K

Charge: 0
Energy: -2102236.7594494

Fe	0.69982	-0.40587	-0.18552
N	0.95857	-2.58464	-0.67762
C	2.32289	-2.88169	-0.22407
C	0.80722	-2.56698	-2.14573
C	-0.08481	-3.32786	0.03762
H	1.66138	-2.01094	-2.53916
H	-0.89378	-3.59538	-0.64631
H	0.29622	-4.27504	0.44179
H	2.28718	-3.04980	0.85701
H	2.73498	-3.78107	-0.70088
C	-0.49461	-1.85814	-2.52543
H	-1.35208	-2.53755	-2.43018
H	-0.45552	-1.58695	-3.58898
N	2.62962	-0.50117	-0.60498
N	-0.06139	-1.35944	1.46773
C	-0.40242	-0.71896	2.74166
N	-0.68544	-0.67173	-1.68616
C	-1.95480	-0.17567	-1.73972
O	-2.90083	-0.72455	-2.35084
K	-3.41158	-1.43716	0.44718
N	-2.20159	0.94356	-0.93193
H	-1.33312	1.35830	-0.59730
C	-2.98545	2.42391	-2.77576
H	-1.96476	2.79707	-2.91871
H	-3.14565	1.57931	-3.45156
C	-4.62926	1.47316	-1.11679
H	-5.35083	2.25789	-1.36945
H	-4.81597	0.60693	-1.75544
C	-3.19107	1.98531	-1.31413
H	-3.03788	2.85836	0.68274
H	-1.93014	3.58043	-0.49921
H	-3.65628	3.97119	-0.55657
H	0.83514	-3.58466	-2.56506
H	-4.80145	1.20647	-0.06287
H	-3.68388	3.22512	-3.04363
C	-2.93730	3.16811	-0.36450
C	3.26797	-1.70305	-0.47839
O	4.48058	-1.90470	-0.52962
C	3.48871	0.64568	-0.90913
C	2.87141	1.64833	-1.92742
H	1.78531	1.52959	-1.98213
H	3.26319	1.45215	-2.93195
C	3.87428	1.49460	0.31947
H	3.00047	1.62906	0.96663
H	4.65637	1.00989	0.91289
H	4.41631	0.24387	-1.32946
C	4.29825	2.83278	-0.30055
C	3.25737	3.06494	-1.41919
H	5.30311	2.73536	-0.73342
H	4.33071	3.65339	0.42391
H	3.64049	3.70901	-2.21794
H	2.37995	3.56785	-0.99890
C	-0.67397	-2.52369	1.20011
O	-1.67664	-2.99421	1.78672
C	-1.56376	0.32424	2.70414
H	-1.72266	0.67542	1.68031
H	-2.49485	-0.13823	3.06212
C	0.78900	0.04098	3.35195
H	1.52356	-0.64060	3.79398
H	1.30128	0.61286	2.57048
H	-0.69585	-1.51591	3.43511
C	-1.12755	1.49547	3.62691
C	0.12870	0.98362	4.36608
H	0.78687	1.79610	4.68991
H	-0.16300	0.41871	5.26190
H	-0.86606	2.37130	3.02526
H	-1.91989	1.80637	4.31607
N	0.41747	1.47062	0.27669
N	0.61080	2.54435	0.78297
N	0.77712	3.58134	1.26378

[6]FeH1CYPNCSK
Charge: 0
Energy: -2307346.2668220

Fe	0.67902	-0.57592	-0.15474
N	0.86762	-2.79643	-0.41864
C	2.21173	-3.08904	0.09528
C	0.74345	-2.92252	-1.88391
C	-0.21298	-3.42674	0.34728
H	1.62682	-2.44473	-2.31353
H	-1.02962	-3.71224	-0.32001
H	0.12002	-4.35252	0.83476
H	2.14935	-3.13572	1.18714
H	2.59922	-4.04855	-0.27187
C	-0.52213	-2.20478	-2.35918
H	-1.40696	-2.83895	-2.22244
H	-0.44818	-2.03334	-3.44148
N	2.60333	-0.77425	-0.53084
N	-0.12298	-1.32720	1.57440
C	-0.43250	-0.55178	2.78066
N	-0.68888	-0.93769	-1.63894
C	-1.95541	-0.43297	-1.72775
O	-2.91878	-1.03997	-2.24903
K	-3.46740	-1.38457	0.59440
N	-2.17444	0.78236	-1.06744
H	-1.30200	1.23149	-0.80257
C	-2.99279	2.02515	-3.06487
H	-1.97523	2.37676	-3.27025
H	-3.16529	1.10430	-3.62881
C	-4.60837	1.29377	-1.27259
H	-5.33073	2.04544	-1.60892
H	-4.81154	0.35668	-1.79566
C	-3.17323	1.77322	-1.55666
H	-2.98508	2.88908	0.31224
H	-1.90489	3.46156	-0.96757
H	-3.63427	3.83384	-1.04497
H	0.73520	-3.97774	-2.19743
H	-4.76425	1.16509	-0.19055
H	-3.69567	2.78887	-3.41699
C	-2.90617	3.06464	-0.76726
C	3.20044	-1.97711	-0.26807
O	4.40536	-2.22032	-0.28495
C	3.49610	0.29974	-0.97406
C	2.90139	1.18559	-2.10499
H	1.80816	1.13943	-2.09987
H	3.22903	0.81929	-3.08453
C	3.91607	1.28478	0.13460
H	3.04421	1.55353	0.74003
H	4.66847	0.84620	0.79828
H	4.40796	-0.17976	-1.34511
C	4.41543	2.49920	-0.66039
C	3.39681	2.62997	-1.81676
H	5.41762	2.29108	-1.05898
H	4.48453	3.40949	-0.05572
H	3.83176	3.10878	-2.70057
H	2.55830	3.25506	-1.49358
C	-0.76867	-2.49631	1.42901
O	-1.77823	-2.87693	2.06494
C	-1.55868	0.51883	2.64416
H	-1.68263	0.80269	1.59460
H	-2.51239	0.11213	3.01096
C	0.78434	0.22810	3.30861
H	1.51155	-0.43133	3.79450
H	1.29098	0.72858	2.47687
H	-0.74562	-1.26679	3.55076
C	-1.10175	1.73900	3.49037
C	0.15545	1.26150	4.25213
H	0.83345	2.08441	4.49942
H	-0.13226	0.77658	5.19491
H	-0.83701	2.57019	2.83033
H	-1.88529	2.09996	4.16498
N	0.48540	1.39244	0.14876
C	0.56357	2.55816	0.39888
S	0.64930	4.12579	0.73784

[6]FeH1CYPOH
Charge: 0
Energy: -2046763.1747696

O	0.32206	1.37587	0.76118
Fe	0.78172	-0.25650	-0.06576
N	1.29893	-2.28186	-0.98515
C	2.71084	-2.48558	-0.63705
C	1.07915	-1.98650	-2.41492
C	0.37686	-3.28109	-0.42772
H	1.85197	-1.27228	-2.71020
H	-0.30292	-3.65420	-1.19913
H	0.92182	-4.15842	-0.05774
H	2.75266	-2.89420	0.37763
H	3.21168	-3.19327	-1.31194
C	-0.29712	-1.35387	-2.62039
H	-1.08213	-2.12406	-2.55011
H	-0.36579	-0.97143	-3.64781
N	2.72405	-0.06053	-0.46180
N	-0.00528	-1.59606	1.28198
C	-0.62304	-1.17554	2.54392
N	-0.49672	-0.28726	-1.64281
C	-1.73822	0.29899	-1.69685
O	-2.68952	-0.17686	-2.37163
K	-3.21086	-1.78760	-0.20351
N	-1.91236	1.38970	-0.88401
H	-1.09071	1.69046	-0.35314
C	-3.28158	2.88768	-2.30077
H	-2.38987	3.44639	-2.60617
H	-3.45771	2.08960	-3.02619
C	-4.35600	1.55357	-0.44832
H	-5.20246	2.24773	-0.39888
H	-4.60313	0.76584	-1.16567
C	-3.07571	2.28962	-0.89623
H	-2.59391	2.99167	1.11552
H	-1.85631	3.95212	-0.18145
H	-3.58835	4.11832	0.16403
H	1.18883	-2.89213	-3.03269
H	-4.21763	1.12779	0.55513
H	-4.13792	3.57270	-2.30870

C	-2.75920	3.40491	0.11381
C	3.49867	-1.16938	-0.63116
O	4.72433	-1.20640	-0.75100
C	3.42967	1.22103	-0.49459
C	2.66434	2.34659	-1.25980
H	1.62283	2.06416	-1.43851
H	3.12312	2.50745	-2.24144
C	3.73432	1.80951	0.90208
H	2.88440	1.62580	1.57454
H	4.61065	1.33714	1.35685
H	4.38986	1.04552	-0.98965
C	3.89627	3.31149	0.63278
C	2.76740	3.61558	-0.37459
H	4.87298	3.49907	0.16693
H	3.84271	3.92697	1.53792
H	2.94691	4.52736	-0.95394
H	1.82372	3.77407	0.16697
C	-0.45866	-2.73273	0.73551
O	-1.48332	-3.37477	1.07265
C	-1.82954	-0.18590	2.40974
H	-1.89735	0.20244	1.38934
H	-2.76817	-0.70187	2.66167
C	0.38137	-0.45115	3.46264
H	1.02602	-1.15390	4.00139
H	1.01551	0.19503	2.84705
H	-0.98056	-2.07972	3.04945
C	-1.55350	0.97361	3.39591
C	-0.50435	0.40931	4.37312
H	0.05231	1.19192	4.90044
H	-0.98976	-0.21793	5.13417
H	-1.11154	1.80289	2.83476
H	-2.45762	1.33859	3.89593
H	1.01706	2.01421	0.97035

[6]FeH1CYPOHK
Charge: 0
Energy: -2046763.1732071

Fe	0.78155	-0.25642	-0.06557
N	1.30004	-2.28041	-0.98721
C	2.71205	-2.48368	-0.63933
C	1.08015	-1.98361	-2.41668
C	0.37859	-3.28090	-0.43102
H	1.85260	-1.26868	-2.71118
H	-0.30063	-3.65390	-1.20299
H	0.92417	-4.15809	-0.06162
H	2.75411	-2.89292	0.37510
H	3.21324	-3.19065	-1.31471
C	-0.29640	-1.35143	-2.62162
H	-1.08103	-2.12217	-2.55255
H	-0.36504	-0.96780	-3.64861
N	2.72376	-0.05887	-0.46164
N	-0.00517	-1.59799	1.28038
C	-0.62305	-1.17940	2.54287
N	-0.49671	-0.28611	-1.64281
C	-1.73803	0.30047	-1.69722
O	-2.68878	-0.17418	-2.37354
K	-3.20865	-1.78715	-0.20585
N	-1.91276	1.38981	-0.88257
H	-1.09126	1.69001	-0.35124
C	-3.28027	2.89053	-2.29819
H	-2.38812	3.44947	-2.60186
H	-3.45599	2.09372	-3.02511
C	-4.35669	1.55348	-0.44900
H	-5.20314	2.24763	-0.39940
H	-4.60314	0.76682	-1.16775
C	-3.07586	2.29009	-0.89446
H	-2.59561	2.98859	1.11889
H	-1.85683	3.95119	-0.17580
H	-3.58913	4.11702	0.16853
H	1.19030	-2.88852	-3.03541
H	-4.21939	1.12621	0.55397
H	-4.13639	3.57584	-2.30576
C	-2.76003	3.40359	0.11775
C	3.49908	-1.16701	-0.63261
O	4.72467	-1.20305	-0.75333
C	3.42841	1.22325	-0.49359
C	2.66179	2.34902	-1.25722
H	1.62055	2.06574	-1.43622
H	3.12035	2.51162	-2.23868
C	3.73347	1.81056	0.90350
H	2.88427	1.62508	1.57639
H	4.61069	1.33869	1.35709
H	4.38841	1.04892	-0.98944
C	3.89349	3.31305	0.63586
C	2.76371	3.61700	-0.37052
H	4.86972	3.50233	0.16968
H	3.83973	3.92740	1.54175
H	2.94178	4.52970	-0.94887
H	1.82012	3.77367	0.17171
C	-0.45772	-2.73435	0.73251
O	-1.48214	-3.37730	1.06860
C	-1.82963	-0.18970	2.41022
H	-1.89704	0.20077	1.39062
H	-2.76832	-0.70630	2.66062
C	0.38125	-0.45627	3.46270
H	1.02626	-1.15973	4.00010
H	1.01503	0.19122	2.84812
H	-0.98048	-2.08435	3.04711
C	-1.55415	0.96794	3.39878
C	-0.50467	0.40224	4.37483
H	0.05178	1.18410	4.90350
H	-0.98974	-0.22656	5.13482
H	-1.11266	1.79860	2.83928
H	-2.45844	1.33145	3.89955
O	0.32127	1.37453	0.76374
H	1.01631	2.01234	0.97438

[6]FeH3BueaBrK
Charge: 0
Energy: -3685548.6153030

Fe	0.19443	-0.36946	0.50434
N	-1.61454	-0.03409	1.21010
C	-2.83736	-0.45395	0.71453
N	-2.78628	-1.59012	-0.03532
C	-3.84033	-2.06075	-0.95851
C	-3.22685	-3.23495	-1.73687
N	0.47064	-0.63312	2.92894
C	1.51324	0.35439	3.26360
C	2.35727	0.62900	2.01450
N	1.48676	1.06012	0.91302
C	1.22982	2.41182	0.89219
N	0.51140	2.83666	-0.25314
C	0.69461	4.22743	-0.75949
C	0.01291	5.22934	0.18684
N	0.70528	-2.24314	0.61420
C	2.00564	-2.55321	0.19046
N	2.26879	-2.10664	-1.07759
C	3.61510	-1.94731	-1.65767
C	4.46990	-1.04481	-0.74695
C	0.89060	-2.04161	3.05687
C	0.32097	-2.85720	1.88603
C	-0.85699	-0.33274	3.48746
C	-1.61111	0.59960	2.52921
O	2.83521	-3.13909	0.89720
O	1.57164	3.20470	1.77613
O	-3.89535	0.19331	0.89224
C	2.19012	4.57109	-0.91325
C	0.02638	4.28419	-2.14456
C	-5.05945	-2.53133	-0.14680
C	-4.24716	-0.94793	-1.94466
C	3.41960	-1.27014	-3.02284
C	4.28301	-3.32251	-1.83847
K	-2.45960	2.25133	-0.38742
H	-1.42033	-1.26734	3.56518
H	1.03531	1.29294	3.55512
H	2.13120	0.00880	4.10620
H	3.11102	1.39190	2.23264
H	2.87109	-0.28576	1.70082
H	1.97850	-2.09036	2.98654
H	0.58799	-2.45998	4.02961
H	-1.09004	1.56849	2.49471
H	-2.63354	0.77578	2.88225
H	0.69041	-3.88655	1.94622
H	-0.77419	-2.87242	1.93338
H	1.48940	-1.72373	-1.59869
H	-1.86809	-2.00158	-0.15516
H	0.63953	2.15514	-1.00072
H	2.67531	3.85973	-1.59213
H	2.31416	5.57823	-1.32784
H	-4.77620	-3.34757	0.52717
H	0.11725	6.24882	-0.20171
H	-5.45146	-1.70527	0.45147
H	-4.97573	-1.33337	-2.66700
H	-4.71081	-0.11713	-1.40474
H	-1.05867	4.11643	-2.08358
H	-2.35831	-2.90461	-2.31885
H	-2.90792	-4.03204	-1.05421
H	-3.96440	-3.65579	-2.42762
H	0.44228	3.53313	-2.82572
H	0.17211	5.27198	-2.59318
H	2.80113	-1.88955	-3.68333
H	2.92948	-0.29592	-2.91195
H	4.38961	-1.11820	-3.50746
H	3.68013	-3.95332	-2.50159
H	5.27891	-3.20518	-2.28257
H	4.37760	-3.82287	-0.87265
H	5.45819	-0.87952	-1.19155
H	3.97846	-0.07442	-0.61075
H	0.45548	5.17236	1.18155
H	-1.06312	5.01715	0.27446
H	-0.77777	0.09996	4.49680
H	4.60287	-1.51254	0.23195
H	-3.36914	-0.59017	-2.49320
H	-5.84767	-2.89345	-0.81749
H	2.69055	4.52744	0.05619
Br	-0.39027	0.02233	-2.08617

^{6}FeH3BueaClK
Charge: 0
Energy: -2359019.6506622

Fe	-0.29518	-0.99772	0.08903
N	1.51928	-1.74973	-0.42042
C	2.76193	-1.35426	0.04618
N	2.90044	-1.31539	1.39968
C	3.95323	-0.56165	2.11601
C	3.57136	-0.60192	3.60429
N	-0.85034	-2.47954	-1.71124
C	-1.21766	-1.57341	-2.81732
C	-1.82591	-0.29181	-2.24552
N	-0.90108	0.33615	-1.29482
C	-0.35596	1.52193	-1.70162
N	0.42230	2.17491	-0.72320
C	0.46113	3.66438	-0.65827
C	1.30062	4.24340	-1.81096
N	-1.81150	-1.98352	0.81811
C	-3.04374	-1.31571	0.93097
N	-2.96065	-0.15054	1.63625
C	-3.95848	0.93395	1.59793
C	-4.20712	1.37175	0.14125
C	-1.97891	-3.29924	-1.21887
C	-1.91656	-3.34855	0.31294
C	0.37223	-3.25964	-1.94249
C	1.59416	-2.37636	-1.74182
O	-4.08895	-1.74067	0.41929
O	-0.43480	1.99000	-2.85384
O	3.70900	-1.06303	-0.72877
C	-0.96471	4.24579	-0.70357
C	1.12677	4.00897	0.68372
C	5.31452	-1.24476	1.90160
C	4.00285	0.90508	1.63991
C	-3.35209	2.10122	2.39244
C	-5.27083	0.47055	2.25465
K	2.58547	0.93012	-2.03878
H	0.40248	-4.06178	-1.19945
H	-0.31255	-1.31343	-3.37435
H	-1.90774	-2.06945	-3.51723
H	-2.06415	0.40013	-3.05759
H	-2.75244	-0.53308	-1.71299
H	-2.91694	-2.81300	-1.48898
H	-1.96234	-4.30151	-1.67339
H	1.63238	-1.63964	-2.56657
H	2.50794	-2.97360	-1.84040
H	-2.80957	-3.84808	0.70297
H	-1.03029	-3.90243	0.64480
H	-2.05118	0.07223	2.02424
H	2.03694	-1.44678	1.90996
H	0.25588	1.78114	0.20212
H	-1.56744	3.83773	0.11575
H	-0.94270	5.33701	-0.60189
H	5.28541	-2.27390	2.27617
H	1.32809	5.33682	-1.74572
H	5.56125	-1.26961	0.83805
H	4.70704	1.48096	2.25114
H	4.34368	0.95105	0.60084
H	2.13354	3.57793	0.74569
H	2.60957	-0.10582	3.77527
H	3.49860	-1.63769	3.95668
H	4.33479	-0.09271	4.20153
H	0.54541	3.61990	1.52718
H	1.20996	5.09520	0.79590
H	-3.15201	1.80865	3.42995
H	-2.40696	2.43072	1.94420
H	-4.04415	2.94957	2.40249
H	-5.09284	0.18124	3.29652
H	-6.01011	1.28060	2.24008
H	-5.67295	-0.39121	1.71794
H	-4.90249	2.21871	0.10993
H	-3.26401	1.67179	-0.32884
H	0.87837	3.95497	-2.77519
H	2.34356	3.89593	-1.74659
H	0.37333	-3.72163	-2.94348
H	-4.63710	0.54723	-0.43284
H	3.01111	1.36188	1.72237
H	6.09962	-0.70159	2.44133
H	-1.44936	3.99323	-1.65057
Cl	0.26405	0.40152	1.99366

^{6}FeH3BueaFK
Charge: 0
Energy: -2132899.3100982

Fe	0.55391	-0.98715	-0.37209
N	-1.18860	-2.00998	-0.29895
C	-2.43844	-1.52849	-0.63672
N	-2.46995	-0.58483	-1.62311
C	-3.67910	0.09556	-2.11226
C	-3.19596	1.10685	-3.16488
N	1.16237	-2.77158	0.99348
C	1.13839	-2.22981	2.36790
C	1.54055	-0.75027	2.35561
N	0.74011	-0.00700	1.38427
C	-0.07973	0.96431	1.87271
N	-0.75330	1.71299	0.89499
C	-1.06500	3.15122	1.11580
C	-2.27065	3.30688	2.06135
N	2.25298	-1.49803	-1.18671
C	3.29208	-0.56244	-1.09455
N	2.92573	0.69207	-1.51532
C	3.60931	1.92813	-1.08955
C	3.70485	1.98384	0.44858
C	2.51463	-3.17998	0.54620
C	2.65538	-2.87875	-0.95043
C	0.13613	-3.79192	0.71957
C	-1.24452	-3.15543	0.60533
O	4.41874	-0.84224	-0.66488
O	-0.33288	1.14867	3.08612
O	-3.48199	-1.89977	-0.03819
C	0.15199	3.89884	1.69472
C	-1.41799	3.73150	-0.26293
C	-4.63212	-0.92570	-2.75896
C	-4.40917	0.84875	-0.97912
C	2.73939	3.08876	-1.59685
C	5.00960	2.00355	-1.72156
K	-2.71852	-0.22052	2.01131
H	0.38488	-4.25434	-0.23953
H	0.11771	-2.31513	2.75333
H	1.79083	-2.81751	3.03232
H	1.42292	-0.32742	3.35773
H	2.59531	-0.65841	2.06680
H	3.25265	-2.56752	1.06815
H	2.70381	-4.23733	0.78966
H	-1.59781	-2.87464	1.61582
H	-1.96506	-3.90368	0.25447
H	3.69205	-3.04509	-1.25918
H	2.00630	-3.53489	-1.54294
H	1.95159	0.79333	-1.78349
H	-1.57392	-0.18930	-1.89827
H	-0.41601	1.51689	-0.04892
H	1.01318	3.80138	1.02506
H	-0.07200	4.96549	1.81235
H	-4.13338	-1.43060	-3.59334
H	-2.51261	4.36627	2.20309
H	-4.93063	-1.67756	-2.02459
H	-5.24373	1.43502	-1.38007
H	-4.80996	0.13454	-0.25438
H	-2.26949	3.20600	-0.70833
H	-2.50031	1.83096	-2.72436
H	-2.67904	0.59482	-3.98446
H	-4.04549	1.65522	-3.58467
H	-0.57146	3.65157	-0.95455
H	-1.68030	4.79065	-0.17074
H	2.64837	3.06178	-2.68919
H	1.73135	3.03287	-1.16827
H	3.18064	4.04936	-1.31143
H	4.93405	1.98332	-2.81462
H	5.51241	2.93189	-1.42376
H	5.60977	1.15040	-1.39938
H	4.15632	2.92864	0.77395
H	2.70692	1.89607	0.89211
H	-2.04310	2.86901	3.03631
H	-3.16200	2.82603	1.63271
H	0.14094	-4.58350	1.48657
H	4.31988	1.15841	0.81633
H	-3.72044	1.54097	-0.47964
H	-5.52916	-0.42471	-3.14247
H	0.42360	3.48907	2.67084
F	0.05961	0.49068	-1.48582

^{6}FeH3BueaN_3K
Charge: 0
Energy: -2173279.2197487

Fe	-0.33760	-0.99910	0.11778
N	1.45541	-1.80967	-0.34088
C	2.68409	-1.28946	0.02630
N	2.87106	-1.11615	1.36202
C	4.03871	-0.47266	2.00025
C	3.79271	-0.51731	3.51659
N	-0.93035	-2.66407	-1.50903
C	-1.31353	-1.89633	-2.71007
C	-1.91245	-0.55344	-2.28995
N	-0.98263	0.16483	-1.41591
C	-0.47139	1.32611	-1.91671
N	0.34102	2.03929	-1.00796
C	0.38729	3.52778	-1.02679
C	1.20903	4.03106	-2.22711
N	-1.80971	-1.94237	1.00570
C	-3.02634	-1.26000	1.13218
N	-2.89214	-0.02973	1.72402
C	-3.85414	1.07881	1.58241
C	-4.14118	1.35240	0.09301
C	-2.05458	-3.41830	-0.91294
C	-1.94504	-3.34073	0.61363

C	0.28656	-3.47090	-1.67126
C	1.51436	-2.57500	-1.58529
O	-4.10903	-1.71796	0.74310
O	-0.59269	1.72497	-3.09263
O	3.57807	-1.00469	-0.81169
C	-1.03294	4.12137	-1.08091
C	1.08378	3.94069	0.28033
C	5.31973	-1.25998	1.66476
C	4.16679	0.99053	1.53308
C	-3.17963	2.30656	2.21484
C	-5.15511	0.74415	2.33169
K	2.40314	0.70387	-2.41384
H	0.32606	-4.18806	-0.84655
H	-0.41553	-1.70826	-3.30691
H	-2.01233	-2.47189	-3.33701
H	-2.14587	0.04388	-3.17567
H	-2.84249	-0.72478	-1.73490
H	-2.99201	-2.93560	-1.19339
H	-2.07253	-4.45472	-1.28466
H	1.54343	-1.93407	-2.48678
H	2.42549	-3.18426	-1.63061
H	-2.83179	-3.79452	1.06851
H	-1.05733	-3.88090	0.96430
H	-1.93941	0.23213	1.94505
H	2.09383	-1.38155	1.95027
H	0.20298	1.68857	-0.06081
H	-1.62608	3.77024	-0.22932
H	-0.99758	5.21631	-1.04411
H	5.23149	-2.29415	2.01635
H	1.24331	5.12614	-2.23154
H	5.49006	-1.27270	0.58672
H	5.01963	1.47236	2.02469
H	4.33134	1.02445	0.45222
H	2.08089	3.48924	0.35422
H	2.90101	0.05346	3.79463
H	3.67641	-1.55257	3.86036
H	4.64794	-0.08254	4.04372
H	0.50979	3.62697	1.16028
H	1.19570	5.02906	0.32401
H	-2.94534	2.12647	3.27069
H	-2.24535	2.55052	1.69320
H	-3.84006	3.17751	2.15348
H	-4.94868	0.57479	3.39444
H	-5.86970	1.57144	2.24266
H	-5.60074	-0.16179	1.91574
H	-4.80861	2.21500	-0.01852
H	-3.20645	1.55749	-0.44038
H	0.76456	3.68699	-3.16322
H	2.25080	3.68094	-2.16022
H	0.27280	-4.03920	-2.61589
H	-4.61848	0.48153	-0.36359
H	3.26428	1.55690	1.78406
H	6.18291	-0.80015	2.16012
H	-1.53688	3.81799	-2.00246
N	0.14907	0.39667	1.46159
N	0.59195	0.99681	2.40357
N	1.00994	1.60493	3.29532

^{6}FeH3BueaNCSK
Charge: 0
Energy: -2378390.3097504

Fe	0.38636	-1.01152	-0.36050
N	-1.36959	-1.99558	-0.19958
C	-2.62640	-1.46414	-0.43199
N	-2.79522	-0.86206	-1.64109
C	-3.92435	0.02032	-2.00677
C	-3.63578	0.52953	-3.42780
N	1.05436	-3.07027	0.66540
C	1.40416	-2.69080	2.04868
C	1.94311	-1.25901	2.06380
N	0.97716	-0.34334	1.44867
C	0.35776	0.52360	2.30034
N	-0.48035	1.46967	1.66783
C	-0.60055	2.85428	2.21542
C	-1.44169	2.86259	3.50451
N	1.90694	-1.55165	-1.46690
C	3.09133	-0.81546	-1.30394
N	2.90575	0.52961	-1.46376
C	3.83091	1.57979	-0.99987
C	4.13382	1.39147	0.49917
C	2.20959	-3.55514	-0.12181
C	2.10480	-2.99508	-1.54580
C	-0.12465	-3.94014	0.55414
C	-1.39325	-3.11914	0.73626
O	4.18097	-1.33131	-1.02285
O	0.41730	0.47778	3.54493
O	-3.55791	-1.54496	0.40902
C	0.79271	3.44822	2.49504
C	-1.31783	3.67835	1.13542
C	-5.23690	-0.78349	-2.00593
C	-4.01818	1.21255	-1.03374
C	3.10484	2.91591	-1.21830
C	5.12948	1.53794	-1.82450
K	-2.52274	-0.31776	2.48484
H	-0.13246	-4.36500	-0.45366
H	0.49938	-2.72986	2.66284
H	2.12849	-3.39948	2.47926
H	2.15804	-0.95389	3.09145
H	2.87315	-1.21057	1.48638
H	3.12726	-3.15867	0.31443
H	2.26275	-4.65456	-0.10433
H	-1.45419	-2.79826	1.79349
H	-2.27443	-3.75035	0.57078
H	3.01380	-3.24027	-2.10516
H	1.24354	-3.42731	-2.06868
H	1.97539	0.81763	-1.73170
H	-1.95011	-0.76042	-2.18696
H	-0.30677	1.49129	0.66555
H	1.39712	3.44761	1.58105
H	0.70929	4.48261	2.84760
H	-5.17076	-1.61572	-2.71543
H	-1.52649	3.88421	3.89088
H	-5.43732	-1.18968	-1.01299
H	-4.81205	1.90041	-1.34565
H	-4.25541	0.85489	-0.02683
H	-2.29441	3.24253	0.89154
H	-2.72267	1.13298	-3.46301
H	-3.53240	-0.31055	-4.12481
H	-4.46294	1.15769	-3.77357
H	-0.73536	3.73025	0.20909
H	-1.47882	4.70240	1.48850
H	2.84749	3.06181	-2.27354
H	2.17566	2.95750	-0.63725
H	3.74246	3.74768	-0.90205
H	4.91104	1.69793	-2.88629
H	5.81860	2.32241	-1.48929
H	5.61207	0.56484	-1.71028
H	4.77324	2.20391	0.86342
H	3.20168	1.39053	1.07491
H	-0.98321	2.23184	4.26819
H	-2.46730	2.51602	3.30299
H	-0.08165	-4.77338	1.27461
H	4.64823	0.44176	0.66531
H	-3.07423	1.76604	-1.01030
H	-6.07044	-0.13806	-2.30714
H	1.31288	2.86085	3.25672
N	-0.21655	0.71578	-1.28964
C	-0.38631	1.71518	-1.92103
S	-0.61885	3.07901	-2.74702

^{6}FeH3BueaOH
Charge: 0
Energy: -2117804.6662446

O	0.12015	0.38203	1.37309
Fe	-0.31307	-0.97605	0.09240
N	1.51951	-1.84924	-0.25410
C	2.67123	-1.26032	0.18574
N	2.68551	-1.00985	1.54790
C	3.80167	-0.39115	2.29198
C	3.33521	-0.29445	3.75375
N	-0.81130	-2.58192	-1.62622
C	-1.10116	-1.78367	-2.83264
C	-1.69662	-0.43292	-2.43370
N	-0.82851	0.22692	-1.45976
C	-0.40515	1.48718	-1.78979
N	0.32671	2.13520	-0.78034
C	0.35853	3.61626	-0.68558
C	1.23681	4.21591	-1.80004
N	-1.76166	-1.99022	0.92365
C	-2.94027	-1.28572	1.18094
N	-2.72263	-0.10416	1.85243
C	-3.62837	1.05712	1.76103
C	-3.89583	1.40872	0.28335
C	-1.99091	-3.31365	-1.11360
C	-1.94477	-3.34395	0.41778
C	0.39787	-3.41065	-1.73364
C	1.64158	-2.54900	-1.52930
O	-4.05982	-1.68033	0.82766
O	-0.53475	2.01065	-2.91603
O	3.62591	-0.91882	-0.55508
C	-1.06093	4.21118	-0.76476
C	0.98156	3.93689	0.68292
C	5.07464	-1.25175	2.19401
C	4.06116	1.02529	1.74617
C	-2.89595	2.22158	2.44674
C	-4.94861	0.76141	2.49259
K	2.44903	0.84904	-2.15277
H	0.36573	-4.15909	-0.93711
H	-0.16072	-1.60774	-3.36570
H	-1.76830	-2.33229	-3.51652
H	-1.82919	0.19343	-3.32057
H	-2.68336	-0.58584	-1.97619
H	-2.88936	-2.76043	-1.39516
H	-2.05198	-4.32130	-1.55596
H	1.74063	-1.86250	-2.39095
H	2.54105	-3.17811	-1.55076

H	-2.87366	-3.78114	0.79851
H	-1.10389	-3.95850	0.76394
H	-1.74444	0.11796	2.02654
H	2.08177	-1.62795	2.07634
H	0.20400	1.67260	0.13244
H	-1.68933	3.80329	0.03375
H	-1.03052	5.30175	-0.65485
H	4.89612	-2.24800	2.61543
H	1.27045	5.30818	-1.71609
H	5.37036	-1.36296	1.14820
H	4.80329	1.53924	2.36693
H	4.43987	0.97485	0.72298
H	1.99249	3.51696	0.76092
H	2.42502	0.31111	3.83841
H	3.12685	-1.28885	4.16862
H	4.11372	0.16671	4.36964
H	0.37889	3.52038	1.49805
H	1.04992	5.02058	0.82603
H	-2.70016	1.99154	3.50090
H	-1.93436	2.41682	1.95743
H	-3.50175	3.13284	2.39999
H	-4.75392	0.52859	3.54569
H	-5.61406	1.63247	2.44529
H	-5.44423	-0.09651	2.03430
H	-4.52098	2.30609	0.20330
H	-2.95012	1.58996	-0.23883
H	0.83865	3.94740	-2.78057
H	2.27440	3.85664	-1.71183
H	0.44069	-3.94401	-2.69767
H	-4.41036	0.58051	-0.21146
H	3.13581	1.61331	1.75718
H	5.89731	-0.78779	2.75094
H	-1.52028	3.96820	-1.72612
H	1.02080	0.25581	1.71884

^{6}FeH3BueaOHK
Charge: 0
Energy: -2117807.3291814

Fe	0.47074	-1.01417	-0.42929
N	-1.29879	-2.00075	-0.21016
C	-2.55721	-1.50428	-0.49521
N	-2.62540	-0.59623	-1.51192
C	-3.84343	0.09761	-1.95338
C	-3.40581	1.03510	-3.09127
N	1.08961	-2.77315	1.00090
C	1.11922	-2.16150	2.34426
C	1.56133	-0.69638	2.25070
N	0.75814	0.03240	1.26981
C	0.00876	1.07118	1.73097
N	-0.63590	1.81412	0.73477
C	-0.94739	3.25585	0.92208
C	-2.15718	3.43683	1.85848
N	2.19633	-1.55672	-1.21400
C	3.28028	-0.68348	-1.07820
N	2.99383	0.61674	-1.43557
C	3.79033	1.77815	-0.99438
C	3.89508	1.80838	0.54350
C	2.41468	-3.23591	0.53052
C	2.52877	-2.95658	-0.97295
C	0.03272	-3.77795	0.80806
C	-1.33772	-3.11650	0.73147
O	4.39640	-1.04577	-0.68186
O	-0.21162	1.31842	2.94055
O	-3.57170	-1.82993	0.17733
C	0.26500	4.01722	1.49336
C	-1.29291	3.80116	-0.47270
C	-4.87273	-0.92008	-2.47721
C	-4.46729	0.93616	-0.81678
C	3.03093	3.01986	-1.48899
C	5.18896	1.73859	-1.63285
K	-2.62028	-0.06913	2.07607
H	0.23081	-4.27726	-0.14478
H	0.10855	-2.20060	2.76197
H	1.77503	-2.73096	3.02162
H	1.48500	-0.22606	3.23569
H	2.61031	-0.65086	1.93215
H	3.18941	-2.64841	1.02691
H	2.56980	-4.29718	0.78085
H	-1.64532	-2.79975	1.74614
H	-2.08643	-3.86092	0.43487
H	3.54336	-3.18714	-1.31268
H	1.82378	-3.58015	-1.53638
H	2.00669	0.81011	-1.57229
H	-1.72868	-0.21779	-1.82723
H	-0.31113	1.59412	-0.20771
H	1.13199	3.90830	0.83355
H	0.03811	5.08575	1.58614
H	-4.44804	-1.48884	-3.31159
H	-2.40040	4.49977	1.96735
H	-5.14731	-1.61879	-1.68373
H	-5.32147	1.51621	-1.18431
H	-4.82171	0.27552	-0.02008
H	-2.14281	3.26396	-0.90751
H	-2.65046	1.74960	-2.74335
H	-2.97421	0.46075	-3.91909
H	-4.26392	1.59667	-3.47488
H	-0.44280	3.69909	-1.15733
H	-1.55283	4.86299	-0.40984
H	2.94521	3.01543	-2.58200
H	2.01896	3.05326	-1.06659
H	3.55453	3.93315	-1.18771
H	5.10596	1.72527	-2.72554
H	5.76381	2.62505	-1.33805
H	5.72209	0.84119	-1.31506
H	4.44554	2.69546	0.87897
H	2.89462	1.82444	0.98995
H	-1.93043	3.03147	2.84775
H	-3.04635	2.94210	1.44329
H	0.05385	-4.54465	1.60038
H	4.42031	0.91744	0.89774
H	-3.72733	1.64123	-0.41901
H	-5.77493	-0.40637	-2.83084
H	0.52940	3.62786	2.47949
O	-0.00315	0.38360	-1.70597
H	0.36498	0.19567	-2.58504

^{6}FeH3BueaBr
Charge: -1
Energy: -2908623.2641102

C	1.53171	-0.65782	-2.26395
C	2.58727	-0.80749	-1.16752
C	-0.56101	2.95188	-0.44581
C	1.52084	2.29588	0.56386
C	-0.55689	-1.09506	2.77604
C	2.58322	-0.60027	1.29253
C	1.52891	-1.62875	1.70495
C	-0.54517	-1.86837	-2.32767
C	2.58037	1.42809	-0.11639
Fe	-0.22332	0.00153	-0.00056
H	1.73823	-1.34563	-3.09079
H	1.55083	0.36572	-2.66461
H	3.59572	-0.54260	-1.53014
H	2.60995	-1.85604	-0.85743
H	1.72283	3.35729	0.38524
H	1.53934	2.12674	1.65043
H	3.58781	1.61410	0.29452
H	2.60082	1.68570	-1.17912
H	1.73245	-2.00081	2.71457
H	1.55482	-2.48689	1.01788
H	3.59272	-1.04461	1.24793
H	2.60104	0.19271	2.04566
N	0.21953	-0.93700	-1.69201
N	2.21630	0.00628	0.00220
N	0.21391	-0.99942	1.65657
N	0.21050	1.93614	0.03320
O	-0.25332	-1.65503	3.83335
O	-0.23782	-2.50714	-3.33801
O	-0.25987	4.14826	-0.48707
H	-1.52011	-2.01050	-1.82997
H	-1.53475	2.58943	-0.81861
H	-1.53335	-0.59689	2.64728
Br	-2.74460	-0.00362	-0.00515

^{6}FeH3BueaCl
Charge: -1
Energy: -1582095.1029012

C	1.69219	-1.67030	1.26214
C	0.61516	-1.28322	2.27419
C	1.52502	2.55205	-0.93626
C	0.59977	2.30122	1.26128
C	-2.97270	0.04416	-0.93681
C	-1.41986	0.10916	2.27357
C	-2.29308	-0.63021	1.26117
C	1.44823	-2.59685	-0.93556
C	0.80344	1.17531	2.27366
Fe	0.00003	-0.00002	-0.50839
H	2.05389	-2.68518	1.46077
H	2.55685	-0.99491	1.34997
H	1.01594	-1.24060	3.30205
H	-0.16598	-2.04823	2.25093
H	1.29775	3.12205	1.45956
H	-0.41757	2.71204	1.34905
H	0.56632	1.50138	3.30145
H	1.85650	0.88140	2.25009
H	-3.35295	-0.43605	1.45932
H	-2.14045	-1.71669	1.34907
H	-1.58381	-0.25930	3.30132
H	-1.69179	1.16818	2.25022
N	1.12599	-1.58821	-0.07871
N	-0.00036	0.00033	1.89565
N	-1.93837	-0.18105	-0.07955
N	0.81175	1.76944	-0.07940
O	-4.17504	-0.08458	-0.68631
O	2.16081	-3.57367	-0.68462
O	2.01551	3.65727	-0.68553

H	0.98714	-2.45912	-1.92843
H	1.63617	2.08353	-1.92898
H	-2.62262	0.37455	-1.92958
Cl	0.00068	-0.00035	-2.82455

^{6}FeH3BueaF
Charge: -1
Energy: -1355969.8864568

C	2.33691	-0.60503	1.16244
C	1.14325	-0.85136	2.08961
C	-0.69114	2.83854	-1.16934
C	-0.64485	2.32526	1.16303
C	-2.11334	-2.01678	-1.16988
C	-1.30779	-0.56474	2.09023
C	-1.69178	-1.72126	1.16271
C	2.80377	-0.82025	-1.17021
C	0.16592	1.41489	2.08974
Fe	-0.00005	-0.00013	-0.63516
H	3.08661	-1.39327	1.30923
H	2.84154	0.34088	1.41702
H	1.42147	-0.70684	3.14891
H	0.82571	-1.89020	1.96710
H	-0.33779	3.36879	1.31027
H	-1.71630	2.28833	1.41774
H	-0.09781	1.58343	3.14917
H	1.22427	1.65933	1.96666
H	-2.74917	-1.97651	1.30993
H	-1.12468	-2.63126	1.41668
H	-1.32095	-0.87845	3.14938
H	-2.04873	0.22981	1.96887
N	1.87014	-0.58268	-0.21511
N	0.00039	-0.00030	1.71844
N	-1.43983	-1.32770	-0.21489
N	-0.43045	1.91058	-0.21472
O	-2.92534	-2.92919	-0.98135
O	4.00006	-1.06684	-0.98189
O	-1.07561	3.99780	-0.98034
H	2.37074	-0.77134	-2.18695
H	-0.51675	2.43984	-2.18632
H	-1.85504	-1.66590	-2.18663
F	-0.00024	-0.00027	-2.43494

^{6}FeH3BueaN_3
Charge: -1
Energy: -1396356.8391481

C	-2.08410	-0.51215	1.89234
C	-2.55993	-1.00727	0.52734
C	0.72324	2.88856	-0.76621
C	-1.42405	2.04741	-1.34039
C	1.59966	-2.14271	-1.44995
C	-1.83702	-0.98224	-1.82745
C	-0.75163	-2.05437	-1.75428
C	-0.02928	-0.38285	3.08002
C	-2.46309	1.12156	-0.70987
Fe	0.27853	0.05446	0.12763
H	-2.38980	-1.22341	2.66990
H	-2.56531	0.44360	2.15398
H	-3.66033	-0.96967	0.44426
H	-2.25080	-2.04933	0.41366
H	-1.75421	3.08974	-1.24958
H	-1.33013	1.85475	-2.42090
H	-3.40214	1.11163	-1.29058
H	-2.69225	1.49439	0.29158
H	-0.54954	-2.44404	-2.75983
H	-1.09079	-2.91832	-1.16102
H	-2.81553	-1.41548	-2.09962
H	-1.56052	-0.26517	-2.60450
N	-0.63482	-0.36700	1.86435
N	-1.92305	-0.24068	-0.55788
N	0.45197	-1.47261	-1.17322
N	-0.14569	1.84944	-0.66987
O	1.70221	-3.16566	-2.13428
O	-0.58885	-0.51425	4.17339
O	0.52516	3.95617	-1.35485
H	1.06709	-0.26484	3.00218
H	1.67387	2.68935	-0.23814
H	2.48769	-1.66987	-0.99214
N	2.10965	0.30742	0.70554
N	3.30896	0.31603	0.70353
N	4.46729	0.32955	0.71882

^{6}FeH3BueaNCS
Charge: -1
Energy: -1601466.2668646

C	-1.75441	2.12542	-1.14069
C	-2.66645	1.41637	-0.14109
C	0.56214	-2.48143	-1.59605
C	-1.75393	-2.05029	-1.27081
C	0.56110	-0.14308	2.94688
C	-2.66649	-0.58684	1.29596
C	-1.75499	-0.07517	2.41011
C	0.56183	2.62439	-1.34818
C	-2.66543	-0.82962	-1.15761
Fe	0.02681	0.00005	-0.00018
H	-1.89752	3.21057	-1.06689
H	-2.01868	1.85771	-2.17578
H	-3.72906	1.51054	-0.42411
H	-2.53646	1.88611	0.83697
H	-1.89652	-2.52903	-2.24752
H	-2.01919	-2.81280	-0.52177
H	-3.72831	-1.12116	-1.09925
H	-2.53351	-0.21750	-2.05317
H	-1.89822	-0.68146	3.31309
H	-2.01974	0.95506	2.69550
H	-3.72925	-0.38928	1.51874
H	-2.53596	-1.66866	1.21388
N	-0.37135	1.76606	-0.85490
N	-2.28279	-0.00005	-0.00076
N	-0.37167	-0.14278	1.95655
N	-0.37083	-1.62351	-1.10167
O	0.32972	-0.09949	4.15831
O	0.33108	3.65213	-1.99122
O	0.33076	-3.55278	-2.16319
H	1.59322	2.31028	-1.10888
H	1.59378	-2.11810	-1.44324
H	1.59272	-0.19236	2.55571
N	2.01058	0.00012	0.00008
C	3.20213	0.00015	-0.00008
S	4.81766	0.00011	-0.00034

^{6}FeH3BueaNMeBr
Charge: -1
Energy: -3086933.7137029

C	2.40026	-0.12770	1.29724
C	4.39256	-1.89163	-2.06714
C	1.30131	4.19579	0.74262
C	1.86894	-1.36560	2.05107
C	-0.01032	2.31658	1.64253
C	-4.64760	-0.53964	-0.85345
C	-1.27580	0.41646	2.35449
C	-2.54621	-1.64828	-0.24828
C	-0.26345	-2.61313	1.70488
C	-0.45305	-2.72778	0.17924
C	2.41318	-0.89508	-1.03747
C	-0.23563	-0.49965	3.02917
Fe	-0.09704	0.06309	-0.26752
H	3.50097	-0.12303	1.33991
H	2.06708	0.78030	1.80796
H	2.28761	-1.40357	3.07458
H	2.21904	-2.25625	1.51728
H	0.03178	2.87604	-0.33263
H	-1.68956	1.09449	3.11194
H	-2.09214	-0.18778	1.94702
H	-0.71231	-1.08464	3.83590
H	0.51592	0.14922	3.48541
H	-1.00371	-3.64790	-0.04954
H	0.51804	-2.76727	-0.32545
H	0.27681	-3.49395	2.09617
H	-2.68319	0.06806	-1.37040
H	-1.26110	-2.60905	2.15365
H	4.33728	-0.64378	-0.39276
N	3.75417	-1.29155	-0.90684
N	1.86870	-0.11691	-0.05733
N	0.41479	-1.36969	2.05589
N	0.30145	3.16471	0.60206
N	-3.20710	-0.55070	-0.76041
N	-1.16921	-1.56202	-0.32262
N	-0.68671	1.17393	1.25535
O	-3.16572	-2.59657	0.26097
O	1.75017	-1.27751	-2.01309
O	0.30205	2.58300	2.81722
H	-5.03055	-1.10810	-1.71714
H	-4.99585	0.49560	-0.93702
H	-5.06617	-0.99021	0.04986
H	2.29137	3.87349	0.38040
H	1.38323	4.44478	1.80271
H	1.00881	5.09354	0.18415
H	5.36129	-2.30910	-1.76870
H	4.54708	-1.18243	-2.89505
H	3.75363	-2.69395	-2.43993
Br	-0.70663	1.49878	-2.34159

^{6}FeH3BueaNMeCl
Charge: -1
Energy: -1760405.1625218

C	2.26378	0.34517	1.19919
C	4.38227	-2.51950	-1.18309
C	1.31473	4.22618	-0.91771
C	1.64618	-0.55759	2.28851
C	-0.09359	2.79181	0.50285
C	-4.60756	-0.68698	-1.26522
C	-1.44641	1.25800	1.74588
C	-2.60927	-1.55083	-0.13350

C	-0.50796	-1.81605	2.22733
C	-0.59720	-2.43663	0.81881
C	2.39509	-1.16890	-0.73317
C	-0.48062	0.61976	2.76340
Fe	-0.11520	0.03486	-0.53802
H	3.35967	0.35917	1.31632
H	1.92617	1.37503	1.34717
H	2.00416	-0.25132	3.29015
H	1.99574	-1.58098	2.11173
H	0.06640	2.62291	-1.53597
H	-1.88521	2.15791	2.19615
H	-2.25415	0.55631	1.51486
H	-1.02567	0.35716	3.68826
H	0.26432	1.37755	3.01881
H	-1.16629	-3.37247	0.87132
H	0.40471	-2.65873	0.43602
H	-0.03542	-2.52463	2.93190
H	-2.58219	-0.28843	-1.75810
H	-1.53310	-1.64393	2.56883
H	4.27043	-0.80144	0.00018
N	3.68952	-1.55397	-0.34600
N	1.82322	-0.09642	-0.11494
N	0.19637	-0.53989	2.19762
N	0.28721	3.22652	-0.75018
N	-3.18206	-0.68386	-1.04170
N	-1.22915	-1.50330	-0.10372
N	-0.77141	1.58759	0.49634
O	-3.30497	-2.27114	0.60133
O	1.79218	-1.82361	-1.59751
O	0.16309	3.44898	1.52791
H	-4.93705	-1.48319	-1.95356
H	-4.91235	0.27926	-1.68246
H	-5.11524	-0.84493	-0.31056
H	2.31055	3.78313	-1.08415
H	1.35070	4.82928	-0.00799
H	1.08334	4.87660	-1.77041
H	5.28678	-2.86063	-0.66600
H	4.66317	-2.11961	-2.16999
H	3.72072	-3.37073	-1.35226
Cl	-0.53647	0.67078	-2.79455

^{6}FeH3BueaNMeF
Charge: -1
Energy: -1534292.5446667

C	-2.55308	-1.01194	-1.43725
C	-3.92626	2.72985	1.29447
C	2.62641	3.45107	-1.04206
C	-1.89882	-2.33993	-1.05279
C	2.04253	1.13968	-1.52077
C	3.51869	0.69915	1.70762
C	1.58723	-1.18179	-1.75569
C	1.69876	-0.92649	1.90122
C	0.07029	-3.03583	0.26983
C	-0.17010	-2.39785	1.64649
C	-3.28692	0.76733	-0.00446
C	0.37378	-2.07804	-1.99089
Fe	-0.31075	0.03288	0.09509
H	-3.63817	-1.13609	-1.51312
H	-2.19249	-0.69185	-2.42841
H	-2.05189	-3.11145	-1.82796
H	-2.36572	-2.69337	-0.12853
H	0.88628	2.42612	-0.43818
H	2.15389	-1.08059	-2.68833
H	2.27008	-1.64493	-1.02624
H	0.67905	-3.08836	-2.31373
H	-0.23054	-1.63669	-2.78919
H	0.31997	-3.00796	2.41467
H	-1.24519	-2.35794	1.86292
H	-0.36980	-4.04420	0.18682
H	1.44455	1.09094	1.78747
H	1.15091	-3.12173	0.14277
H	-1.97607	1.93983	1.05270
N	-2.96197	1.70816	0.95634
N	-2.22564	-0.01383	-0.42916
N	-0.46373	-2.14375	-0.78033
N	1.62935	2.40543	-1.13352
N	2.13592	0.38494	2.02416
N	0.34216	-1.03535	1.64874
N	1.13452	0.12413	-1.28364
O	2.47458	-1.88824	2.02304
O	-4.45585	0.64540	-0.40642
O	3.14854	0.96943	-2.06192
H	3.77896	1.67327	2.13766
H	3.71058	0.72982	0.62431
H	4.15862	-0.06701	2.15048
H	2.12288	4.41758	-0.92698
H	3.22336	3.46376	-1.95694
H	3.32185	3.31678	-0.19579
H	-4.03671	3.50259	0.51413
H	-3.61866	3.22045	2.22496
H	-4.90686	2.26959	1.43898
F	-0.16408	1.78494	0.85256

^{6}FeH3BueaNMeN$_3$
Charge: -1
Energy: -1574650.7035337

C	1.13891	2.88146	-0.47454
C	3.67765	-0.61310	-2.61102
C	-5.10111	-1.78195	-0.83305
C	0.54110	2.96272	0.93266
C	-2.92496	-0.75503	-0.40375
C	2.89698	-2.63129	3.10273
C	-2.85584	1.62495	-0.00356
C	1.44931	-1.24936	1.69603
C	-0.94477	1.52882	2.32178
C	0.11113	0.48903	2.73079
C	2.35666	1.22329	-1.66787
C	-1.81109	2.69746	0.33415
Fe	-0.13475	0.17805	-0.26344
H	2.10532	3.40174	-0.49292
H	0.50512	3.42179	-1.19851
H	0.30995	4.00440	1.22373
H	1.27874	2.56921	1.63577
H	-4.60896	0.22986	-1.04812
H	-3.47339	2.03185	-0.82908
H	-3.55084	1.48818	0.84210
H	-2.26579	3.51244	0.92802
H	-1.44387	3.13790	-0.59605
H	-0.31584	-0.05538	3.59608
H	1.01728	0.99115	3.11053
H	-1.04144	2.30384	3.10456
H	1.29332	-1.45162	3.72897
H	-1.90277	1.01282	2.23450
H	2.45023	-0.67874	-0.88873
N	2.88966	-0.03806	-1.54745
N	1.29412	1.47740	-0.80966
N	-0.65281	2.11142	1.00893
N	-4.32687	-0.59035	-0.52479
N	1.96697	-1.52095	2.97650
N	0.42033	-0.37285	1.60879
N	-2.17879	0.38808	-0.33400
O	1.97370	-1.79431	0.70694
O	2.83548	2.07505	-2.43615
O	-2.46045	-1.89596	-0.32347
H	2.43153	-3.61244	2.92150
H	3.33281	-2.62192	4.10895
H	3.69136	-2.50624	2.36508
H	-6.16971	-1.54142	-0.77454
H	-4.86468	-2.55360	-0.09813
H	-4.88042	-2.20192	-1.82673
H	3.06102	-1.17671	-3.33071
H	4.42909	-1.29663	-2.19725
H	4.18216	0.19658	-3.14367
N	0.07589	-1.14115	-1.66311
N	0.09249	-2.33979	-1.76679
N	0.12466	-3.48442	-1.92708

^{6}FeH3BueaNMeNCS
Charge: -1
Energy: -1779760.9156120

C	-1.23906	-1.21688	-2.62828
C	-3.59389	2.42270	-0.51114
C	4.97978	1.39678	1.26528
C	-0.57827	-2.48479	-2.08689
C	2.85528	0.44472	0.53173
C	-2.78475	-1.76881	3.88669
C	2.80475	-0.94115	-1.46005
C	-1.34347	-1.20481	1.99091
C	0.99691	-3.02523	-0.24240
C	-0.01625	-2.93506	0.91044
C	-2.39767	0.64186	-1.69889
C	1.75314	-1.76279	-2.22137
Fe	0.11664	-0.12201	-0.18791
H	-2.22204	-1.46517	-3.04934
H	-0.66058	-0.80079	-3.46992
H	-0.35538	-3.20994	-2.89056
H	-1.27109	-2.95679	-1.38662
H	4.49658	0.74123	-0.65336
H	3.36713	-0.35559	-2.21284
H	3.54666	-1.60610	-0.98734
H	2.21164	-2.65270	-2.68980
H	1.33604	-1.14840	-3.02293
H	0.44929	-3.44429	1.77650
H	-0.92461	-3.51458	0.67188
H	1.09984	-4.07040	-0.58600
H	-1.20547	-2.90427	3.12090
H	1.96483	-2.69391	0.13778
H	-2.43832	0.86584	0.33929
N	-2.88706	1.15972	-0.52645
N	-1.36313	-0.27782	-1.52787
N	0.63676	-2.12443	-1.34389
N	4.24339	0.57741	0.31396
N	-1.86671	-2.19071	2.84118
N	-0.32990	-1.54728	1.16649
N	2.12731	-0.12776	-0.47476

O	-1.84287	-0.06215	1.99360
O	-2.87387	0.92355	-2.80962
O	2.36428	0.80057	1.60659
H	-2.29931	-1.17963	4.67994
H	-3.25264	-2.65361	4.33399
H	-3.55638	-1.14140	3.43783
H	6.05214	1.31999	1.04997
H	4.78769	1.02247	2.27260
H	4.68096	2.45539	1.24716
H	-2.91698	3.26767	-0.31522
H	-4.37033	2.41221	0.26382
H	-4.06460	2.56336	-1.48667
N	-0.03517	1.84242	0.12465
C	-0.03463	3.02169	0.23730
S	-0.04735	4.64474	0.38294

^{6}FeH3BueaNMeOH
Charge: -1
Energy: -1519197.7822388

C	-1.49753	2.21594	-0.17494
C	-4.02655	-1.47779	-1.87933
C	-3.11211	-1.39325	1.86046
C	-0.13261	2.88694	-0.29353
C	-0.84735	-0.53319	2.22250
C	3.48922	-2.83210	0.38566
C	1.30798	0.51412	2.14470
C	3.00259	-0.77684	-0.84324
C	2.23741	2.20641	-0.41398
C	2.30543	1.34259	-1.68289
C	-2.71601	0.43850	-1.16262
C	0.98868	1.95274	1.70818
Fe	0.18372	-0.17400	-0.41775
H	-2.25610	2.85030	-0.64761
H	-1.78797	2.12529	0.88349
H	-0.13265	3.87077	0.20909
H	0.07768	3.05376	-1.35523
H	-1.34773	-1.96409	0.84708
H	1.27972	0.45811	3.23975
H	2.31265	0.23295	1.80518
H	1.71913	2.67855	2.10485
H	0.00608	2.20005	2.11451
H	3.31279	1.40556	-2.11114
H	1.58635	1.70834	-2.42717
H	2.42918	3.27375	-0.62152
H	1.68410	-2.31291	-0.55965
H	3.01806	1.84507	0.25929
H	-1.93545	-1.40386	-1.57147
N	-2.74713	-0.81176	-1.76067
N	-1.45895	0.89946	-0.81028
N	0.92863	2.01875	0.23531
N	-1.67409	-1.52126	1.70041
N	2.68123	-2.10310	-0.57147
N	1.95513	-0.03202	-1.35065
N	0.35365	-0.41419	1.55126
O	4.15050	-0.34042	-0.65075
O	-3.76551	1.08187	-0.98754
O	-1.18779	0.14657	3.20324
O	-0.27540	-1.98290	-0.99773
H	3.35187	-3.90991	0.23977
H	3.23193	-2.58803	1.42961
H	4.53861	-2.57890	0.22274
H	-3.54776	-0.62671	1.20214
H	-3.32346	-1.11772	2.89602
H	-3.58885	-2.35559	1.64260
H	-4.44409	-1.79656	-0.90926
H	-3.90989	-2.36370	-2.51419
H	-4.75139	-0.80098	-2.33866
H	0.06178	-2.11612	-1.89947

^{6}FeH3BueaOH
Charge: -1
Energy: -1340877.0026731

C	-0.12641	2.37438	1.20091
C	0.48078	1.29794	2.10430
C	-2.58982	-1.42556	-1.14624
C	-2.00350	-1.35730	1.16118
C	2.61153	-1.35388	-1.18286
C	0.95175	-1.12220	2.06870
C	2.16628	-1.12174	1.13885
C	-0.05684	2.94657	-1.11534
C	-1.37688	-0.32517	2.10159
Fe	-0.00186	0.01177	-0.65171
H	0.38826	3.32920	1.36922
H	-1.18243	2.55209	1.46084
H	0.26881	1.50338	3.16927
H	1.56570	1.31472	1.97139
H	-3.08665	-1.40281	1.33170
H	-1.62062	-2.36709	1.38072
H	-1.44382	-0.64928	3.15605
H	-1.93715	0.60842	2.00370
H	2.73070	-2.05398	1.27284
H	2.86341	-0.31092	1.40505
H	1.25928	-1.05720	3.12823
H	0.42040	-2.06825	1.93507
N	-0.00315	1.95815	-0.18803
N	0.01504	-0.04383	1.71839
N	1.71633	-0.97699	-0.23844
N	-1.71154	-0.98269	-0.21502
O	3.73725	-1.82691	-0.98781
O	-0.18498	4.15592	-0.89169
O	-3.59532	-2.11832	-0.95000
O	-0.02101	0.00408	-2.50902
H	0.03197	2.55226	-2.14497
H	-2.31455	-1.08434	-2.16303
H	2.22435	-1.18863	-2.20671
H	-0.06486	-0.86228	-2.94157

^{6}FeMeBzImTPABrA
Charge: 2+
Energy: -3245405.1442799

Fe	0.36477	0.15967	0.52393
N	-1.51000	-0.38959	-0.12443
N	-2.89660	-0.99406	-1.75771
N	0.72831	-0.11085	-1.71486
N	1.02961	-1.90044	0.32758
N	2.49734	0.53997	0.24492
N	-0.03262	2.12146	-0.22542
C	-2.80246	-0.40112	0.40648
C	-3.28159	-0.10541	1.68655
C	-4.65402	-0.21784	1.89048
C	-5.52912	-0.60919	0.85594
C	-5.06255	-0.90280	-0.42355
C	-3.68662	-0.78737	-0.62006
C	-3.42176	-1.43620	-3.04930
C	-1.61721	-0.74227	-1.40875
C	-0.40915	-0.87603	-2.29238
C	0.77638	-2.90056	1.18580
C	1.22840	-4.19817	0.94743
C	1.95595	-4.45371	-0.21483
C	2.21578	-3.40618	-1.10722
C	1.73740	-2.14030	-0.79656
C	2.00530	-0.89112	-1.62690
C	3.01292	-0.04860	-0.85534
C	4.35272	0.07319	-1.19763
C	5.18680	0.82850	-0.36425
C	4.65080	1.43202	0.77299
C	3.29352	1.26538	1.04609
C	0.88164	1.24241	-2.31651
C	0.12524	2.31139	-1.55289
C	-0.31639	3.47541	-2.17490
C	-0.92138	4.47104	-1.40367
C	-1.07406	4.27004	-0.03148
C	-0.62251	3.07592	0.52039
H	2.39594	-1.15603	-2.61637
H	4.73902	-0.40752	-2.09073
H	6.23941	0.94176	-0.60446
H	5.26750	2.02101	1.44306
H	2.78003	-3.57346	-2.01920
H	2.31937	-5.45414	-0.42847
H	1.01340	-4.98447	1.66280
H	0.20949	-2.63724	2.07229
H	-0.13124	-1.93326	-2.36423
H	-0.62192	-0.53664	-3.31161
H	0.57916	1.23578	-3.36937
H	1.94329	1.50574	-2.30073
H	-0.18332	3.60505	-3.24452
H	-1.26970	5.38741	-1.87010
H	-2.61945	-1.49240	-3.78508
H	-4.17775	-0.72700	-3.39616
H	-3.87568	-2.42505	-2.94107
H	-5.73669	-1.20537	-1.21778
H	-6.59188	-0.68481	1.06159
H	-5.06286	-0.00112	2.87207
H	-2.60943	0.19023	2.48329
H	2.82144	1.70383	1.91833
H	-0.72746	2.85508	1.57650
H	-1.53897	5.01666	0.60293
Br	0.24279	0.39339	2.90682

^{6}FeMeBzImTPAClA
Charge: 2+
Energy: -1918877.2604676

Fe	0.36872	0.15155	0.74423
N	-1.48534	-0.36373	0.03345
N	-2.86349	-0.88331	-1.63350
N	0.76492	-0.01302	-1.51587
N	1.02936	-1.89311	0.45201
N	2.49670	0.52832	0.51018
N	-0.00308	2.14199	0.07396
C	-2.77819	-0.40057	0.55835
C	-3.25696	-0.16960	1.85152
C	-4.63020	-0.28950	2.04621
C	-5.50320	-0.62575	0.99051
C	-5.03514	-0.85516	-0.30188

C	-3.65861	-0.73295	-0.48963
C	-3.38280	-1.25823	-2.94852
C	-1.58516	-0.65138	-1.26705
C	-0.36828	-0.74347	-2.14482
C	0.76064	-2.92469	1.26619
C	1.20851	-4.21393	0.97886
C	1.94682	-4.42447	-0.18577
C	2.22365	-3.34226	-1.03084
C	1.74954	-2.08746	-0.67266
C	2.03703	-0.80257	-1.44079
C	3.03245	-0.00230	-0.60930
C	4.37947	0.13438	-0.91515
C	5.19604	0.84032	-0.02266
C	4.63786	1.38055	1.13575
C	3.27446	1.20397	1.36981
C	0.93320	1.36739	-2.04721
C	0.17501	2.40177	-1.23839
C	-0.24829	3.60257	-1.80025
C	-0.85496	4.55910	-0.98198
C	-1.02795	4.28430	0.37512
C	-0.59431	3.05729	0.86578
H	2.44666	-1.02344	-2.43337
H	4.78504	-0.29772	-1.82439
H	6.25375	0.96378	-0.23367
H	5.24208	1.92803	1.85084
H	2.79800	-3.47512	-1.94218
H	2.30658	-5.41737	-0.43735
H	0.98209	-5.02837	1.65827
H	0.18520	-2.69274	2.15628
H	-0.09294	-1.79667	-2.26822
H	-0.56942	-0.35127	-3.14736
H	0.64235	1.41612	-3.10227
H	1.99626	1.62267	-2.00688
H	-0.10008	3.79053	-2.85917
H	-1.18918	5.50313	-1.40113
H	-2.57665	-1.27673	-3.68206
H	-4.13674	-0.53156	-3.26203
H	-3.83756	-2.25106	-2.89346
H	-5.70888	-1.11540	-1.11129
H	-6.56658	-0.70953	1.18973
H	-5.04170	-0.12266	3.03639
H	-2.58253	0.08302	2.66164
H	2.78131	1.59228	2.25444
H	-0.71436	2.77603	1.90602
H	-1.49497	4.99932	1.04346
Cl	0.19107	0.29471	2.94172

^{6}FeMeBzImTPAFA
Charge: 2+
Energy: -1692751.5030913

Fe	-0.36157	0.15699	-0.85291
N	1.47139	-0.32192	-0.09617
N	2.86954	-0.80698	1.55912
N	-0.78357	-0.00394	1.43467
N	-0.96276	-1.91035	-0.55027
N	-2.49280	0.45464	-0.65613
N	-0.08215	2.15126	-0.17343
C	2.75440	-0.34656	-0.63484
C	3.19761	-0.11984	-1.94038
C	4.56861	-0.22065	-2.15952
C	5.46414	-0.53423	-1.11439
C	5.02633	-0.75909	0.19022
C	3.65164	-0.65678	0.40412
C	3.40524	-1.15735	2.87413
C	1.58291	-0.59557	1.20402
C	0.36525	-0.69222	2.08459
C	-0.64109	-2.94502	-1.34093
C	-1.03733	-4.24712	-1.03604
C	-1.77685	-4.46784	0.12587
C	-2.10484	-3.38359	0.94961
C	-1.68213	-2.11542	0.57348
C	-2.02677	-0.83412	1.32662
C	-3.02921	-0.07203	0.46496
C	-4.38406	0.03635	0.74752
C	-5.20455	0.70554	-0.16957
C	-4.64413	1.24058	-1.32964
C	-3.27299	1.09640	-1.53906
C	-1.00668	1.37440	1.94984
C	-0.28581	2.42891	1.12948
C	0.08114	3.65966	1.66614
C	0.65602	4.61994	0.82892
C	0.85601	4.32219	-0.52039
C	0.47881	3.06699	-0.98556
H	-2.45918	-1.06638	2.30702
H	-4.79313	-0.38961	1.65808
H	-6.26807	0.80544	0.02409
H	-5.25211	1.76011	-2.06216
H	-2.67902	-3.52534	1.85973
H	-2.09688	-5.47039	0.39242
H	-0.76954	-5.06329	-1.69813
H	-0.06166	-2.70858	-2.22782
H	0.11495	-1.74796	2.23786
H	0.55748	-0.26882	3.07621
H	-0.72115	1.44896	3.00488
H	-2.07873	1.58913	1.90457
H	-0.08448	3.86741	2.71877
H	0.94669	5.58673	1.22828
H	2.60376	-1.18243	3.61281
H	4.14743	-0.41337	3.17499
H	3.87805	-2.14216	2.82736
H	5.72152	-1.00040	0.98728
H	6.52491	-0.60352	-1.33243
H	4.96211	-0.05669	-3.15747
H	2.49208	0.11700	-2.73064
H	-2.77447	1.48587	-2.42095
H	0.61969	2.75517	-2.01516
H	1.30129	5.04124	-1.19915
F	-0.05759	0.41556	-2.56830

^{6}FeMeBzImTPAN$_3$A
Charge: 2+
Energy: -1733139.2397741

Fe	0.37437	0.17390	0.65622
N	-1.49472	-0.35584	-0.04974
N	-2.88396	-0.89432	-1.70258
N	0.74595	-0.00173	-1.61458
N	1.02850	-1.89802	0.34014
N	2.51698	0.54656	0.38248
N	-0.02818	2.16132	-0.03555
C	-2.78146	-0.40252	0.48333
C	-3.24831	-0.16772	1.77994
C	-4.61722	-0.29715	1.99283
C	-5.49882	-0.64741	0.94772
C	-5.04390	-0.87951	-0.34809
C	-3.66995	-0.74723	-0.55349
C	-3.40890	-1.27709	-3.01240
C	-1.60242	-0.64789	-1.34491
C	-0.39365	-0.72923	-2.23602
C	0.75483	-2.94687	1.12974
C	1.18995	-4.23471	0.81862
C	1.92329	-4.42903	-0.35205
C	2.20082	-3.33296	-1.17746
C	1.73696	-2.08104	-0.79320
C	2.01640	-0.79196	-1.55756
C	3.02862	0.00415	-0.74211
C	4.37059	0.13084	-1.07728
C	5.20980	0.84184	-0.21150
C	4.67729	1.40103	0.95028
C	3.31827	1.23195	1.21176
C	0.90946	1.37670	-2.15031
C	0.13454	2.40721	-1.35191
C	-0.32130	3.58924	-1.92930
C	-0.94761	4.54200	-1.12206
C	-1.10783	4.28205	0.23977
C	-0.63946	3.07304	0.74307
H	2.41399	-1.01260	-2.55550
H	4.75406	-0.31154	-1.99120
H	6.26336	0.95786	-0.44619
H	5.29744	1.95850	1.64372
H	2.76580	-3.45264	-2.09651
H	2.27447	-5.41955	-0.62426
H	0.95639	-5.06055	1.48172
H	0.17499	-2.73489	2.02206
H	-0.11848	-1.78065	-2.37410
H	-0.60779	-0.32829	-3.23265
H	0.62952	1.42109	-3.20881
H	1.96968	1.64140	-2.09933
H	-0.18419	3.76500	-2.99180
H	-1.30797	5.47109	-1.55282
H	-2.60597	-1.29755	-3.74957
H	-4.16615	-0.55448	-3.32779
H	-3.86073	-2.27101	-2.95147
H	-5.72521	-1.14856	-1.14829
H	-6.55915	-0.73864	1.15961
H	-5.02050	-0.12682	2.98586
H	-2.56611	0.10066	2.57934
H	2.84662	1.64586	2.09680
H	-0.75094	2.80198	1.78732
H	-1.59137	4.99413	0.89945
N	0.22123	0.30444	2.50036
N	0.32191	0.20806	3.70561
N	0.40724	0.12275	4.84645

^{6}FeMeBzImTPANCSA
Charge: 2+
Energy: -1938247.5147369

Fe	-0.37832	-0.34645	0.38121
N	1.47352	0.45417	-0.07084
N	2.82697	1.66545	-1.35581
N	-0.80372	0.79806	-1.58480
N	-1.02686	1.64728	1.01386
N	-2.52551	-0.56867	0.03090
N	-0.01138	-1.83216	-1.12149
C	2.77138	0.27746	0.40546
C	3.26491	-0.48777	1.46639

C	4.63819	-0.45023	1.68716
C	5.49769	0.32282	0.87744
C	5.01551	1.08635	-0.18305
C	3.63749	1.04334	-0.39864
C	3.32357	2.58129	-2.38154
C	1.55310	1.27830	-1.11422
C	0.32523	1.72751	-1.85782
C	-0.73083	2.24206	2.17863
C	-1.16198	3.53554	2.47201
C	-1.91446	4.22288	1.51952
C	-2.21700	3.59944	0.30298
C	-1.75619	2.30636	0.08998
C	-2.06546	1.47880	-1.15295
C	-3.06210	0.40280	-0.73649
C	-4.41346	0.42617	-1.05610
C	-5.23417	-0.59176	-0.55588
C	-4.67557	-1.59195	0.24003
C	-3.30854	-1.54614	0.51100
C	-0.99306	-0.21049	-2.66152
C	-0.20939	-1.48427	-2.40951
C	0.21902	-2.29993	-3.45335
C	0.85412	-3.50780	-3.15448
C	1.04968	-3.86301	-1.81902
C	0.60737	-2.99113	-0.82975
H	-2.48856	2.11092	-1.94295
H	-4.81850	1.21655	-1.67998
H	-6.29454	-0.60068	-0.78841
H	-5.28193	-2.39430	0.64593
H	-2.79928	4.10915	-0.45815
H	-2.26263	5.23216	1.71621
H	-0.91101	3.98700	3.42565
H	-0.13968	1.65763	2.87613
H	0.05219	2.73530	-1.52576
H	0.51650	1.79413	-2.93435
H	-0.73886	0.20926	-3.64133
H	-2.05428	-0.47307	-2.70350
H	0.05403	-1.99883	-4.48327
H	1.19369	-4.15883	-3.95415
H	2.50617	2.90482	-3.02634
H	4.07879	2.07480	-2.98827
H	3.77055	3.45896	-1.90646
H	5.67975	1.68005	-0.80209
H	6.56234	0.32325	1.08736
H	5.06222	-1.02704	2.50281
H	2.59981	-1.07717	2.08783
H	-2.81536	-2.29331	1.12393
H	0.74551	-3.19940	0.22567
H	1.54048	-4.79056	-1.54550
N	-0.16775	-1.29255	1.98010
C	-0.04838	-1.87909	3.03178
S	0.12011	-2.64622	4.40162

^{6}FeMeBzImTPAOHA
Charge: 2+
Energy: -1677667.4842593

Fe	-0.36847	0.16907	-0.88426
N	1.46904	-0.34719	-0.11599
N	2.84466	-0.85235	1.55535
N	-0.79380	0.00107	1.41194
N	-1.01323	-1.90555	-0.55105
N	-2.51229	0.51769	-0.64631
N	-0.01711	2.14938	-0.18187
C	2.75989	-0.38260	-0.63670
C	3.22848	-0.15336	-1.93330
C	4.60111	-0.26585	-2.13300
C	5.47882	-0.59416	-1.07709
C	5.01854	-0.82115	0.21831
C	3.64144	-0.70596	0.41226
C	3.36036	-1.21483	2.87443
C	1.56359	-0.62561	1.18290
C	0.34116	-0.71198	2.05652
C	-0.70139	-2.95697	-1.32291
C	-1.12047	-4.24925	-1.00840
C	-1.87756	-4.44446	0.14695
C	-2.19282	-3.34541	0.95470
C	-1.74292	-2.08880	0.56883
C	-2.05485	-0.79873	1.31989
C	-3.04906	-0.01266	0.47198
C	-4.39796	0.12202	0.77457
C	-5.21408	0.82803	-0.11736
C	-4.65369	1.37473	-1.27209
C	-3.28975	1.19842	-1.50157
C	-0.97748	1.38314	1.92948
C	-0.20732	2.41486	1.12603
C	0.21744	3.61671	1.68538
C	0.83911	4.56354	0.86685
C	1.02587	4.28021	-0.48710
C	0.58847	3.05296	-0.97451
H	-2.48244	-1.02097	2.30513
H	-4.80418	-0.30942	1.68387
H	-6.27219	0.95036	0.09241
H	-5.25636	1.92842	-1.98374
H	-2.77506	-3.46647	1.86272
H	-2.21716	-5.43832	0.42167
H	-0.85597	-5.07783	-1.65629
H	-0.10264	-2.74240	-2.20223
H	0.07368	-1.76502	2.19800
H	0.53669	-0.30277	3.05373
H	-0.70707	1.44394	2.98973
H	-2.04024	1.63566	1.86729
H	0.06051	3.81251	2.74164
H	1.17571	5.50769	1.28395
H	2.55049	-1.23299	3.60410
H	4.10829	-0.48177	3.18789
H	3.82149	-2.20536	2.83002
H	5.69836	-1.07331	1.02526
H	6.54200	-0.67241	-1.27990
H	5.01115	-0.09915	-3.12391
H	2.53943	0.09718	-2.73343
H	-2.79169	1.60045	-2.37769
H	0.71578	2.75423	-2.00970
H	1.50665	4.98864	-1.15269
O	-0.12003	0.37618	-2.64894
H	-0.44525	0.04556	-3.50033

^{6}FeMeBzImTPAOH
Charge: 2+
Energy: -1677667.4849182

Fe	-0.36833	0.16905	-0.88422
N	1.46933	-0.34651	-0.11585
N	2.84500	-0.85159	1.55547
N	-0.79373	0.00085	1.41197
N	-1.01229	-1.90579	-0.55115
N	-2.51233	0.51688	-0.64627
N	-0.01785	2.14948	-0.18186
C	2.76019	-0.38168	-0.63654
C	3.22874	-0.15233	-1.93314
C	4.60140	-0.26459	-2.13283
C	5.47915	-0.59279	-1.07691
C	5.01890	-0.81990	0.21848
C	3.64178	-0.70495	0.41241
C	3.36074	-1.21403	2.87454
C	1.56389	-0.62503	1.18301
C	0.34148	-0.71172	2.05663
C	-0.69995	-2.95704	-1.32304
C	-1.11842	-4.24954	-1.00855
C	-1.87540	-4.44513	0.14679
C	-2.19119	-3.34625	0.95458
C	-1.74188	-2.08941	0.56874
C	-2.05441	-0.79951	1.31983
C	-3.04893	-0.01386	0.47192
C	-4.39792	0.12009	0.77442
C	-5.21434	0.82575	-0.11751
C	-4.65414	1.37288	-1.27214
C	-3.29008	1.19730	-1.50152
C	-0.97808	1.38283	1.92952
C	-0.20872	2.41505	1.12592
C	0.21469	3.61746	1.68514
C	0.83568	4.56471	0.86660
C	1.02318	4.28125	-0.48724
C	0.58711	3.05348	-0.97450
H	-2.48195	-1.02198	2.30505
H	-4.80400	-0.31166	1.68363
H	-6.27253	0.94751	0.09218
H	-5.25704	1.92633	-1.98378
H	-2.77337	-3.46761	1.86260
H	-2.21453	-5.43916	0.42150
H	-0.85353	-5.07797	-1.65647
H	-0.10132	-2.74215	-2.20236
H	0.07437	-1.76483	2.19826
H	0.53689	-0.30231	3.05378
H	-0.70740	1.44381	2.98968
H	-2.04101	1.63474	1.86765
H	0.05725	3.81334	2.74130
H	1.17122	5.50929	1.28358
H	2.55072	-1.23318	3.60403
H	4.10797	-0.48044	3.18843
H	3.82273	-2.20415	2.82988
H	5.69875	-1.07197	1.02542
H	6.54235	-0.67084	-1.27972
H	5.01142	-0.09780	-3.12373
H	2.53965	0.09807	-2.73328
H	-2.79218	1.59973	-2.37755
H	0.71503	2.75465	-2.00959
H	1.50351	4.98998	-1.15283
O	-0.11982	0.37576	-2.64893
H	-0.44562	0.04583	-3.50037

^{6}FebisMeBzImTPABr
Charge: 2+
Energy: -3352690.6043530

Fe	0.43486	-0.00007	-0.55296
N	2.10101	1.41923	-0.38398
N	2.10098	-1.41941	-0.38402
N	-0.78922	-1.47716	0.21200

N	-0.78910	1.47711	0.21202
N	1.03303	-0.00012	1.70117
N	-1.52778	-2.72232	1.90229
N	-1.52762	2.72226	1.90234
C	2.35737	2.43253	-1.22526
C	3.43022	3.30013	-1.02108
C	4.24995	3.10577	0.09022
C	3.97641	2.04917	0.96700
C	2.89247	1.22569	0.69107
C	2.52011	-0.00012	1.51466
H	3.05449	-0.00015	2.47231
C	2.89245	-1.22590	0.69102
C	3.97641	-2.04937	0.96689
C	4.24995	-3.10594	0.09006
C	3.43019	-3.30027	-1.02123
C	2.35733	-2.43268	-1.22535
C	0.50109	-1.24362	2.32185
C	-0.61956	-1.80774	1.49231
C	-1.65689	-3.36008	3.21134
C	-2.35372	-3.00572	0.80887
C	-3.44371	-3.86680	0.67754
C	-4.05507	-3.90012	-0.57317
C	-3.59439	-3.10474	-1.64360
C	-2.50674	-2.24814	-1.50499
C	-1.88261	-2.21039	-0.25409
C	-0.61945	1.80763	1.49235
C	0.50110	1.24336	2.32191
C	-1.65637	3.36035	3.21126
C	-2.35340	3.00590	0.80886
C	-3.44321	3.86720	0.67748
C	-4.05450	3.90065	-0.57325
C	-3.59393	3.10519	-1.64368
C	-2.50643	2.24839	-1.50503
C	-1.88236	2.21053	-0.25410
H	-0.91541	2.95948	3.90324
H	-2.65708	3.17549	3.61067
H	-1.50131	4.43816	3.11097
H	-4.10233	3.16522	-2.60054
H	-2.15115	1.63882	-2.32732
H	1.30719	1.98232	2.38761
H	0.17262	1.05045	3.34865
H	1.30714	-1.98263	2.38741
H	0.17269	-1.05078	3.34864
H	-2.65619	-3.17149	3.61257
H	-0.91306	-2.96240	3.90207
H	-1.50616	-4.43844	3.11046
H	-3.79908	-4.47908	1.49956
H	-4.90686	-4.55431	-0.72820
H	-4.10285	-3.16466	-2.60045
H	-2.15139	-1.63861	-2.32729
H	1.68731	-2.53025	-2.07253
H	3.61377	-4.10581	-1.72383
H	5.09204	-3.76525	0.27639
H	4.59509	-1.87149	1.84081
H	1.68737	2.53013	-2.07246
H	3.61381	4.10569	-1.72365
H	5.09204	3.76508	0.27659
H	4.59506	1.87125	1.84093
H	-3.79846	4.47959	1.49946
H	-4.90615	4.55501	-0.72833
Br	0.16815	-0.00005	-2.93768

[6]FebisMeBzImTPACl
Charge: 2+
Energy: -2026162.8290623

Fe	0.42787	-0.00008	-0.74538
N	2.09289	1.40913	-0.59123
N	2.09278	-1.40940	-0.59128
N	-0.77181	-1.47607	0.04579
N	-0.77163	1.47605	0.04581
N	1.05587	-0.00014	1.52051
N	-1.49587	-2.73270	1.73185
N	-1.49558	2.73270	1.73191
C	2.33512	2.41219	-1.44780
C	3.40891	3.28378	-1.26582
C	4.24154	3.10243	-0.16173
C	3.98254	2.05358	0.72922
C	2.89757	1.22463	0.47512
C	2.53928	-0.00018	1.30785
H	3.09196	-0.00022	2.25507
C	2.89749	-1.22498	0.47507
C	3.98244	-2.05399	0.72911
C	4.24137	-3.10281	-0.16190
C	3.40871	-3.28408	-1.26597
C	2.33496	-2.41244	-1.44789
C	0.53077	-1.24392	2.14606
C	-0.59420	-1.81075	1.32338
C	-1.61667	-3.37625	3.03884
C	-2.32372	-3.01641	0.63919
C	-3.40895	-3.88294	0.50432
C	-4.02047	-3.91349	-0.74669
C	-3.56524	-3.11113	-1.81451
C	-2.48254	-2.24864	-1.67288
C	-1.86015	-2.21378	-0.42126
C	-0.59401	1.81066	1.32342
C	0.53085	1.24364	2.14611
C	-1.61599	3.37659	3.03877
C	-2.32326	3.01669	0.63919
C	-3.40828	3.88348	0.50427
C	-4.01974	3.91418	-0.74676
C	-3.56465	3.11173	-1.81456
C	-2.48214	2.24900	-1.67290
C	-1.85980	2.21400	-0.42126
H	-0.87669	2.97162	3.73020
H	-2.61718	3.20122	3.44123
H	-1.45234	4.45275	2.93445
H	-4.07343	3.17149	-2.77125
H	-2.12738	1.63297	-2.49111
H	1.33856	1.98139	2.20711
H	0.20865	1.05099	3.17495
H	1.33841	-1.98175	2.20692
H	0.20865	-1.05132	3.17493
H	-2.61646	-3.19708	3.44314
H	-0.87444	-2.97449	3.72900
H	-1.45743	-4.45300	2.93394
H	-3.76084	-4.50135	1.32323
H	-4.86858	-4.57187	-0.90417
H	-4.07407	-3.17077	-2.77117
H	-2.12769	-1.63268	-2.49109
H	1.65288	-2.49667	-2.28726
H	3.58316	-4.08237	-1.97907
H	5.08386	-3.76615	0.00761
H	4.61354	-1.88616	1.59610
H	1.65306	2.49648	-2.28717
H	3.58341	4.08209	-1.97889
H	5.08405	3.76573	0.00782
H	4.61362	1.88569	1.59622
H	-3.76002	4.50202	1.32315
H	-4.86768	4.57277	-0.90428
Cl	0.11052	-0.00004	-2.93184

[6]FebisMeBzImTPAF
Charge: 2+
Energy: -1800037.1440817

Fe	-0.38309	-0.00719	-0.83775
N	-2.02712	-1.43531	-0.71657
N	-2.07594	1.36292	-0.71631
N	0.73010	1.49722	-0.00142
N	0.78269	-1.47134	-0.00164
N	-1.05946	-0.01934	1.45884
N	1.40162	2.80746	1.66043
N	1.50048	-2.75670	1.66030
C	-2.22999	-2.44370	-1.57673
C	-3.28118	-3.34535	-1.40987
C	-4.12963	-3.18971	-0.31383
C	-3.90902	-2.13696	0.58294
C	-2.84612	-1.27540	0.34314
C	-2.53276	-0.04480	1.18870
H	-3.12347	-0.05520	2.11286
C	-2.88862	1.17451	0.34357
C	-3.98061	1.99875	0.58392
C	-4.23765	3.04360	-0.31237
C	-3.39535	3.22883	-1.40854
C	-2.31372	2.36404	-1.57603
C	-0.56893	1.23432	2.09280
C	0.53806	1.84056	1.26954
C	1.50042	3.46947	2.95987
C	2.21349	3.11062	0.55889
C	3.26103	4.01791	0.39438
C	3.85466	4.04945	-0.86610
C	3.42184	3.21176	-1.91723
C	2.37776	2.30787	-1.74739
C	1.77894	2.27316	-0.48532
C	0.60287	-1.82138	1.26930
C	-0.52573	-1.25562	2.09204
C	1.62277	-3.41496	2.95965
C	2.32292	-3.03048	0.55890
C	3.40235	-3.89962	0.39456
C	3.99697	-3.90982	-0.86581
C	3.53459	-3.08814	-1.91698
C	2.45873	-2.22228	-1.74733
C	1.85879	-2.20912	-0.48537
H	0.88001	-3.02075	3.65381
H	2.62234	-3.23960	3.36627
H	1.46410	-4.49059	2.84305
H	4.03279	-3.13673	-2.87984
H	2.08513	-1.58472	-2.54219
H	-1.32741	-1.99967	2.16120
H	-0.20189	-1.05506	3.11891
H	-1.39628	1.94951	2.16409
H	-0.23675	1.04397	3.11895
H	2.50584	3.33042	3.36609
H	0.77274	3.04834	3.65420
H	1.30274	4.53866	2.84363
H	3.59902	4.66561	1.19633
H	4.67318	4.73912	-1.04505

H	3.91781	3.27821	-2.88017
H	2.02705	1.65731	-2.54215
H	-1.61988	2.45570	-2.40569
H	-3.56752	4.02528	-2.12423
H	-5.08600	3.70185	-0.15249
H	-4.61910	1.83022	1.44534
H	-1.53312	-2.51101	-2.40619
H	-3.42560	-4.14699	-2.12590
H	-4.95478	-3.87692	-0.15440
H	-4.55316	-1.99091	1.44426
H	3.76320	-4.53482	1.19656
H	4.83971	-4.56970	-1.04463
F	0.10130	0.00178	-2.53181

^{6}FebisMeBzImTPAN$_3$
Charge: 2+
Energy: -1840424.6330551

Fe	-0.42712	-0.00035	0.66863
N	-2.10245	1.42299	0.47920
N	-2.10154	-1.42462	0.48016
N	0.78536	-1.47738	-0.13084
N	0.78437	1.47710	-0.13171
N	-1.03678	-0.00115	-1.61455
N	1.52457	-2.72924	-1.81517
N	1.52229	2.72904	-1.81656
C	-2.35426	2.44594	1.30860
C	-3.42310	3.31721	1.10044
C	-4.24434	3.11583	-0.00892
C	-3.97369	2.05212	-0.87737
C	-2.89257	1.22577	-0.59523
C	-2.52097	-0.00160	-1.41890
H	-3.06426	-0.00209	-2.37196
C	-2.89175	-1.22867	-0.59443
C	-3.97230	-2.05595	-0.87603
C	-4.24225	-3.11924	-0.00685
C	-3.42092	-3.31928	1.10269
C	-2.35269	-2.44714	1.31029
C	-0.50514	-1.24366	-2.23670
C	0.61663	-1.80930	-1.40775
C	1.65444	-3.36864	-3.12283
C	2.34726	-3.01118	-0.71913
C	3.43646	-3.87208	-0.57488
C	4.03986	-3.89755	0.67979
C	3.57529	-3.09490	1.74416
C	2.48918	-2.23928	1.59248
C	1.87334	-2.21039	0.33773
C	0.61524	1.80838	-1.40872
C	-0.50598	1.24133	-2.23745
C	1.65108	3.36847	-3.12431
C	2.34466	3.01232	-0.72063
C	3.43293	3.87445	-0.57672
C	4.03638	3.90098	0.67791
C	3.57275	3.09816	1.74257
C	2.48755	2.24135	1.59122
C	1.87162	2.21141	0.33654
H	0.91049	2.96692	-3.81642
H	2.65169	3.18509	-3.52487
H	1.49461	4.44617	-3.02440
H	4.07844	3.15342	2.70121
H	2.12866	1.61860	2.40339
H	-1.31160	1.98079	-2.30495
H	-0.17750	1.04822	-3.26442
H	-1.31023	-1.98377	-2.30351
H	-0.17699	-1.05102	-3.26387
H	2.65333	-3.18031	-3.52543
H	0.91031	-2.97160	-3.81374
H	1.50382	-4.44706	-3.02187
H	3.79776	-4.48964	-1.39037
H	4.89046	-4.55115	0.84370
H	4.08096	-3.14932	2.70286
H	2.12950	-1.61671	2.40443
H	-1.67501	-2.55629	2.15060
H	-3.59907	-4.13306	1.79717
H	-5.08099	-3.78128	-0.19851
H	-4.59017	-1.87658	-1.75025
H	-1.67661	2.55621	2.14879
H	-3.60176	4.13136	1.79435
H	-5.08354	3.77716	-0.20101
H	-4.59146	1.87172	-1.75145
H	3.79348	4.49219	-1.39240
H	4.88627	4.55556	0.84156
N	-0.14544	0.00047	2.50256
N	-0.24257	0.00338	3.71102
N	-0.32120	0.00605	4.85611

^{6}FebisMeBzImTPANCS
Charge: 2+
Energy: -2045532.9740884

Fe	-0.42349	0.00000	0.54234
N	-2.10475	1.41705	0.46190
N	-2.10473	-1.41706	0.46190
N	0.73103	-1.47917	-0.33750
N	0.73101	1.47919	-0.33750
N	-1.17593	0.00000	-1.70590
N	1.36219	-2.73382	-2.06270
N	1.36234	2.73366	-2.06279
C	-2.30431	2.43146	1.31541
C	-3.38367	3.30431	1.17950
C	-4.27045	3.11265	0.12004
C	-4.05532	2.05523	-0.77164
C	-2.95981	1.22636	-0.56281
C	-2.64352	-0.00001	-1.41144
H	-3.24980	-0.00001	-2.32574
C	-2.95980	-1.22637	-0.56281
C	-4.05531	-2.05525	-0.77164
C	-4.27043	-3.11267	0.12005
C	-3.38365	-3.30431	1.17950
C	-2.30430	-2.43147	1.31541
C	-0.68588	-1.24248	-2.36016
C	0.48334	-1.81111	-1.60144
C	1.40985	-3.37428	-3.37538
C	2.24924	-3.01804	-1.01854
C	3.34212	-3.88271	-0.94034
C	4.01980	-3.91077	0.27583
C	3.62233	-3.10757	1.36657
C	2.53210	-2.24800	1.28121
C	1.84291	-2.21585	0.06511
C	0.48337	1.81107	-1.60147
C	-0.68589	1.24249	-2.36015
C	1.40974	3.37445	-3.37531
C	2.24929	3.01799	-1.01857
C	3.34215	3.88268	-0.94035
C	4.01979	3.91077	0.27585
C	3.62230	3.10759	1.36659
C	2.53206	2.24804	1.28123
C	1.84290	2.21586	0.06511
H	0.62939	2.97149	-4.02139
H	2.38457	3.19386	-3.83617
H	1.25699	4.45169	-3.26508
H	4.18366	3.16498	2.29362
H	2.22269	1.62778	2.11499
H	-1.49483	1.98128	-2.37833
H	-0.42035	1.04987	-3.40529
H	-1.49483	-1.98125	-2.37841
H	-0.42026	-1.04982	-3.40528
H	2.38313	-3.18994	-3.83808
H	0.62661	-2.97456	-4.01996
H	1.26152	-4.45209	-3.26478
H	3.65132	-4.50137	-1.77615
H	4.87640	-4.56743	0.38812
H	4.18372	-3.16493	2.29358
H	2.22277	-1.62772	2.11496
H	-1.57828	-2.52950	2.11583
H	-3.52023	-4.11195	1.89035
H	-5.11916	-3.77593	-0.01517
H	-4.72670	-1.88126	-1.60661
H	-1.57830	2.52950	2.11583
H	-3.52026	4.11194	1.89034
H	-5.11918	3.77591	-0.01518
H	-4.72670	1.88124	-1.60661
H	3.65134	4.50138	-1.77613
H	4.87638	4.56745	0.38815
N	-0.00610	-0.00003	2.36536
C	0.26436	-0.00002	3.54386
S	0.63573	0.00002	5.07957

^{6}FebisMeBzImTPAOH
Charge: 2+
Energy: -1784952.6342675

Fe	0.41084	-0.00034	-0.87576
N	2.09090	1.41662	-0.70690
N	2.08990	-1.41828	-0.70720
N	-0.75782	-1.47539	-0.02970
N	-0.75658	1.47570	-0.02973
N	1.08036	-0.00064	1.43037
N	-1.47871	-2.73134	1.65630
N	-1.47613	2.73259	1.65614
C	2.31232	2.44350	-1.54002
C	3.37426	3.32755	-1.35120
C	4.21941	3.13412	-0.25842
C	3.97874	2.06637	0.61406
C	2.90248	1.22682	0.35273
C	2.55628	-0.00119	1.18763
H	3.13217	-0.00148	2.12156
C	2.90154	-1.22934	0.35254
C	3.97707	-2.06984	0.61382
C	4.21690	-3.13766	-0.25882
C	3.37168	-3.33018	-1.35172
C	2.31051	-2.44519	-1.54049
C	0.55849	-1.24305	2.05879
C	-0.57505	-1.80885	1.24431
C	-1.59660	-3.37353	2.96352
C	-2.31040	-3.01236	0.56558
C	-3.39963	-3.87370	0.42405
C	-4.00803	-3.89520	-0.82879

C	-3.54876	-3.09061	-1.89452
C	-2.46260	-2.23393	-1.74738
C	-1.84600	-2.20931	-0.49322
C	-0.57342	1.80911	1.24423
C	0.55937	1.24209	2.05889
C	-1.59276	3.37566	2.96304
C	-2.30739	3.01455	0.56532
C	-3.39556	3.87720	0.42359
C	-4.00393	3.89917	-0.82926
C	-3.54563	3.09382	-1.89482
C	-2.46048	2.23589	-1.74751
C	-1.84391	2.21081	-0.49336
H	-0.85295	2.96790	3.65246
H	-2.59319	3.20199	3.36835
H	-1.42712	4.45181	2.86088
H	-4.05574	3.14886	-2.85118
H	-2.09405	1.60970	-2.55440
H	1.36575	1.98188	2.11523
H	0.24467	1.05079	3.09062
H	1.36424	-1.98357	2.11455
H	0.24435	-1.05176	3.09069
H	-2.59455	-3.19263	3.37181
H	-0.85160	-2.97166	3.65079
H	-1.43920	-4.45083	2.86056
H	-3.75732	-4.49437	1.23877
H	-4.85905	-4.54894	-0.99026
H	-4.05891	-3.14524	-2.85087
H	-2.09540	-1.60837	-2.55440
H	1.61234	-2.54577	-2.36518
H	3.52587	-4.14829	-2.04684
H	5.05081	-3.80984	-0.08190
H	4.61344	-1.89775	1.47614
H	1.61415	2.54489	-2.36461
H	3.52909	4.14565	-2.04620
H	5.05392	3.80556	-0.08145
H	4.61502	1.89359	1.47631
H	-3.75244	4.49855	1.23814
H	-4.85414	4.55393	-0.99086
O	0.00412	-0.00087	-2.62414
H	0.44833	0.00004	-3.48604

^{3}FeMeHPyTACNBrOH
Charge: 2+
Energy: -2937127.4263999

H	-0.88389	-3.66331	0.65175
H	-3.09411	-2.56871	-1.03820
H	-2.10804	-2.54970	1.21875
C	-1.11197	-2.60109	0.78103
H	-3.34415	-1.03639	0.90042
H	-0.20346	-2.26637	2.72473
C	-2.51095	-1.63943	-1.01710
H	-1.95677	-0.75044	2.66459
H	-4.12011	-0.30899	-0.48763
C	-0.36199	-2.71067	-1.56086
C	-3.15131	-0.61989	-0.08856
N	-1.11679	-1.91607	-0.55578
C	-0.07963	-1.95667	1.68083
H	-2.44439	-1.25029	-2.03416
H	0.92041	-2.25080	1.36320
C	-1.34801	0.09730	2.34567
H	-1.00938	0.60333	3.25411
H	-3.16947	1.19380	1.90187
N	-0.15593	-0.45190	1.59328
N	-2.25854	0.59128	0.06029
C	-2.16249	1.06908	1.48514
H	1.45971	-0.36268	2.99556
C	-2.79655	1.68064	-0.81868
C	1.17544	0.08604	2.03690
H	-1.68459	2.04736	1.45593
Fe	-0.32784	0.05105	-0.39698
H	1.09110	1.16703	2.16931
C	2.16661	-0.23268	0.94264
N	1.61766	-0.38138	-0.29048
H	3.95701	-0.24539	2.12621
C	3.53585	-0.35326	1.13177
C	2.39405	-0.61651	-1.36327
H	1.88315	-0.69006	-2.31533
C	4.35296	-0.60384	0.02420
C	3.77411	-0.73977	-1.23859
H	5.42784	-0.69049	0.14923
H	4.37614	-0.93027	-2.12042
H	-2.14611	2.55064	-0.77930
H	-3.79920	1.95498	-0.47349
H	-2.84664	1.30570	-1.84139
H	0.64212	-2.90467	-1.18042
H	-0.30121	-2.14667	-2.49084
H	-0.87329	-3.66316	-1.74171
O	-0.47331	0.14399	-2.13330
H	-0.26026	1.01776	-2.51735
Br	0.48389	2.39742	-0.25329

^{3}FeMeHPyTACNClOH
Charge: 2+
Energy: -1610599.7927819

H	0.61974	3.11025	1.63419
H	2.88393	2.70889	-0.25278
H	1.90304	1.94386	1.86856
C	0.90619	2.07102	1.44848
H	3.24355	0.67975	1.13131
H	0.01562	1.12172	3.18644
C	2.36627	1.78173	-0.52816
H	1.86385	-0.19848	2.70397
H	4.05440	0.44781	-0.40148
C	0.15243	2.83415	-0.76644
C	3.07123	0.56957	0.06030
N	0.95391	1.81548	-0.03370
C	-0.08838	1.13205	2.09553
H	2.32631	1.71787	-1.61643
H	-1.10443	1.44871	1.86103
C	1.30751	-0.94557	2.13534
H	0.99981	-1.71863	2.84509
H	3.19102	-1.75417	1.41730
N	0.08460	-0.26632	1.56013
N	2.24870	-0.67609	-0.17366
C	2.17887	-1.56671	1.03871
H	-1.52706	-0.88820	2.82320
C	2.83255	-1.42345	-1.33477
C	-1.20786	-0.99989	1.78071
H	1.75869	-2.51456	0.70623
Fe	0.29527	-0.13149	-0.48231
H	-1.04733	-2.06026	1.57476
C	-2.21463	-0.42616	0.81166
N	-1.67386	0.13883	-0.29775
H	-4.00641	-0.90968	1.89019
C	-3.59012	-0.46866	0.99012
C	-2.46040	0.63614	-1.26826
H	-1.95254	1.03821	-2.13623
C	-4.41893	0.05369	-0.00851
C	-3.84660	0.61473	-1.15121
H	-5.49785	0.02007	0.10687
H	-4.45742	1.02426	-1.94843
H	2.21382	-2.28559	-1.57112
H	3.84366	-1.75382	-1.07351
H	2.87281	-0.75209	-2.19306
H	-0.86201	2.84436	-0.36528
H	0.12893	2.57852	-1.82479
H	0.60584	3.82330	-0.63729
O	0.44536	0.31182	-2.16336
H	0.27712	-0.43393	-2.77414
Cl	-0.28289	-2.26901	-0.95964

^{3}FeMeHPyTACNFOH
Charge: 2+
Energy: -1384480.0916250

H	0.60239	1.35167	3.11734
H	2.87676	2.20057	1.39408
H	1.87706	0.28521	2.56821
C	0.88136	0.65379	2.32299
H	3.26021	-0.23565	1.16264
H	-0.02315	-1.16872	3.09172
C	2.35305	1.66294	0.59476
H	1.88308	-1.84833	1.86478
H	4.02613	0.55242	-0.20141
C	0.14457	2.64381	1.07395
C	3.05832	0.35177	0.26616
N	0.93576	1.38088	1.00176
C	-0.12077	-0.48295	2.24240
H	2.30937	2.30728	-0.28470
H	-1.13739	-0.08917	2.24484
C	1.30261	-2.10806	0.97829
H	1.00845	-3.15600	1.08799
H	3.13054	-2.33557	-0.17702
N	0.07431	-1.23112	0.95484
N	2.20627	-0.46663	-0.66981
C	2.12228	-1.92290	-0.29846
H	-1.52163	-2.57696	1.42537
C	2.69684	-0.32976	-2.07698
C	-1.18615	-1.95777	0.58605
H	1.63979	-2.42290	-1.13726
Fe	0.28529	0.15234	-0.53409
H	-0.96522	-2.60227	-0.26759
C	-2.21067	-0.92152	0.19104
N	-1.68640	0.23984	-0.27001
H	-3.99021	-2.03159	0.65426
C	-3.58506	-1.10227	0.26690
C	-2.48442	1.23377	-0.69731
H	-1.98654	2.11636	-1.08044
C	-4.42684	-0.07321	-0.16817
C	-3.86969	1.11061	-0.65501
H	-5.50452	-0.19711	-0.12572
H	-4.49147	1.92748	-1.00497
H	1.98466	-0.81020	-2.74633
H	3.67731	-0.80963	-2.16580
H	2.77902	0.73029	-2.31783
H	-0.87199	2.40643	1.39082

H	0.12360	3.11008	0.08992
H	0.60257	3.32743	1.79680
O	0.39884	1.51753	-1.61108
H	0.20107	1.24638	-2.53127
F	-0.09559	-1.04322	-1.77228

^{3}FeMeHPyTACNN$_3$OH
Charge: 2+
Energy: -1424868.6968248

H	-1.13244	-3.46708	0.30603
H	-3.22737	-2.09437	-1.30628
H	-2.30236	-2.33997	0.95197
C	-1.29900	-2.40989	0.53280
H	-3.46685	-0.72054	0.74165
H	-0.43282	-2.32458	2.52479
C	-2.59380	-1.20582	-1.19305
H	-2.12016	-0.71198	2.53369
H	-4.13695	0.17989	-0.60014
C	-0.50305	-2.34739	-1.79125
C	-3.20730	-0.23092	-0.19750
N	-1.22557	-1.59592	-0.72898
C	-0.25892	-1.92005	1.52101
H	-2.47838	-0.73597	-2.17056
H	0.73379	-2.23871	1.20250
C	-1.44535	0.12243	2.33623
H	-1.12001	0.50041	3.30991
H	-3.15848	1.40434	1.96198
N	-0.25954	-0.41646	1.57165
N	-2.24476	0.89471	0.09324
C	-2.15407	1.23242	1.55668
H	1.32007	-0.46316	3.01995
C	-2.65225	2.10433	-0.68713
C	1.07065	0.04460	2.08116
H	-1.59379	2.16438	1.62474
Fe	-0.34751	0.29379	-0.36010
H	1.00681	1.11886	2.27474
C	2.08625	-0.24034	0.99774
N	1.57062	-0.26479	-0.25894
H	3.83440	-0.44511	2.22823
C	3.43984	-0.45552	1.21720
C	2.36673	-0.47616	-1.32319
H	1.88041	-0.45390	-2.29108
C	4.27622	-0.68057	0.11788
C	3.73245	-0.69398	-1.16775
H	5.33906	-0.84370	0.26730
H	4.35137	-0.86267	-2.04231
H	-1.90720	2.88769	-0.55882
H	-3.62523	2.45667	-0.32828
H	-2.72564	1.83008	-1.74008
H	0.47592	-2.64564	-1.41221
H	-0.37920	-1.70408	-2.66144
H	-1.07087	-3.24163	-2.07198
O	-0.42648	0.53715	-2.10032
H	-0.26175	1.45358	-2.39100
N	0.20320	2.03055	0.06582
N	1.30163	2.46319	-0.30478
N	2.29645	2.93195	-0.61130

^{3}FeMeHPyTACNNCSOH
Charge: 2+
Energy: -1629974.3953404

H	-2.33005	-3.08323	0.50269
H	-3.90095	-1.19232	-1.14044
H	-3.03155	-1.60178	1.10946
C	-2.12416	-2.02353	0.67822
H	-3.61344	0.28839	0.82922
H	-1.21731	-2.14580	2.64924
C	-3.01364	-0.54939	-1.09026
H	-2.26610	-0.06001	2.59745
H	-3.99435	1.29637	-0.54919
C	-1.43887	-2.34405	-1.65521
C	-3.23986	0.61870	-0.14080
N	-1.82371	-1.33498	-0.62767
C	-0.95007	-1.86706	1.62327
H	-2.78542	-0.18949	-2.09407
H	-0.13116	-2.51347	1.30655
C	-1.35890	0.48774	2.33722
H	-0.89480	0.78856	3.28136
H	-2.56184	2.24854	1.91746
N	-0.45101	-0.45088	1.58523
N	-1.94400	1.36332	0.06392
C	-1.69201	1.72694	1.49986
H	1.08824	-0.95183	2.99294
C	-1.95224	2.59226	-0.78683
C	0.97476	-0.43472	2.03280
H	-0.85198	2.42219	1.50109
Fe	-0.39501	0.12913	-0.38400
H	1.27774	0.60692	2.17126
C	1.79837	-1.08623	0.94227
N	1.25036	-1.01097	-0.29574
H	3.43297	-1.78331	2.15056
C	3.01803	-1.71697	1.14983
C	1.89263	-1.52742	-1.35724
H	1.39662	-1.40619	-2.31289
C	3.69208	-2.26211	0.05167
C	3.12160	-2.16680	-1.21855
H	4.64804	-2.75752	0.19032
H	3.61539	-2.57767	-2.09245
H	-0.99590	3.10505	-0.70303
H	-2.75481	3.26181	-0.45926
H	-2.11201	2.29429	-1.82301
H	-0.59836	-2.92913	-1.27828
H	-1.14641	-1.82620	-2.56679
H	-2.28341	-3.01138	-1.85913
O	-0.45130	0.31253	-2.15072
H	0.15537	0.99242	-2.49352
N	0.82273	1.56706	-0.16852
C	1.75524	2.30736	-0.20136
S	2.99113	3.33774	-0.23298

^{3}FeMeHPyTACNOHBr
Charge: 2+
Energy: -2937126.6230058

H	0.28439	-1.57722	3.24535
H	2.73087	-0.06027	2.69176
H	1.52501	-2.11729	2.13712
C	0.58648	-1.56779	2.19449
H	3.01712	-1.70579	0.87315
H	-0.51984	-3.30015	1.49372
C	2.28434	0.16405	1.71501
H	1.43300	-3.22340	0.20861
H	3.97857	-0.30062	0.46774
C	0.09521	0.78167	2.66962
C	2.95266	-0.64793	0.61525
N	0.81487	-0.14497	1.74175
C	-0.47873	-2.21591	1.33682
H	2.39047	1.23243	1.52503
H	-1.45941	-1.80696	1.58038
C	0.96317	-2.71811	-0.63659
H	0.60131	-3.50059	-1.31013
H	2.92585	-2.35268	-1.48239
N	-0.20398	-1.92351	-0.10929
N	2.18712	-0.51210	-0.67904
C	1.96762	-1.83044	-1.37680
H	-1.92624	-3.03944	-0.70448
C	2.92248	0.40363	-1.60839
C	-1.46976	-2.06097	-0.89327
H	1.59883	-1.58936	-2.37268
Fe	0.23646	0.05834	-0.29994
H	-1.22328	-1.98431	-1.95496
C	-2.38271	-0.92752	-0.48685
N	-1.75636	0.19707	-0.04094
H	-4.24499	-1.90942	-0.89944
C	-3.76691	-0.99968	-0.55037
C	-2.48252	1.26571	0.34304
H	-1.92832	2.13555	0.67009
C	-4.52570	0.10888	-0.15930
C	-3.87340	1.25268	0.30066
H	-5.60968	0.07318	-0.20883
H	-4.42408	2.13172	0.61759
H	2.29357	0.61610	-2.47097
H	3.84695	-0.08846	-1.93071
H	3.15760	1.33288	-1.09309
H	-0.96537	0.52567	2.67344
H	0.22193	1.80975	2.33697
H	0.49950	0.67281	3.68194
O	-0.02519	0.01530	-2.03650
H	-0.30385	0.87420	-2.41076
Br	0.63168	2.46135	-0.29832

^{3}FeMeHPyTACNOHCl
Charge: 2+
Energy: -1610599.1134590

H	-0.48952	0.55923	3.41750
H	-2.78554	-1.01333	2.47118
H	-1.76277	1.22577	2.41965
C	-0.78087	0.75630	2.38203
H	-3.20111	0.97324	1.05609
H	0.17989	2.68476	2.09874
C	-2.31148	-0.96878	1.48287
H	-1.74229	2.73381	0.77324
H	-4.03094	-0.38263	0.32300
C	-0.08104	-1.59146	2.32897
C	-3.04121	0.00820	0.57342
N	-0.87846	-0.54299	1.62175
C	0.23282	1.65979	1.71398
H	-2.31262	-1.97069	1.05278
H	1.24239	1.28877	1.89130
C	-1.22575	2.46160	-0.14845
H	-0.92253	3.39621	-0.62907
H	-3.14836	2.12836	-1.09642
N	0.00055	1.66583	0.22902
N	-2.25320	0.22634	-0.69514
C	-2.14907	1.67746	-1.08699

H	1.63157	3.02042	-0.04505
C	-2.87755	-0.54265	-1.81693
C	1.26351	2.07635	-0.46246
H	-1.75784	1.69210	-2.10304
Fe	-0.26945	-0.24356	-0.39252
H	1.04046	2.22019	-1.52230
C	2.26137	0.95436	-0.28936
N	1.71956	-0.28378	-0.12589
H	4.05011	2.13269	-0.42014
C	3.63673	1.13637	-0.29977
C	2.51544	-1.36156	0.01184
H	2.01918	-2.31843	0.11011
C	4.47096	0.02184	-0.15623
C	3.90201	-1.24153	0.00641
H	5.54975	0.14356	-0.16880
H	4.51459	-2.12931	0.12040
H	-2.22684	-0.49465	-2.68796
H	-3.85120	-0.09878	-2.05241
H	-3.00409	-1.58113	-1.51624
H	0.95012	-1.24836	2.42509
H	-0.10733	-2.51835	1.75967
H	-0.50255	-1.76088	3.32582
O	0.00781	0.20587	-2.06916
H	0.31842	-0.55115	-2.60479
Cl	-0.45424	-2.42244	-0.84020

^{3}FeMeHPyTACNOHF
Charge: 2+
Energy: -1384476.9241580

H	0.59160	1.37851	3.11779
H	2.85144	2.24573	1.36811
H	1.87212	0.31728	2.57339
C	0.87568	0.68123	2.32404
H	3.24959	-0.19548	1.17844
H	-0.02932	-1.14325	3.09451
C	2.32755	1.68704	0.58312
H	1.86698	-1.83573	1.88838
H	4.01976	0.58889	-0.18585
C	0.10792	2.64163	1.04560
C	3.05008	0.38092	0.27433
N	0.91878	1.39308	1.00162
C	-0.12217	-0.45759	2.24471
H	2.27097	2.31386	-0.30823
H	-1.13901	-0.06326	2.24299
C	1.30384	-2.09522	0.99077
H	1.00836	-3.14320	1.09280
H	3.16558	-2.30133	-0.11264
N	0.06773	-1.21984	0.95922
N	2.22325	-0.46055	-0.66471
C	2.15316	-1.91170	-0.27073
H	-1.53345	-2.53510	1.50143
C	2.72215	-0.31468	-2.06800
C	-1.20356	-1.95038	0.63573
H	1.70696	-2.43738	-1.11338
Fe	0.29237	0.11698	-0.54707
H	-0.99693	-2.62653	-0.19698
C	-2.22388	-0.91571	0.21914
N	-1.68772	0.20700	-0.32367
H	-4.01913	-1.95276	0.78233
C	-3.59988	-1.05786	0.33364
C	-2.46900	1.19420	-0.79758
H	-1.95573	2.03658	-1.24694
C	-4.42667	-0.03413	-0.14482
C	-3.85603	1.10397	-0.71865
H	-5.50569	-0.12868	-0.07059
H	-4.46883	1.91078	-1.10596
H	2.03635	-0.82392	-2.74214
H	3.72386	-0.75203	-2.13812
H	2.75416	0.74595	-2.31760
H	-0.90530	2.39652	1.36898
H	0.07821	3.07856	0.04821
H	0.55131	3.35534	1.74857
O	-0.03388	-1.12519	-1.79331
H	-0.82856	-0.90528	-2.31411
F	0.42384	1.47643	-1.58869

^{3}FeMeHPyTACNOHN$_3$
Charge: 2+
Energy: -1424868.6631212

H	0.36864	-2.39277	2.68897
H	2.78112	-0.65063	2.67758
H	1.66589	-2.49228	1.52201
C	0.69717	-2.03030	1.71059
H	3.11518	-1.61405	0.42696
H	-0.28342	-3.49803	0.44112
C	2.30218	-0.15632	1.82321
H	1.67835	-2.88259	-0.69976
H	4.01292	-0.11511	0.50662
C	0.09531	0.03435	2.88992
C	3.00299	-0.53364	0.52311
N	0.85510	-0.53329	1.74166
C	-0.30978	-2.42133	0.64578
H	2.34653	0.92218	1.98433
H	-1.31777	-2.17100	0.97755
C	1.16684	-2.17533	-1.35445
H	0.85011	-2.73758	-2.23793
H	3.08203	-1.41691	-2.04014
N	-0.04188	-1.65505	-0.61764
N	2.22446	-0.01961	-0.66198
C	2.09224	-1.03154	-1.76764
H	-1.67991	-2.62168	-1.60071
C	2.87576	1.21540	-1.19728
C	-1.28635	-1.61034	-1.44658
H	1.68017	-0.49750	-2.62292
Fe	0.28855	0.30997	-0.11973
H	-1.02603	-1.18022	-2.41678
C	-2.27676	-0.72419	-0.72720
N	-1.71137	0.22517	0.06384
H	-4.08879	-1.61609	-1.45843
C	-3.65673	-0.84264	-0.83146
C	-2.48807	1.07666	0.76127
H	-1.96939	1.80860	1.36864
C	-4.46918	0.04381	-0.11671
C	-3.87638	1.01298	0.69487
H	-5.55004	-0.02817	-0.18886
H	-4.47363	1.71380	1.26816
H	2.22447	1.66878	-1.94299
H	3.83670	0.95225	-1.65226
H	3.04583	1.91018	-0.37388
H	-0.94859	-0.27485	2.81132
H	0.15509	1.12176	2.86067
H	0.51038	-0.32930	3.83648
O	0.03851	0.90592	-1.78953
H	-0.82494	1.33933	-1.91873
N	0.50284	1.95756	0.63733
N	0.49477	2.99065	-0.04637
N	0.50227	3.98170	-0.60717

^{3}FeMeHPyTACNOHNCS
Charge: 2+
Energy: -1629974.2889713

H	-0.48933	-1.88075	3.12604
H	2.41983	-1.36648	2.67389
H	0.52168	-2.77458	2.01531
C	-0.14519	-1.91604	2.08815
H	2.06036	-2.86725	0.73724
H	-1.76668	-3.07054	1.21164
C	2.08829	-0.92914	1.72362
H	0.10244	-3.61804	-0.06114
H	3.50195	-1.92706	0.43010
C	0.29253	0.40957	2.73134
C	2.41821	-1.85298	0.55721
N	0.61541	-0.66098	1.75103
C	-1.33084	-2.06672	1.15244
H	2.58994	0.03304	1.60134
H	-2.10843	-1.35230	1.42349
C	-0.12918	-2.91428	-0.86265
H	-0.74706	-3.45344	-1.58642
H	1.84747	-3.22344	-1.70694
N	-0.91596	-1.77380	-0.26473
N	1.78837	-1.32859	-0.70453
C	1.14259	-2.40114	-1.53494
H	-2.91336	-2.14313	-0.94673
C	2.82035	-0.62684	-1.52604
C	-2.12800	-1.38617	-1.05397
H	0.90338	-1.94058	-2.49255
Fe	0.20895	-0.11933	-0.24826
H	-1.83393	-1.31522	-2.10337
C	-2.57756	-0.03255	-0.55530
N	-1.59503	0.72870	-0.00705
H	-4.65713	-0.20336	-1.06468
C	-3.88634	0.42715	-0.63317
C	-1.88302	1.95523	0.46807
H	-1.05590	2.51165	0.89106
C	-4.18723	1.70329	-0.14871
C	-3.17088	2.47696	0.41532
H	-5.20250	2.08346	-0.20519
H	-3.36664	3.46899	0.80757
H	2.32547	-0.11819	-2.35134
H	3.54505	-1.35433	-1.90765
H	3.33698	0.10137	-0.89980
H	-0.78646	0.57359	2.73664
H	0.79377	1.33214	2.43914
H	0.61981	0.12351	3.73738
O	0.00937	0.11589	-2.01364
H	-0.19679	1.04222	-2.23290
N	1.17185	1.47849	-0.05349
C	1.76317	2.50758	-0.16943
S	2.56716	3.89274	-0.29178

^{4}FeMeHPyTACNOHOH
Charge: 2+
Energy: -1369399.4145696

H	0.51897	1.37612	3.11548

H	2.82872	2.22859	1.43781
H	1.81728	0.32263	2.60334
C	0.82514	0.68034	2.32885
H	3.21685	-0.20769	1.24223
H	-0.07883	-1.14596	3.09019
C	2.32181	1.68201	0.63307
H	1.84415	-1.82924	1.91811
H	4.02573	0.57625	-0.09718
C	0.10325	2.65318	1.05305
C	3.04258	0.37259	0.33549
N	0.90048	1.39646	1.00811
C	-0.16244	-0.46735	2.23343
H	2.29718	2.31646	-0.25393
H	-1.18158	-0.07998	2.21416
C	1.29263	-2.09558	1.01519
H	1.00401	-3.14550	1.12078
H	3.16306	-2.31026	-0.06901
N	0.05899	-1.22748	0.95644
N	2.23468	-0.46287	-0.62608
C	2.15436	-1.91379	-0.23525
H	-1.53647	-2.57317	1.44004
C	2.79957	-0.33712	-2.00525
C	-1.19290	-1.96506	0.59560
H	1.71196	-2.43484	-1.08330
Fe	0.29453	0.13090	-0.57107
H	-0.96119	-2.62483	-0.24426
C	-2.21951	-0.93393	0.18504
N	-1.68990	0.20543	-0.33072
H	-4.00276	-2.00008	0.73104
C	-3.59415	-1.08995	0.30368
C	-2.48631	1.20371	-0.75580
H	-1.98216	2.06867	-1.17042
C	-4.43236	-0.05817	-0.13425
C	-3.87188	1.10383	-0.66841
H	-5.51010	-0.16225	-0.05461
H	-4.49198	1.92250	-1.01732
H	2.13722	-0.83823	-2.70917
H	3.79289	-0.79773	-2.03281
H	2.87783	0.72186	-2.25382
H	-0.91868	2.41397	1.35271
H	0.09708	3.10778	0.06318
H	0.53911	3.35127	1.77632
O	0.00647	-1.07089	-1.86700
O	0.44470	1.53202	-1.61263
H	0.40828	1.27998	-2.55546
H	-0.89224	-1.01767	-2.24026

^{4}FeL2Br
Charge: -2
Energy: -3174928.6973333

C	2.92778	-3.52459	-1.43747
C	2.21229	-2.36478	-1.20045
N	2.82369	-1.20619	-0.69498
C	4.18827	-1.31377	-0.44868
C	4.93373	-2.43891	-0.69067
C	4.31676	-3.61015	-1.21520
C	0.73694	-2.30716	-1.51351
Fe	1.95345	0.50759	-0.14396
N	-0.07481	0.04925	0.62773
C	-0.04059	-0.92207	1.72428
C	0.23308	-2.24291	0.96479
N	-0.20462	-1.99394	-0.41922
C	-0.85146	-0.67987	-0.46078
C	-0.53689	1.40211	0.96871
C	-0.23070	2.34868	-0.16993
N	1.00268	2.12766	-0.77839
C	1.36583	3.03231	-1.75533
C	0.56685	4.07807	-2.16245
C	-0.70656	4.27011	-1.57725
C	-1.07854	3.36303	-0.55592
H	-2.04529	3.44304	-0.06393
H	-1.36978	5.06873	-1.89544
H	0.92810	4.74198	-2.94686
H	2.34247	2.85610	-2.19951
H	4.63675	-0.42799	-0.00912
H	5.99754	-2.41981	-0.45827
H	4.87498	-4.52123	-1.41099
H	2.38008	-4.38840	-1.81367
H	0.75849	-0.65574	2.42222
H	-1.00611	-0.95764	2.25317
H	1.30025	-2.48450	0.99072
H	-0.31558	-3.07950	1.42189
H	0.45984	-3.27217	-1.96571
H	0.57071	-1.54386	-2.28987
H	-1.60618	1.41614	1.22003
H	0.04741	1.70440	1.84930
H	-0.60491	-0.16259	-1.39486
C	-2.34939	-0.70170	-0.28474
C	-3.14697	0.36029	-0.79963
C	-3.03879	-1.73130	0.41251
C	-4.51243	0.40944	-0.61603
H	-2.65450	1.16004	-1.35240
C	-4.40484	-1.70099	0.60709
H	-2.47384	-2.58774	0.77444
C	-5.21248	-0.61763	0.10955
H	-5.09886	1.22805	-1.02556
H	-4.89423	-2.51543	1.13491
C	-6.61934	-0.53279	0.28012
O	-7.40588	0.35659	-0.12492
O	-7.19161	-1.60961	1.00550
H	-8.12827	-1.34914	0.99750
Br	3.27278	1.29384	2.00687

^{4}FeL2Cl
Charge: -2
Energy: -1848396.8637882

C	3.38793	-3.17185	-1.37286
C	2.60448	-2.07106	-1.07772
N	3.12975	-0.93464	-0.44297
C	4.48234	-1.00369	-0.12556
C	5.29516	-2.06778	-0.42133
C	4.76682	-3.21353	-1.08209
C	1.14448	-2.05477	-1.46075
Fe	2.17600	0.69724	0.22678
N	0.11988	0.09635	0.81471
C	0.13680	-0.95907	1.83007
C	0.51757	-2.19989	0.98605
N	0.14135	-1.85900	-0.39580
C	-0.55847	-0.57197	-0.37321
C	-0.42173	1.39823	1.22876
C	-0.09514	2.44182	0.18422
N	1.18103	2.31742	-0.36239
C	1.55989	3.31517	-1.23873
C	0.74106	4.35783	-1.61103
C	-0.57420	4.45104	-1.09445
C	-0.96371	3.44912	-0.17189
H	-1.95952	3.45145	0.26618
H	-1.25280	5.24539	-1.39019
H	1.11873	5.09784	-2.31584
H	2.56816	3.21479	-1.63352
H	4.86071	-0.14252	0.41728
H	6.34255	-2.02239	-0.12591
H	5.37931	-4.07769	-1.32330
H	2.90392	-4.02381	-1.85014
H	0.88121	-0.71784	2.59465
H	-0.85438	-1.08069	2.29514
H	1.59301	-2.39163	1.05397
H	-0.01111	-3.09561	1.34455
H	0.93381	-2.99670	-1.99109
H	0.97819	-1.24720	-2.19071
H	-1.50294	1.34857	1.41730
H	0.09704	1.65393	2.16392
H	-0.28115	0.02976	-1.24595
C	-2.06194	-0.67072	-0.29029
C	-2.87958	0.39560	-0.76278
C	-2.73914	-1.78617	0.27411
C	-4.25422	0.36827	-0.66029
H	-2.39581	1.26102	-1.21494
C	-4.11402	-1.83322	0.38599
H	-2.15444	-2.64532	0.59609
C	-4.94392	-0.74752	-0.06791
H	-4.85545	1.19270	-1.03529
H	-4.59237	-2.71132	0.81210
C	-6.36068	-0.74027	0.02169
O	-7.16598	0.14492	-0.35518
O	-6.92027	-1.90053	0.61740
H	-7.86653	-1.68186	0.57242
Cl	3.30359	1.31774	2.28790

^{4}FeL2F
Charge: -2
Energy: -1622262.0272723

C	3.56601	-3.04072	-1.22649
C	2.69386	-2.00903	-0.93875
N	3.14639	-0.74792	-0.51676
C	4.53047	-0.59402	-0.52377
C	5.43256	-1.58227	-0.82384
C	4.97149	-2.88323	-1.17511
C	1.20776	-2.20273	-1.17907
Fe	2.28169	0.67446	0.65029
N	0.15587	0.13808	1.02365
C	0.13196	-0.90032	2.05652
C	0.65269	-2.11858	1.26746
N	0.25938	-1.85712	-0.12036
C	-0.40984	-0.55382	-0.20060
C	-0.42793	1.44087	1.36915
C	0.02808	2.48424	0.37631
N	1.37723	2.37357	0.02576
C	1.86706	3.39117	-0.77694
C	1.10169	4.42677	-1.25910
C	-0.28170	4.50541	-0.94259
C	-0.78960	3.48471	-0.09349
H	-1.83753	3.47572	0.20086
H	-0.91892	5.29397	-1.33139
H	1.57314	5.17922	-1.89182

H	2.92641	3.31177	-1.01582
H	4.88064	0.40277	-0.25542
H	6.49698	-1.35077	-0.79116
H	5.65160	-3.69655	-1.41174
H	3.13808	-3.99736	-1.52786
H	0.80305	-0.61185	2.87078
H	-0.88776	-1.06884	2.43759
H	1.74539	-2.18203	1.35765
H	0.22217	-3.05847	1.64815
H	1.06320	-3.25811	-1.46185
H	0.90448	-1.61257	-2.05648
H	-1.52383	1.39786	1.43300
H	-0.02338	1.68843	2.36286
H	-0.04088	0.02217	-1.05754
C	-1.91674	-0.64125	-0.25653
C	-2.68532	0.40971	-0.83205
C	-2.64286	-1.73168	0.29402
C	-4.06422	0.38858	-0.84277
H	-2.15965	1.25970	-1.26685
C	-4.02275	-1.77212	0.29491
H	-2.08485	-2.57590	0.69513
C	-4.80663	-0.70337	-0.26866
H	-4.62855	1.20070	-1.29428
H	-4.53949	-2.63157	0.71449
C	-6.22560	-0.69010	-0.29660
O	-6.99455	0.18056	-0.77240
O	-6.83924	-1.82579	0.29636
H	-7.77683	-1.60567	0.16316
F	2.92535	0.67198	2.37346

^{4}FeL2N$_3$
Charge: -2
Energy: -1662657.8117013

C	-1.27836	-0.78737	3.62660
C	-1.50010	-1.03982	2.28438
N	-2.28211	-0.19412	1.48695
C	-2.79908	0.91637	2.13039
C	-2.61304	1.19968	3.46090
C	-1.83868	0.32923	4.27357
C	-0.93479	-2.26211	1.61718
Fe	-2.32505	-0.23800	-0.52374
N	-0.15861	-0.47092	-1.05342
C	0.10325	-1.72175	-1.77405
C	-0.09685	-2.77392	-0.67005
N	0.12223	-2.06025	0.59798
C	0.56923	-0.69836	0.28055
C	0.17385	0.74194	-1.82081
C	-0.60089	1.93220	-1.32209
N	-1.95039	1.66176	-1.08345
C	-2.73353	2.77243	-0.81538
C	-2.23997	4.05217	-0.68938
C	-0.85528	4.30267	-0.85135
C	-0.04806	3.18510	-1.18883
H	1.02083	3.29970	-1.35936
H	-0.43265	5.29625	-0.73578
H	-2.93221	4.86402	-0.46659
H	-3.79561	2.56372	-0.70057
H	-3.36394	1.59150	1.49499
H	-3.05924	2.10380	3.87152
H	-1.66454	0.52690	5.32712
H	-0.64838	-1.48365	4.17786
H	-0.61739	-1.83821	-2.58937
H	1.12923	-1.74083	-2.17298
H	-1.12556	-3.15487	-0.71853
H	0.59087	-3.62375	-0.79551
H	-1.77736	-2.78280	1.12772
H	-0.55616	-2.93661	2.40060
H	1.25482	0.93024	-1.83260
H	-0.14937	0.53328	-2.85331
H	0.14816	0.02207	0.98425
C	2.06469	-0.52324	0.22463
C	2.63118	0.77575	0.37514
C	2.97391	-1.58721	-0.02043
C	3.98611	1.00334	0.26351
H	1.96222	1.61302	0.57930
C	4.33425	-1.38139	-0.13359
H	2.58513	-2.60159	-0.08514
C	4.90923	-0.06694	-0.00970
H	4.39429	2.00305	0.38820
H	4.99701	-2.22525	-0.30711
C	6.29785	0.20545	-0.12359
O	6.89259	1.30514	-0.02074
O	7.10277	-0.93357	-0.38640
H	7.98317	-0.52238	-0.41923
N	-3.30000	-1.57435	-1.65514
N	-4.33030	-2.05214	-2.03145
N	-5.31290	-2.54817	-2.42528

^{4}FeL2NCS
Charge: -2
Energy: -1867773.5298175

C	-0.91208	1.39635	3.62178
C	-1.24509	0.50977	2.61264
N	-2.08600	0.87017	1.55409
C	-2.59351	2.15640	1.61736
C	-2.29996	3.06569	2.60475
C	-1.42711	2.70570	3.66161
C	-0.74069	-0.91075	2.64857
Fe	-2.17870	-0.00524	-0.26129
N	-0.11681	-0.73649	-0.64990
C	-0.05230	-2.20201	-0.66965
C	-0.31335	-2.54138	0.80488
N	0.13495	-1.35883	1.55157
C	0.68837	-0.38054	0.60888
C	0.27425	-0.09659	-1.91670
C	-0.30021	1.29156	-2.01669
N	-1.63014	1.38285	-1.61098
C	-2.22853	2.61157	-1.81946
C	-1.57139	3.71303	-2.32441
C	-0.20542	3.62645	-2.67685
C	0.41227	2.36252	-2.50872
H	1.45955	2.21379	-2.76309
H	0.34450	4.48099	-3.05938
H	-2.12254	4.64482	-2.44659
H	-3.28135	2.65919	-1.55128
H	-3.25246	2.42841	0.79837
H	-2.74734	4.05690	2.55556
H	-1.16464	3.39926	4.45487
H	-0.23476	1.04999	4.40046
H	-0.82747	-2.60217	-1.32983
H	0.93809	-2.55131	-0.99951
H	-1.38965	-2.70724	0.95352
H	0.21896	-3.45594	1.10813
H	-1.62019	-1.57692	2.65105
H	-0.23277	-1.06016	3.61428
H	1.36312	-0.09870	-2.05230
H	-0.17451	-0.71436	-2.71061
H	0.38852	0.63444	0.88289
C	2.18305	-0.43293	0.44304
C	2.88345	0.70406	-0.05477
C	2.95957	-1.59344	0.70748
C	4.24055	0.68193	-0.29388
H	2.31835	1.61519	-0.25606
C	4.31970	-1.63536	0.47716
H	2.46568	-2.46305	1.13745
C	5.02845	-0.49754	-0.04914
H	4.75429	1.56385	-0.66782
H	4.88057	-2.53769	0.70618
C	6.42409	-0.48399	-0.31122
O	7.12808	0.45377	-0.75518
O	7.08941	-1.70232	-0.02242
H	8.00098	-1.46896	-0.26708
N	-3.45934	-1.52673	-0.65850
C	-4.23130	-2.39600	-0.88369
S	-5.30214	-3.60809	-1.19666

^{4}FeL2OH
Charge: -2
Energy: -1607166.2181461

C	-2.36761	-1.90101	2.62864
C	-2.08542	-1.90469	1.27856
N	-2.91531	-1.27393	0.34050
C	-4.13867	-0.83140	0.84922
C	-4.46873	-0.81751	2.18388
C	-3.55670	-1.32464	3.14452
C	-0.91613	-2.72666	0.75892
Fe	-2.42102	0.05891	-1.11536
N	-0.17994	-0.10658	-1.28777
C	0.09241	-1.08157	-2.34496
C	-0.33476	-2.37933	-1.64674
N	-0.01328	-2.14997	-0.23397
C	0.39674	-0.75371	-0.03815
C	0.21258	1.28366	-1.55003
C	-0.50831	2.20794	-0.60160
N	-1.85017	1.86954	-0.40711
C	-2.57070	2.73427	0.39904
C	-2.04339	3.86362	0.97837
C	-0.67678	4.20383	0.77632
C	0.07805	3.31435	-0.03130
H	1.13829	3.48623	-0.20912
H	-0.22284	5.07010	1.24844
H	-2.68509	4.48205	1.60618
H	-3.60477	2.43854	0.56567
H	-4.84421	-0.47508	0.09823
H	-5.44454	-0.43390	2.48281
H	-3.77605	-1.32167	4.20845
H	-1.66431	-2.39093	3.30236
H	-0.52891	-0.85920	-3.21801
H	1.15865	-1.09785	-2.62310
H	-1.41263	-2.53455	-1.79614
H	0.20270	-3.25358	-2.04913
H	-1.30671	-3.65110	0.30261
H	-0.32393	-3.04362	1.63079
H	1.30116	1.42400	-1.50316
H	-0.12441	1.48973	-2.58065

H	-0.14607	-0.30569	0.80362
C	1.88406	-0.57846	0.15174
C	2.40310	0.56125	0.82887
C	2.83554	-1.49115	-0.37763
C	3.75819	0.78605	0.95226
H	1.69985	1.27958	1.24995
C	4.19624	-1.28551	-0.26529
H	2.46861	-2.39800	-0.85537
C	4.72804	-0.12447	0.40077
H	4.13011	1.66129	1.47910
H	4.89071	-2.01612	-0.67249
C	6.11473	0.14129	0.54438
O	6.67600	1.11007	1.11260
O	6.96760	-0.83464	-0.03866
H	7.83640	-0.45660	0.17941
O	-3.16135	-0.15901	-2.86454
H	-3.13745	0.69287	-3.32656

^{6}FeLABrOH
Charge: 1+
Energy: -3016953.5023740

Fe	0.12282	-0.32266	-0.75522
N	0.09600	0.23690	1.57501
N	-1.94533	-0.48736	-0.15004
N	2.14309	0.17579	-0.22758
N	-1.37977	3.68495	-1.03938
H	-1.81766	4.45719	-1.52408
N	-0.34861	1.79030	-0.69100
C	-1.04841	-0.53316	2.10354
H	-1.33439	-0.20480	3.11235
H	-0.73605	-1.58125	2.16405
C	-2.23502	-0.47914	1.16420
C	-3.55438	-0.50321	1.61055
H	-3.76740	-0.49079	2.67480
C	-4.58577	-0.55277	0.67105
H	-5.62094	-0.57823	0.99767
C	-4.27149	-0.56713	-0.68878
H	-5.04482	-0.60685	-1.44813
C	-2.93091	-0.52624	-1.05948
H	-2.60600	-0.52137	-2.09485
C	1.41169	-0.24608	2.04837
H	1.37620	-1.33998	2.06587
H	1.64444	0.10508	3.06303
C	2.49625	0.16373	1.07303
C	3.79777	0.46310	1.46740
H	4.06037	0.45567	2.52055
C	4.74952	0.76253	0.49040
H	5.77112	0.99333	0.77653
C	4.37219	0.76715	-0.85313
H	5.08240	0.99703	-1.63977
C	3.05046	0.47095	-1.17183
H	2.67949	0.45863	-2.19149
C	-0.04788	1.70970	1.76442
H	0.94651	2.11393	1.98262
H	-0.67626	1.92875	2.63678
C	-0.57919	2.38050	0.53094
C	-1.22749	3.57175	0.33251
H	-1.57435	4.33387	1.01321
C	-0.84255	2.58698	-1.62158
H	-0.83960	2.37827	-2.68090
O	0.04837	-0.23070	-2.58377
H	0.18110	-1.06947	-3.05774
Br	0.49741	-2.74886	-0.32867

^{6}FeLAClOH
Charge: 1+
Energy: -1690425.3273911

Fe	0.13280	-0.47356	-0.87684
N	0.13932	-0.30360	1.51074
N	-1.94934	-0.60467	-0.28660
N	2.18177	-0.14869	-0.29750
N	-1.10557	3.61928	-0.47848
H	-1.48571	4.48991	-0.82556
N	-0.21489	1.62403	-0.45567
C	-1.04086	-1.09815	1.90790
H	-1.30275	-0.94555	2.96410
H	-0.78339	-2.15346	1.77037
C	-2.22909	-0.81180	1.01325
C	-3.54453	-0.83499	1.47131
H	-3.74969	-0.99722	2.52476
C	-4.58301	-0.65600	0.55546
H	-5.61565	-0.67601	0.89042
C	-4.27913	-0.44949	-0.79094
H	-5.05839	-0.30841	-1.53196
C	-2.94059	-0.42422	-1.17158
H	-2.62251	-0.25590	-2.19542
C	1.42972	-0.92867	1.87449
H	1.33789	-2.00382	1.69308
H	1.68147	-0.77899	2.93342
C	2.53288	-0.40339	0.97816
C	3.84589	-0.23286	1.40995
H	4.10739	-0.43485	2.44387
C	4.81008	0.19226	0.49355
H	5.84043	0.32647	0.80857
C	4.43427	0.44721	-0.82593
H	5.15429	0.78048	-1.56526
C	3.10083	0.26754	-1.18203
H	2.72987	0.44991	-2.18539
C	0.06935	1.11882	1.95245
H	1.07844	1.42554	2.24849
H	-0.56390	1.21717	2.84303
C	-0.40525	2.02006	0.84862
C	-0.96535	3.27122	0.85459
H	-1.25859	3.93361	1.65443
C	-0.64712	2.59646	-1.23807
H	-0.65514	2.56520	-2.31724
O	0.05919	-0.05944	-2.66254
H	0.14396	-0.81148	-3.27344
Cl	0.36518	-2.75194	-0.80217

^{6}FeLAFOH
Charge: 1+
Energy: -1464300.5541630

Fe	-0.13707	-0.33222	1.08963
N	-0.14991	-0.93693	-1.20989
N	1.96182	-0.54929	0.55589
N	-2.19960	-0.18432	0.45413
N	0.99606	3.45583	-0.69903
H	1.35374	4.40147	-0.67624
N	0.15366	1.55296	-0.02381
C	1.03992	-1.80692	-1.29539
H	1.28503	-2.07176	-2.33337
H	0.80215	-2.72574	-0.75079
C	2.23216	-1.17809	-0.60276
C	3.53787	-1.28719	-1.07502
H	3.73597	-1.79203	-2.01524
C	4.57762	-0.74430	-0.31646
H	5.60367	-0.82149	-0.66334
C	4.28389	-0.10117	0.88660
H	5.06514	0.33078	1.50258
C	2.95220	-0.01982	1.28600
H	2.63847	0.47605	2.19929
C	-1.43056	-1.67136	-1.29557
H	-1.31563	-2.58378	-0.70370
H	-1.68660	-1.95076	-2.32680
C	-2.54041	-0.85506	-0.66313
C	-3.84203	-0.81539	-1.15659
H	-4.09627	-1.35464	-2.06363
C	-4.80522	-0.07824	-0.46313
H	-5.82699	-0.03666	-0.82815
C	-4.43982	0.60659	0.69630
H	-5.15999	1.19000	1.25949
C	-3.11593	0.53007	1.12164
H	-2.75096	1.03888	2.00827
C	-0.10021	0.24023	-2.11778
H	-1.10772	0.39844	-2.51819
H	0.55193	0.04112	-2.97760
C	0.33657	1.48065	-1.38706
C	0.86572	2.66609	-1.82846
H	1.14467	3.01782	-2.80978
C	0.56163	2.74539	0.36989
H	0.56940	3.09225	1.39239
O	-0.05926	0.62748	2.65570
H	-0.12238	0.11902	3.48154
F	-0.29558	-2.08753	1.41685

^{6}FeLAN$_3$OH
Charge: 1+
Energy: -1504685.1892923

Fe	0.18756	-0.32567	-0.93970
N	0.21935	-0.27527	1.47597
N	-1.91358	-0.31270	-0.31145
N	2.26073	-0.24274	-0.35616
N	-0.76779	3.81892	-0.27496
H	-1.10166	4.72914	-0.56268
N	-0.00682	1.77217	-0.38884
C	-1.03991	-0.93286	1.87514
H	-1.28599	-0.73647	2.92822
H	-0.90544	-2.01516	1.77773
C	-2.20206	-0.53794	0.98270
C	-3.51410	-0.48214	1.44978
H	-3.72514	-0.66277	2.49911
C	-4.54207	-0.20313	0.54830
H	-5.57181	-0.16199	0.89005
C	-4.23095	0.02373	-0.79340
H	-5.00197	0.24266	-1.52408
C	-2.89606	-0.03465	-1.18189
H	-2.57269	0.14524	-2.20244
C	1.43007	-1.07007	1.77008
H	1.20999	-2.11054	1.51122
H	1.70836	-1.03557	2.83282
C	2.58339	-0.61046	0.89938
C	3.90537	-0.59593	1.33692
H	4.14390	-0.88662	2.35516

C	4.90846	-0.20654	0.44613
H	5.94604	-0.19177	0.76572
C	4.56204	0.16956	-0.85202
H	5.31251	0.48176	-1.56999
C	3.21795	0.14133	-1.21426
H	2.86745	0.42529	-2.20147
C	0.33465	1.12375	1.97316
H	1.39169	1.31145	2.19113
H	-0.21052	1.25066	2.91735
C	-0.12655	2.11074	0.94041
C	-0.60467	3.39207	1.03228
H	-0.82617	4.02780	1.87563
C	-0.40155	2.81061	-1.10241
H	-0.44599	2.83765	-2.18085
O	0.16508	0.21899	-2.69963
H	0.15883	-0.48624	-3.36789
N	0.13463	-2.26384	-0.95738
N	-0.68980	-3.07720	-0.59798
N	-1.46427	-3.85327	-0.24169

^{6}FeLANCSOH
Charge: 1+
Energy: -1709793.5355214

Fe	-0.12907	-0.01383	-0.98134
N	-0.15780	0.15446	1.42471
N	1.93950	0.33635	-0.38775
N	-2.17459	-0.33819	-0.35693
N	1.39077	-3.89804	-0.00300
H	1.84800	-4.77307	-0.22235
N	0.33739	-2.00082	-0.26688
C	0.98382	1.03721	1.73806
H	1.25450	0.99023	2.80224
H	0.68078	2.06841	1.52780
C	2.19114	0.73072	0.87355
C	3.49752	0.91395	1.32353
H	3.67999	1.22747	2.34660
C	4.55532	0.69707	0.43919
H	5.58009	0.84030	0.76819
C	4.28073	0.29174	-0.86792
H	5.07539	0.11298	-1.58407
C	2.95151	0.11573	-1.24043
H	2.65725	-0.21159	-2.23265
C	-1.47605	0.76606	1.69628
H	-1.42654	1.82034	1.40833
H	-1.73814	0.73010	2.76302
C	-2.55019	0.09278	0.86326
C	-3.86501	-0.04626	1.30221
H	-4.14557	0.29927	2.29224
C	-4.80607	-0.62783	0.45022
H	-5.83701	-0.74057	0.77161
C	-4.40547	-1.06734	-0.81216
H	-5.10628	-1.52721	-1.50029
C	-3.07207	-0.90641	-1.17735
H	-2.68406	-1.22668	-2.13908
C	-0.04322	-1.19745	2.04196
H	-1.05239	-1.52058	2.31979
H	0.54178	-1.15460	2.96951
C	0.53255	-2.19712	1.08211
C	1.19385	-3.38313	1.26745
H	1.52307	-3.90184	2.15454
C	0.86587	-3.03183	-0.90170
H	0.89502	-3.14766	-1.97471
O	-0.00108	-0.67811	-2.69091
H	-0.11464	-0.03848	-3.41389
N	-0.41779	1.90445	-1.16267
C	-0.42940	3.01671	-0.71624
S	-0.44489	4.47516	-0.05745

^{6}FeLAOHBr
Charge: 1+
Energy: -3016952.9752284

Fe	0.14619	0.47017	-0.63554
N	0.12513	-1.82447	-0.47174
N	-1.98633	-0.04047	-0.65239
N	2.20980	-0.08647	-0.23105
N	-1.08295	0.03620	3.53146
H	-1.45758	0.35001	4.41693
N	-0.19276	0.09621	1.53139
C	-1.06557	-2.19299	-1.26912
H	-1.30160	-3.26160	-1.17642
H	-0.82580	-1.97847	-2.31509
C	-2.25705	-1.33719	-0.89648
C	-3.56204	-1.82238	-0.87044
H	-3.75514	-2.87301	-1.06283
C	-4.60696	-0.93551	-0.60224
H	-5.63297	-1.29022	-0.58152
C	-4.31588	0.40699	-0.36055
H	-5.09923	1.12763	-0.15226
C	-2.98430	0.81491	-0.38911
H	-2.68528	1.84134	-0.20239
C	1.40390	-2.18684	-1.12749
H	1.30750	-1.92530	-2.18515
H	1.61811	-3.26088	-1.04650
C	2.52915	-1.35854	-0.54361
C	3.82195	-1.84419	-0.36756
H	4.05351	-2.87503	-0.61638
C	4.80523	-0.98361	0.12622
H	5.82132	-1.33931	0.26738
C	4.46487	0.33201	0.44013
H	5.19947	1.03004	0.82647
C	3.14769	0.74290	0.24967
H	2.81340	1.75080	0.47269
C	0.06574	-2.30359	0.93996
H	1.07603	-2.61441	1.22651
H	-0.57268	-3.19218	1.01656
C	-0.39536	-1.22384	1.87610
C	-0.95501	-1.28035	3.12599
H	-1.25470	-2.10651	3.75226
C	-0.61840	0.83498	2.54116
H	-0.61716	1.91475	2.56600
O	0.31441	0.26438	-2.44717
H	0.35879	1.06722	-2.99276
Br	0.12170	2.91577	-0.26576

^{6}FeLAOHCl
Charge: 1+
Energy: -1690425.0372244

Fe	0.14926	0.40225	-0.92007
N	0.15233	-1.61703	0.21638
N	-1.96782	-0.09355	-0.70208
N	2.21079	0.08228	-0.33120
N	-1.07180	1.76503	3.04045
H	-1.45126	2.42600	3.70523
N	-0.17520	0.96524	1.21024
C	-1.03551	-2.29807	-0.34352
H	-1.26592	-3.22593	0.19726
H	-0.79774	-2.54936	-1.38170
C	-2.23222	-1.37120	-0.36929
C	-3.53576	-1.80250	-0.13693
H	-3.72587	-2.83523	0.13776
C	-4.58323	-0.88849	-0.27138
H	-5.60808	-1.20343	-0.09975
C	-4.29715	0.43005	-0.62591
H	-5.08336	1.16789	-0.74340
C	-2.96695	0.79064	-0.82764
H	-2.66845	1.79897	-1.09665
C	1.43553	-2.20898	-0.22938
H	1.33493	-2.42726	-1.29638
H	1.66700	-3.14156	0.30249
C	2.54897	-1.19508	-0.06574
C	3.84930	-1.53678	0.29582
H	4.09843	-2.57007	0.51586
C	4.81739	-0.53187	0.36367
H	5.83881	-0.77600	0.63935
C	4.45605	0.78522	0.07992
H	5.17917	1.59232	0.12290
C	3.13265	1.05315	-0.26185
H	2.77882	2.05254	-0.49388
C	0.09775	-1.45206	1.69821
H	1.11052	-1.60496	2.08612
H	-0.53370	-2.22819	2.14769
C	-0.37107	-0.07955	2.08730
C	-0.93429	0.40265	3.24032
H	-1.23130	-0.07582	4.16087
C	-0.60877	2.06345	1.80256
H	-0.61481	3.04815	1.35906
O	0.31581	-0.57639	-2.46264
H	0.34865	-0.08449	-3.30001
Cl	0.09075	2.59482	-1.52901

^{6}FeLAOHF
Charge: 1+
Energy: -1464299.1922980

Fe	-0.15335	-0.38963	1.07523
N	-0.17123	-0.87694	-1.23503
N	1.94458	-0.57128	0.52339
N	-2.21298	-0.15980	0.43821
N	1.11407	3.45066	-0.55178
H	1.51848	4.37552	-0.49077
N	0.16107	1.57163	0.04466
C	1.01404	-1.74852	-1.37486
H	1.25139	-1.95550	-2.42761
H	0.77380	-2.69431	-0.87942
C	2.21186	-1.16143	-0.65517
C	3.51907	-1.26925	-1.12419
H	3.71679	-1.74167	-2.08122
C	4.56054	-0.76672	-0.34059
H	5.58759	-0.84383	-0.68451
C	4.26825	-0.16374	0.88376
H	5.05151	0.23544	1.51900
C	2.93536	-0.08033	1.27875
H	2.62198	0.38253	2.20978
C	-1.45958	-1.59393	-1.36443
H	-1.35807	-2.53728	-0.82020

H	-1.71206	-1.81423	-2.41074
C	-2.56216	-0.79509	-0.69699
C	-3.86634	-0.73437	-1.18216
H	-4.12700	-1.24347	-2.10470
C	-4.82315	-0.01572	-0.46142
H	-5.84656	0.04105	-0.81966
C	-4.44908	0.63185	0.71657
H	-5.16381	1.20033	1.30152
C	-3.12307	0.53741	1.13155
H	-2.75655	1.01717	2.03410
C	-0.11634	0.34259	-2.08952
H	-1.13093	0.54103	-2.45171
H	0.50646	0.16738	-2.97570
C	0.36734	1.53662	-1.31618
C	0.96490	2.70656	-1.70920
H	1.28011	3.07534	-2.67314
C	0.62403	2.72658	0.48453
H	0.63438	3.04266	1.51704
O	-0.33937	-2.20480	1.34209
H	-0.33095	-2.52653	2.25823
F	-0.00635	0.47024	2.62981

^{6}FeLAOHN$_{3}$
Charge: 1+
Energy: -1504684.0052573

Fe	0.16163	0.80733	-0.34633
N	0.12469	-1.45894	-0.93936
N	-1.97069	0.31230	-0.54130
N	2.21402	0.10354	-0.13307
N	-1.14938	-0.96644	3.42758
H	-1.54748	-0.94931	4.35702
N	-0.19400	-0.28220	1.57837
C	-1.05942	-1.53235	-1.81944
H	-1.31054	-2.56884	-2.08462
H	-0.80812	-0.98907	-2.73559
C	-2.24813	-0.83112	-1.19532
C	-3.55742	-1.28769	-1.33068
H	-3.75737	-2.21650	-1.85560
C	-4.59708	-0.53023	-0.78747
H	-5.62552	-0.86455	-0.88504
C	-4.29817	0.65592	-0.11630
H	-5.07757	1.27218	0.31867
C	-2.96325	1.03859	-0.01059
H	-2.65560	1.94082	0.50888
C	1.40844	-1.59448	-1.66266
H	1.32394	-1.00258	-2.57860
H	1.62611	-2.63679	-1.93364
C	2.53024	-1.00395	-0.83226
C	3.81855	-1.53289	-0.80386
H	4.04886	-2.43221	-1.36640
C	4.79840	-0.88655	-0.04710
H	5.81021	-1.27907	-0.01409
C	4.46018	0.26142	0.67001
H	5.19204	0.78911	1.27183
C	3.14787	0.72256	0.60227
H	2.81207	1.60435	1.13878
C	0.04515	-2.36359	0.24167
H	1.05019	-2.75824	0.42601
H	-0.59766	-3.22629	0.02571
C	-0.42411	-1.63683	1.47053
C	-1.02405	-2.08290	2.61989
H	-1.35428	-3.06039	2.93615
C	-0.64279	0.09917	2.75989
H	-0.63134	1.11219	3.13396
O	0.34796	1.17064	-2.13892
H	0.38772	2.07947	-2.47645
N	0.12404	2.47565	0.62102
N	0.22192	3.63226	0.24666
N	0.30966	4.73520	-0.06313

^{6}FeLAOHNCS
Charge: 1+
Energy: -1709792.3566194

Fe	0.21229	0.25468	-0.87333
N	0.65795	-1.84874	-0.03649
N	-1.75885	-0.69605	-0.73152
N	2.30385	0.29524	-0.31021
N	-1.30609	0.66766	3.23613
H	-1.84276	1.09798	3.97753
N	-0.20927	0.43163	1.35195
C	-0.37570	-2.68205	-0.68985
H	-0.39195	-3.70290	-0.28466
H	-0.11838	-2.73169	-1.75222
C	-1.74050	-2.03458	-0.58724
C	-2.91723	-2.76050	-0.41946
H	-2.87821	-3.83840	-0.29798
C	-4.13630	-2.07937	-0.41626
H	-5.06665	-2.62498	-0.29095
C	-4.14334	-0.69295	-0.57156
H	-5.06899	-0.12773	-0.57496
C	-2.92464	-0.03562	-0.72130
H	-2.86124	1.04199	-0.83427
C	2.02536	-2.09717	-0.55187
H	1.94874	-2.18287	-1.63941
H	2.45521	-3.02543	-0.15214
C	2.90898	-0.90667	-0.23957
C	4.26265	-1.01595	0.06799
H	4.72859	-1.99430	0.13044
C	5.00115	0.14907	0.28841
H	6.05885	0.08788	0.52587
C	4.36449	1.38791	0.20704
H	4.90406	2.31371	0.37406
C	3.00496	1.41671	-0.09303
H	2.44487	2.34320	-0.17042
C	0.61075	-1.90907	1.45370
H	1.64206	-1.84952	1.81733
H	0.21151	-2.87469	1.78805
C	-0.17312	-0.76833	2.03187
C	-0.85665	-0.64001	3.21287
H	-1.04983	-1.32935	4.02033
C	-0.90140	1.27820	2.09564
H	-1.14250	2.29978	1.83769
O	0.54738	-0.45183	-2.53754
H	0.43413	0.12551	-3.31013
N	-0.26753	2.11814	-1.10149
C	-0.91693	3.07105	-0.77017
S	-1.80011	4.31909	-0.29995

^{6}FeLBBrOH
Charge: 1+
Energy: -3052457.7926169

Fe	0.17729	-0.19326	-1.03430
N	0.15218	-0.01505	1.42159
N	-0.71148	1.79068	-0.58837
N	3.74489	0.69664	0.98773
N	2.06416	0.56140	-0.42865
N	-3.25558	-1.42202	1.08318
N	-1.77309	-0.79826	-0.41942
C	-0.20761	1.37983	1.76801
H	0.72530	1.92540	1.94937
H	-0.77565	1.41268	2.70776
C	-0.94966	2.14059	0.68505
C	-1.77053	3.22241	1.00103
H	-1.95610	3.48130	2.03921
C	-2.33772	3.96607	-0.03500
H	-2.97923	4.81338	0.18785
C	-2.07172	3.60392	-1.35544
H	-2.49238	4.15502	-2.18954
C	-1.25779	2.49858	-1.58983
H	-1.02960	2.13579	-2.58664
C	1.54220	-0.33443	1.81474
H	1.67330	-1.41881	1.73835
H	1.76756	-0.03221	2.84779
C	2.45189	0.32728	0.82153
C	4.19595	1.17892	-0.23214
H	5.20662	1.53613	-0.35769
C	3.14161	1.09172	-1.09978
H	3.07522	1.36589	-2.14126
C	4.55984	0.52991	2.18934
H	3.96704	0.75877	3.07778
H	5.40039	1.22397	2.14406
H	4.93972	-0.49359	2.25769
C	-0.84488	-1.01147	1.86247
H	-1.20613	-0.81248	2.88182
H	-0.35784	-1.99289	1.86220
C	-1.96849	-1.05017	0.86877
C	-3.89870	-1.40483	-0.14505
H	-4.94109	-1.66821	-0.23924
C	-2.96701	-1.01022	-1.06692
H	-3.06370	-0.86280	-2.13146
C	-3.84652	-1.85920	2.34589
H	-3.57700	-2.89762	2.55984
H	-4.93201	-1.77828	2.27275
H	-3.50454	-1.21813	3.16171
O	0.06944	0.10565	-2.82543
H	0.32872	-0.62298	-3.41472
Br	0.98267	-2.57537	-0.87203

^{6}FeLBClOH
Charge: 1+
Energy: -1725929.4992606

Fe	-0.19554	-0.17228	1.20263
N	-0.22895	-0.63134	-1.20958
N	0.44822	1.71475	0.22059
N	-3.86662	-0.16547	-0.83490
N	-2.16507	0.23528	0.50467
N	3.32389	-1.52076	-0.69372
N	1.81505	-0.68738	0.67564
C	-0.02395	0.64627	-1.92914
H	-1.00921	1.01800	-2.23266
H	0.54534	0.48422	-2.85459
C	0.62243	1.74799	-1.10929
C	1.29236	2.80196	-1.72991
H	1.42907	2.80195	-2.80727

C	1.77269	3.85255	-0.94717
H	2.29623	4.68407	-1.40938
C	1.57362	3.81652	0.43297
H	1.93091	4.61225	1.07759
C	0.91234	2.72021	0.98020
H	0.74588	2.60470	2.04604
C	-1.58375	-1.18085	-1.43536
H	-1.59594	-2.20845	-1.05886
H	-1.85770	-1.20006	-2.50021
C	-2.54258	-0.36207	-0.62112
C	-4.34739	0.58818	0.22561
H	-5.38569	0.87636	0.28684
C	-3.27972	0.83162	1.04631
H	-3.22827	1.38403	1.97182
C	-4.67574	-0.72135	-1.91737
H	-4.11603	-0.69334	-2.85494
H	-5.57566	-0.11518	-2.03171
H	-4.96144	-1.75336	-1.69396
C	0.85984	-1.60873	-1.41041
H	1.17179	-1.67001	-2.46308
H	0.48230	-2.59221	-1.11098
C	2.00585	-1.25560	-0.50809
C	3.99244	-1.09709	0.44460
H	5.06194	-1.20374	0.54271
C	3.04309	-0.57678	1.28254
H	3.14999	-0.13441	2.26098
C	3.93224	-2.21249	-1.82772
H	3.79569	-3.29431	-1.73959
H	4.99932	-1.98612	-1.84630
H	3.48701	-1.86393	-2.76244
O	-0.09085	0.60858	2.84493
H	-0.25971	0.04000	3.61541
Cl	-0.70019	-2.39633	1.59047

^{6}FeLBFOH
Charge: 1+
Energy: -1499804.6834748

Fe	-0.18704	-0.06810	1.35580
N	-0.23104	-1.03221	-0.88972
N	0.31541	1.59997	-0.06917
N	-3.86239	-0.55399	-0.63033
N	-2.19933	0.14885	0.63277
N	3.38154	-1.51423	-0.37140
N	1.86885	-0.53503	0.89544
C	-0.09618	0.03016	-1.90607
H	-1.09358	0.24025	-2.30971
H	0.51249	-0.31448	-2.75340
C	0.45534	1.34572	-1.37819
C	1.01659	2.28252	-2.24653
H	1.12726	2.05019	-3.30176
C	1.42424	3.51619	-1.73854
H	1.86267	4.26072	-2.39635
C	1.26478	3.77604	-0.37694
H	1.57006	4.72143	0.05840
C	0.71187	2.78328	0.42743
H	0.58042	2.89753	1.49856
C	-1.56100	-1.67751	-0.89837
H	-1.50703	-2.53936	-0.22765
H	-1.85637	-2.02733	-1.89794
C	-2.54727	-0.69957	-0.32795
C	-4.36708	0.43461	0.20102
H	-5.40346	0.73274	0.15679
C	-3.32196	0.86317	0.97482
H	-3.29368	1.62464	1.73914
C	-4.64526	-1.34485	-1.57713
H	-4.05117	-1.55712	-2.46865
H	-5.52382	-0.77008	-1.87440
H	-4.96716	-2.28607	-1.12200
C	0.89765	-1.98215	-0.85342
H	1.17890	-2.33291	-1.85688
H	0.57618	-2.84797	-0.26682
C	2.05419	-1.34265	-0.14047
C	4.06229	-0.77379	0.58282
H	5.14088	-0.75150	0.61470
C	3.10889	-0.16692	1.35636
H	3.22180	0.50300	2.19500
C	4.00024	-2.38357	-1.36916
H	4.00295	-3.42355	-1.02972
H	5.02860	-2.05680	-1.53077
H	3.46046	-2.31140	-2.31605
O	-0.08258	1.05898	2.79089
H	-0.20365	0.68146	3.67763
F	-0.49939	-1.77248	1.83139

^{6}FeLBN$_3$OH
Charge: 1+
Energy: -1540189.9359668

Fe	-0.15548	-0.03677	1.20490
N	-0.16461	-0.52916	-1.23463
N	0.87114	1.68597	0.20670
N	-3.73207	0.42616	-0.96837
N	-2.00523	0.67681	0.37899
N	3.15760	-1.99015	-0.54006
N	1.73696	-0.94426	0.77836
C	0.29260	0.68538	-1.94567
H	-0.60070	1.23850	-2.25665
H	0.83245	0.41941	-2.86545
C	1.12320	1.64176	-1.11104
C	2.03832	2.50645	-1.71014
H	2.23045	2.44335	-2.77712
C	2.69022	3.45413	-0.91954
H	3.40550	4.13932	-1.36460
C	2.41128	3.50465	0.44580
H	2.89477	4.22563	1.09610
C	1.50012	2.59225	0.97273
H	1.25585	2.54649	2.02875
C	-1.57678	-0.83807	-1.53906
H	-1.78641	-1.86954	-1.23969
H	-1.79772	-0.76608	-2.61464
C	-2.43805	0.09649	-0.73706
C	-4.13953	1.24752	0.06993
H	-5.14391	1.63970	0.11733
C	-3.05810	1.39791	0.89524
H	-2.95653	1.96458	1.80797
C	-4.59624	-0.11889	-2.01281
H	-4.05809	-0.15693	-2.96288
H	-5.46312	0.53293	-2.12974
H	-4.93035	-1.12382	-1.73842
C	0.74925	-1.67930	-1.36993
H	1.10783	-1.80556	-2.40219
H	0.19082	-2.58290	-1.10204
C	1.88879	-1.52662	-0.40426
C	3.83463	-1.68213	0.62996
H	4.86988	-1.95314	0.77017
C	2.94152	-1.02744	1.43488
H	3.07414	-0.60942	2.42094
C	3.70401	-2.75051	-1.66184
H	3.38148	-3.79483	-1.61622
H	4.79319	-2.71028	-1.61562
H	3.38047	-2.30991	-2.60775
O	0.05168	0.78121	2.82807
H	-0.26425	0.30199	3.61166
N	-1.00279	-1.77252	1.55428
N	-2.11670	-2.16401	1.28814
N	-3.16974	-2.54378	1.00303

^{6}FeLBNCSOH
Charge: 1+
Energy: -1745298.7407484

Fe	0.13906	-0.20618	1.20887
N	0.26515	0.20094	-1.23260
N	-0.84766	-1.94369	0.25805
N	3.81416	-0.70827	-0.76138
N	2.03582	-0.90807	0.52379
N	-3.03063	1.84766	-0.69922
N	-1.72547	0.70065	0.65242
C	-0.10173	-1.07105	-1.89497
H	0.82493	-1.62914	-2.06953
H	-0.54770	-0.88395	-2.88162
C	-1.00135	-1.97498	-1.07630
C	-1.87628	-2.87045	-1.68885
H	-1.98894	-2.86923	-2.76881
C	-2.59221	-3.76765	-0.89447
H	-3.27863	-4.47480	-1.35040
C	-2.41434	-3.73984	0.48828
H	-2.94973	-4.41984	1.14196
C	-1.53680	-2.80233	1.02744
H	-1.36778	-2.69950	2.09400
C	1.68672	0.53964	-1.45982
H	1.84651	1.58127	-1.16414
H	1.97221	0.45216	-2.51892
C	2.51497	-0.36227	-0.59030
C	4.17378	-1.50563	0.31492
H	5.17083	-1.90766	0.41022
C	3.06018	-1.62277	1.10137
H	2.91849	-2.16084	2.02600
C	4.70890	-0.25522	-1.82481
H	4.19700	-0.29771	-2.78914
H	5.57499	-0.91733	-1.86124
H	5.04505	0.76821	-1.63482
C	-0.67017	1.30826	-1.51717
H	-1.03067	1.27795	-2.55595
H	-0.13764	2.25731	-1.38932
C	-1.81417	1.26662	-0.54455
C	-3.74124	1.63541	0.47193
H	-4.74576	2.00936	0.59792
C	-2.92052	0.91760	1.29886
H	-3.09696	0.54285	2.29531
C	-3.47842	2.64512	-1.83867
H	-3.00211	3.62994	-1.82917
H	-4.56031	2.76947	-1.77716
H	-3.23948	2.13276	-2.77397
O	-0.11126	-0.93571	2.86210
H	0.14932	-0.40724	3.63489
N	0.88546	1.59767	1.51441

C	1.03052	2.69739	1.06865
S	1.22351	4.14729	0.39995

^{6}FeLBOHBr
Charge: 1+
Energy: -3052455.4309097

Fe	0.25719	0.62664	-0.69557
N	0.20044	-1.69156	-0.27422
N	-0.41742	0.41958	1.52059
N	3.83869	-1.34756	0.13516
N	2.20517	0.12550	0.01718
N	-3.37942	-1.41926	-1.10268
N	-1.82006	0.12014	-0.88507
C	-0.00143	-1.96452	1.16763
H	0.98598	-2.13029	1.61239
H	-0.56841	-2.89452	1.30824
C	-0.64770	-0.83409	1.94585
C	-1.37018	-1.09866	3.10890
H	-1.54696	-2.12432	3.41913
C	-1.84917	-0.02893	3.86604
H	-2.41337	-0.20982	4.77602
C	-1.59195	1.27060	3.43285
H	-1.94171	2.13366	3.98897
C	-0.87997	1.44859	2.24843
H	-0.67382	2.43520	1.84805
C	1.54095	-2.12533	-0.73630
H	1.54923	-2.05288	-1.82749
H	1.76719	-3.16094	-0.44641
C	2.53571	-1.14610	-0.18220
C	4.35500	-0.12588	0.54159
H	5.38604	-0.02276	0.84360
C	3.32850	0.77724	0.46620
H	3.31325	1.83203	0.69433
C	4.60189	-2.58510	-0.00998
H	3.97879	-3.44159	0.25660
H	5.45697	-2.55366	0.66708
H	4.95899	-2.70058	-1.03750
C	-0.91326	-2.16073	-1.12873
H	-1.22506	-3.18286	-0.87261
H	-0.55310	-2.15580	-2.16193
C	-2.04550	-1.18042	-1.02192
C	-4.02060	-0.19273	-1.01899
H	-5.09600	-0.11471	-1.06702
C	-3.03904	0.75224	-0.87734
H	-3.11685	1.82354	-0.77092
C	-4.03428	-2.70516	-1.33083
H	-4.00803	-2.97099	-2.39167
H	-5.07295	-2.63365	-1.00464
H	-3.54038	-3.48567	-0.74764
O	0.62979	0.11287	-2.42417
H	0.72385	0.83310	-3.06957
Br	0.27730	3.07222	-0.72122

^{6}FeLBOHCl
Charge: 1+
Energy: -1725927.6828027

Fe	0.24426	0.20739	-1.18059
N	0.25971	-1.29772	0.65465
N	-0.39179	1.45791	0.66166
N	3.88866	-0.70901	0.64998
N	2.21350	0.30562	-0.35773
N	-3.33402	-1.68192	-0.05924
N	-1.81664	-0.34674	-0.93224
C	0.07921	-0.57483	1.93477
H	1.07407	-0.40711	2.36205
H	-0.46957	-1.19630	2.65510
C	-0.57906	0.78634	1.80930
C	-1.26947	1.34349	2.88533
H	-1.41263	0.77072	3.79690
C	-1.76086	2.64460	2.77238
H	-2.30058	3.10047	3.59700
C	-1.54907	3.34471	1.58560
H	-1.91151	4.35838	1.45295
C	-0.86708	2.70844	0.55062
H	-0.69584	3.18955	-0.40616
C	1.60756	-1.90523	0.54721
H	1.60286	-2.55693	-0.33102
H	1.86859	-2.50255	1.43209
C	2.57827	-0.78460	0.30816
C	4.37283	0.49253	0.15398
H	5.40244	0.78499	0.29281
C	3.32049	1.11219	-0.46555
H	3.27682	2.06256	-0.97523
C	4.68522	-1.73045	1.32601
H	4.08891	-2.21680	2.10112
H	5.54485	-1.25223	1.79814
H	5.03671	-2.48148	0.61252
C	-0.84747	-2.22615	0.33601
H	-1.12751	-2.84468	1.20018
H	-0.49756	-2.88519	-0.46427
C	-2.00644	-1.42815	-0.18752
C	-4.00860	-0.70383	-0.77395
H	-5.08623	-0.69124	-0.83259
C	-3.05245	0.12139	-1.30444
H	-3.15932	1.00477	-1.91541
C	-3.95492	-2.81744	0.61846
H	-3.93509	-3.70715	-0.01776
H	-4.99084	-2.56530	0.85017
H	-3.43129	-3.02729	1.55387
O	0.61477	-1.30762	-2.16275
H	0.68266	-1.17609	-3.12312
Cl	0.17330	1.93604	-2.61999

^{6}FeLBOHF
Charge: 1+
Energy: -1499802.8447716

Fe	-0.19570	-0.09770	1.36021
N	-0.23600	-1.01739	-0.87614
N	0.31576	1.60188	-0.03896
N	-3.87022	-0.52851	-0.65361
N	-2.21121	0.16573	0.62048
N	3.37801	-1.51478	-0.40393
N	1.88219	-0.53240	0.88148
C	-0.08773	0.05420	-1.88691
H	-1.08159	0.27259	-2.29416
H	0.52292	-0.29211	-2.73166
C	0.46861	1.36198	-1.34769
C	1.04547	2.30436	-2.19964
H	1.16686	2.08440	-3.25634
C	1.45541	3.52890	-1.67103
H	1.90584	4.27870	-2.31455
C	1.28384	3.77343	-0.30772
H	1.59190	4.71113	0.14206
C	0.71590	2.77414	0.47784
H	0.57587	2.87257	1.54921
C	-1.57093	-1.65546	-0.91716
H	-1.53273	-2.53069	-0.26230
H	-1.85049	-1.98239	-1.92893
C	-2.55656	-0.67772	-0.34527
C	-4.37718	0.45658	0.17980
H	-5.41267	0.75727	0.13210
C	-3.33477	0.88013	0.96047
H	-3.31183	1.63711	1.72964
C	-4.64730	-1.31216	-1.61088
H	-4.05317	-1.50493	-2.50696
H	-5.53201	-0.74149	-1.89747
H	-4.95939	-2.26343	-1.16995
C	0.88743	-1.97722	-0.85506
H	1.15324	-2.32674	-1.86302
H	0.56539	-2.83910	-0.26283
C	2.05359	-1.34139	-0.15550
C	4.07163	-0.77492	0.54070
H	5.15057	-0.75398	0.55931
C	3.12880	-0.16568	1.32598
H	3.25581	0.50305	2.16379
C	3.98112	-2.38373	-1.41138
H	3.97292	-3.42637	-1.08028
H	5.01260	-2.06836	-1.57543
H	3.43780	-2.29764	-2.35521
O	-0.51567	-1.84745	1.86116
H	-0.55512	-2.02275	2.81538
F	-0.08032	0.99543	2.75425

^{6}FeLBOHN$_{3}$
Charge: 1+
Energy: -1540187.9564066

Fe	0.25494	0.93957	-0.51894
N	0.19477	-1.46387	-0.56179
N	-0.39466	0.28075	1.58134
N	3.83176	-1.22450	-0.08962
N	2.21595	0.26604	0.07797
N	-3.38551	-1.05937	-1.29514
N	-1.84013	0.43662	-0.81328
C	-0.01488	-2.00614	0.79846
H	0.96434	-2.29590	1.19614
H	-0.61906	-2.92306	0.76229
C	-0.61880	-1.02555	1.78919
C	-1.30556	-1.48199	2.91456
H	-1.48083	-2.54491	3.05289
C	-1.75331	-0.55442	3.85565
H	-2.28912	-0.88623	4.73995
C	-1.50541	0.80125	3.64061
H	-1.83586	1.55627	4.34579
C	-0.82892	1.17536	2.48203
H	-0.62705	2.21314	2.23705
C	1.53363	-1.79334	-1.09911
H	1.54150	-1.50353	-2.15368
H	1.76530	-2.86564	-1.02445
C	2.53203	-0.94563	-0.36447
C	4.36219	-0.11448	0.54976
H	5.39263	-0.08706	0.86973
C	3.34654	0.79858	0.64948
H	3.34665	1.78495	1.08778
C	4.57759	-2.42132	-0.47121

H	3.95226	-3.30810	-0.34573
H	5.44850	-2.51611	0.17919
H	4.91016	-2.35506	-1.51128
C	-0.91480	-1.74876	-1.49438
H	-1.22620	-2.80267	-1.45835
H	-0.55344	-1.52765	-2.50314
C	-2.05251	-0.81699	-1.19183
C	-4.04160	0.11674	-0.96806
H	-5.11872	0.18435	-0.98188
C	-3.06863	1.03215	-0.66460
H	-3.16349	2.05990	-0.34841
C	-4.02682	-2.29076	-1.74936
H	-3.99296	-2.36700	-2.84015
H	-5.06790	-2.28580	-1.42310
H	-3.52931	-3.15776	-1.30868
O	0.63829	0.75755	-2.31635
H	0.61447	1.53879	-2.89112
N	0.21055	2.78693	-0.03526
N	0.39449	3.85098	-0.59472
N	0.55976	4.87667	-1.08637

[6]FeLBOHNCS
Charge: 1+
Energy: -1745295.2727922

Fe	0.19089	0.57688	-0.78968
N	0.54765	-1.71562	-0.24832
N	-0.41002	0.33954	1.44059
N	4.07252	-0.73613	0.10377
N	2.21549	0.43781	-0.07443
N	-3.02681	-2.13687	-1.01441
N	-1.77291	-0.32784	-0.91683
C	0.40166	-1.95175	1.20658
H	1.40475	-1.93223	1.64704
H	-0.00400	-2.95450	1.39754
C	-0.41917	-0.90651	1.93907
C	-1.07776	-1.21951	3.12819
H	-1.07535	-2.23949	3.50127
C	-1.72815	-0.20264	3.82822
H	-2.24695	-0.42124	4.75674
C	-1.70273	1.09371	3.31498
H	-2.19364	1.91551	3.82502
C	-1.03856	1.31690	2.11095
H	-1.00763	2.29763	1.64941
C	1.94010	-1.93003	-0.70764
H	1.92941	-1.90876	-1.80090
H	2.34718	-2.89520	-0.37427
C	2.75373	-0.76853	-0.21412
C	4.37864	0.57169	0.44815
H	5.37765	0.85900	0.73859
C	3.21569	1.28598	0.33656
H	3.02882	2.33299	0.52074
C	5.02936	-1.83662	0.01409
H	4.56417	-2.76537	0.35191
H	5.87931	-1.61837	0.66248
H	5.38235	-1.95951	-1.01402
C	-0.46773	-2.41488	-1.06589
H	-0.58819	-3.46504	-0.76443
H	-0.12163	-2.38769	-2.10340
C	-1.75820	-1.65252	-0.98320
C	-3.88178	-1.04656	-0.97264
H	-4.95385	-1.16962	-0.99376
C	-3.08787	0.06782	-0.90507
H	-3.36432	1.10961	-0.84551
C	-3.43671	-3.53160	-1.15813
H	-3.37121	-3.84996	-2.20271
H	-4.46817	-3.63194	-0.81700
H	-2.80342	-4.17382	-0.54185
O	0.64580	0.02052	-2.49090
H	0.57696	0.68148	-3.19868
N	-0.20186	2.44734	-0.79736
C	-0.53845	3.59947	-0.75422
S	-0.99267	5.12559	-0.67385

[3]FePh2TIPCysOEtBr
Charge: 0
Energy: -3960169.3542670

Fe	1.31165	-0.67393	-0.06044
S	0.47648	-0.82688	2.06973
N	2.32281	0.94849	0.58698
C	1.59584	1.67193	1.64932
C	2.42771	2.83374	2.17353
O	3.62428	2.94884	2.01418
C	1.23766	0.69643	2.77610
O	1.66746	3.69577	2.87355
H	2.52145	1.57606	-0.19481
H	3.24261	0.66865	0.93624
H	0.67433	2.05193	1.20653
H	0.55404	1.18359	3.47619
H	2.14328	0.41626	3.32812
C	-0.67692	0.14192	-2.36650
P	-1.82796	-1.25213	-2.11925
N	-0.28368	0.49038	-3.62939
H	0.91826	2.09572	-4.40774
C	0.48172	1.62010	-3.54362
N	-0.20778	1.01726	-1.47941
C	0.50973	1.95039	-2.20520
H	-0.48742	-0.02997	-4.47146
N	-1.11334	-3.80304	-1.32217
C	-0.75209	-2.48720	-1.28953
N	0.35052	-2.35944	-0.55009
C	-0.22600	-4.52676	-0.56722
N	-2.41025	-0.33691	0.53171
C	0.69486	-3.62481	-0.08476
N	-4.14320	-0.50024	-0.85460
C	-2.83171	-0.66296	-0.73004
C	-3.51059	0.05468	1.23490
C	-4.58966	-0.04463	0.36483
H	-3.43521	0.35450	2.26929
H	-1.45274	-0.37650	0.90897
H	-0.29175	-5.59718	-0.45361
H	-1.91061	-4.16761	-1.82491
C	1.18145	3.10203	-1.58747
C	0.51469	3.88994	-0.63556
H	-0.50762	3.63921	-0.36741
C	1.15614	4.98044	-0.04860
H	0.63006	5.58025	0.68839
C	2.47121	5.29536	-0.40252
H	2.97261	6.14206	0.05829
C	3.14340	4.51455	-1.34602
H	4.17154	4.74448	-1.61037
C	2.50410	3.42442	-1.93817
H	3.03233	2.78779	-2.64245
C	1.83256	-3.90070	0.80663
H	0.66556	-5.15750	2.11282
C	1.65018	-4.74283	1.91420
H	2.55375	-5.65682	3.63872
C	2.71020	-5.01138	2.77860
H	4.78749	-4.64041	3.22893
C	3.96329	-4.43702	2.55039
H	5.12625	-3.16190	1.25346
C	4.15182	-3.60274	1.44626
H	3.25553	-2.71349	-0.30034
C	3.09688	-3.33900	0.57272
C	-6.00611	0.25646	0.60992
H	-6.59808	-0.22438	-1.39722
C	-6.94476	0.11163	-0.42559
C	-8.29180	0.39485	-0.20790
H	-9.00282	0.27713	-1.02187
H	-9.78125	1.04893	1.21413
C	-8.73054	0.82826	1.04588
C	-7.80530	0.97537	2.08251
H	-8.13367	1.31097	3.06296
H	-5.75204	0.81045	2.68553
C	-6.45776	0.69244	1.86728
C	2.37089	4.82388	3.42309
H	3.16417	4.49085	4.09780
H	2.81299	5.41728	2.61795
H	1.62116	5.40236	3.96346
Br	2.82951	-0.72467	-2.09712

[5]FePh2TIPCysOEtCl
Charge: 0
Energy: -2633645.8117975

Fe	-1.53461	0.42714	-0.33102
S	-0.85963	-1.11496	-2.14519
N	0.10277	1.63685	-1.26383
C	1.17942	0.68161	-1.55183
C	2.51317	1.36618	-1.84027
O	2.70280	2.56432	-1.79907
C	0.70940	-0.28217	-2.65021
O	3.47146	0.45094	-2.06728
H	0.44656	2.40979	-0.69659
H	-0.24422	2.05208	-2.12902
H	1.35248	0.09502	-0.63961
H	1.49185	-1.01870	-2.83915
H	0.54972	0.27701	-3.58111
C	0.07470	-0.01218	2.46626
P	-0.02687	-1.83481	2.41753
N	0.87579	0.56265	3.40679
H	1.51957	2.58982	3.75932
C	0.95858	1.90494	3.14309
N	-0.37251	0.91241	1.61707
C	0.17098	2.12483	2.03451
H	1.37442	0.05737	4.12662
N	-2.41897	-3.13361	2.13664
C	-1.66135	-2.09791	1.65982
N	-2.35535	-1.42009	0.74286
C	-3.62459	-3.11816	1.49370
N	1.02581	-2.61771	-0.16000
C	-3.58861	-2.04347	0.62431
N	2.48246	-1.88251	1.36308
C	1.20631	-2.12160	1.10093
C	2.26912	-2.65079	-0.74439
C	3.16763	-2.19380	0.20271
H	2.39567	-2.95320	-1.77202

H	0.16235	-2.49528	-0.72367
H	-4.38915	-3.85848	1.66901
H	-2.12385	-3.79001	2.84647
C	-0.04346	3.42018	1.36864
C	1.06379	4.23008	1.05860
H	2.06590	3.87698	1.28622
C	0.88152	5.45403	0.41546
H	1.74467	6.06396	0.16469
C	-0.40513	5.87779	0.07241
H	-0.54611	6.82544	-0.44038
C	-1.50744	5.07530	0.37694
H	-2.50965	5.38893	0.10051
C	-1.33156	3.85536	1.02863
H	-2.18559	3.22581	1.24403
C	-4.68592	-1.64410	-0.27163
H	-3.44009	-1.14606	-1.96158
C	-4.45399	-1.23067	-1.58997
H	-5.32709	-0.58865	-3.44064
C	-5.52495	-0.91722	-2.42444
H	-7.66887	-0.76377	-2.61211
C	-6.83723	-1.01400	-1.95868
H	-8.09518	-1.48952	-0.26900
C	-7.07759	-1.42393	-0.64495
H	-6.19554	-2.02807	1.22342
C	-6.00876	-1.73587	0.19297
C	4.60763	-1.95956	0.05366
H	4.72308	-0.68780	1.77954
C	5.28217	-1.12103	0.95648
C	6.63834	-0.84363	0.79151
H	7.14264	-0.18864	1.49753
H	8.40641	-1.18352	-0.40271
C	7.34923	-1.39988	-0.27534
C	6.68972	-2.24436	-1.17342
H	7.23443	-2.69289	-2.00026
H	4.83461	-3.19009	-1.70748
C	5.33342	-2.52298	-1.00966
C	4.81359	0.95745	-2.19159
H	4.90088	1.59066	-3.07910
H	5.07954	1.53980	-1.30572
H	5.44916	0.07640	-2.26805
Cl	-3.40086	1.73594	-0.55386

^{5}FePh2TIPCysOEtN$_{3}$
Charge: 0
Energy: -2447906.4937281

Fe	-1.38777	0.32246	-0.51248
N	-3.13068	1.21974	-0.22986
N	-3.83258	1.07065	0.74399
N	-4.52539	0.93525	1.66105
S	-0.65610	-1.17953	-2.31305
N	0.26563	1.56555	-1.43615
C	1.36275	0.60765	-1.62993
C	2.69986	1.29262	-1.89479
O	2.86303	2.49136	-1.98956
C	0.96261	-0.39522	-2.72093
O	3.68491	0.37972	-1.95082
H	0.57556	2.34661	-0.86100
H	-0.00481	1.96943	-2.33329
H	1.49163	0.05849	-0.68929
H	1.74698	-1.14783	-2.81776
H	0.88682	0.12760	-3.68342
C	-0.06510	0.29191	2.46683
P	-0.06515	-1.53382	2.60865
N	0.43812	1.03275	3.49475
H	0.79330	3.14106	3.76201
C	0.45710	2.34790	3.11286
N	-0.37965	1.08549	1.44394
C	-0.05621	2.38200	1.83283
H	0.76336	0.65488	4.37417
N	-2.55609	-2.72369	2.48495
C	-1.65759	-1.93253	1.82393
N	-2.18824	-1.51285	0.67552
C	-3.69525	-2.80527	1.73041
N	0.97389	-2.49541	0.09856
C	-3.46442	-2.04750	0.59976
N	2.45756	-1.73409	1.57760
C	1.17165	-1.93749	1.33297
C	2.21150	-2.61704	-0.48058
C	3.12846	-2.14024	0.43981
H	2.31989	-2.99113	-1.48612
H	0.11620	-2.43438	-0.46812
H	-4.55442	-3.38412	2.03075
H	-2.39711	-3.16053	3.38253
C	-0.18151	3.58929	0.99548
C	0.87622	4.51624	0.97889
H	1.77536	4.31132	1.55388
C	0.79458	5.67168	0.20245
H	1.62503	6.37196	0.19043
C	-0.34108	5.91319	-0.57365
H	-0.40150	6.80822	-1.18682
C	-1.39278	4.99321	-0.56689
H	-2.27860	5.17056	-1.17064
C	-1.32148	3.84028	0.21453
H	-2.12988	3.11654	0.19614
C	-4.40907	-1.80422	-0.50170
H	-2.98395	-2.18506	-2.07315
C	-4.00753	-1.91783	-1.83931
H	-4.59235	-1.77351	-3.89992
C	-4.92038	-1.69099	-2.86757
H	-6.95426	-1.17851	-3.37420
C	-6.24430	-1.35858	-2.57115
H	-7.67800	-0.98163	-1.00208
C	-6.65261	-1.25215	-1.23928
H	-6.03988	-1.33783	0.82688
C	-5.74095	-1.47266	-0.20779
C	4.57892	-1.98365	0.28564
H	4.76615	-0.70372	1.99911
C	5.29952	-1.17548	1.18030
C	6.66951	-0.97819	1.01408
H	7.20991	-0.34622	1.71432
H	8.41663	-1.43311	-0.17293
C	7.34842	-1.58610	-0.04537
C	6.64174	-2.39962	-0.93638
H	7.15987	-2.88623	-1.75876
H	4.73602	-3.23778	-1.46731
C	5.27145	-2.59687	-0.77221
C	5.02421	0.89529	-2.06340
H	5.15572	1.40600	-3.02176
H	5.22645	1.59865	-1.25141
H	5.67555	0.02593	-1.98497

^{5}FePh2TIPCysOEtNCS
Charge: 0
Energy: -2653018.7035079

Fe	-1.31322	0.08220	-0.28215
S	-0.43608	-1.21606	-2.17429
N	0.15429	1.57843	-1.08107
C	1.34342	0.80617	-1.46340
C	2.56088	1.69441	-1.71059
O	2.58640	2.89518	-1.53425
C	0.98260	-0.12354	-2.63035
O	3.62325	0.95457	-2.06923
H	0.40352	2.33266	-0.44311
H	-0.24843	2.03080	-1.90288
H	1.61869	0.18036	-0.60423
H	1.85588	-0.72194	-2.89419
H	0.71805	0.47987	-3.50817
C	0.35536	-0.28402	2.47052
P	0.56562	-2.09236	2.30206
N	1.06396	0.37825	3.42751
H	1.28197	2.46403	3.92920
C	0.84818	1.72454	3.27457
N	-0.31412	0.58621	1.71616
C	-0.02286	1.85224	2.21531
H	1.68913	-0.06007	4.09032
N	-1.61750	-3.71981	1.93712
C	-1.02226	-2.55431	1.53479
N	-1.83508	-1.90532	0.69858
C	-2.83957	-3.81397	1.33035
N	1.69954	-2.54656	-0.31918
C	-2.97919	-2.67486	0.55989
N	3.03498	-1.66694	1.23805
C	1.81105	-2.09366	0.96590
C	2.92587	-2.34800	-0.90725
C	3.74953	-1.80354	0.06147
H	3.08830	-2.56949	-1.95037
H	0.82090	-2.53232	-0.87085
H	-3.49426	-4.66065	1.46479
H	-1.21345	-4.38678	2.58042
C	-0.57166	3.09800	1.65778
C	0.28051	4.18234	1.38576
H	1.34621	4.08887	1.57815
C	-0.23189	5.35261	0.82504
H	0.43617	6.18044	0.60452
C	-1.59396	5.44775	0.52657
H	-1.98885	6.35375	0.07511
C	-2.44699	4.37489	0.79894
H	-3.50317	4.42906	0.55282
C	-1.93925	3.20847	1.36997
H	-2.59573	2.37156	1.57381
C	-4.15822	-2.30910	-0.24172
H	-3.05567	-1.58800	-1.95164
C	-4.03741	-1.76372	-1.52750
H	-5.06927	-0.98878	-3.24230
C	-5.17761	-1.43126	-2.25662
H	-7.33303	-1.37613	-2.28797
C	-6.44809	-1.64986	-1.72051
H	-7.56229	-2.36930	-0.01751
C	-6.57723	-2.20630	-0.44618
H	-5.53889	-2.93228	1.29588
C	-5.43919	-2.53120	0.29020
C	5.13313	-1.33704	-0.07669
H	5.05917	-0.14300	1.70636
C	5.67320	-0.44450	0.86389
C	6.96756	0.05067	0.71207
H	7.36740	0.74409	1.44760

H	8.75849	0.04821	-0.49610
C	7.74954	-0.33767	-0.37908
C	7.22532	-1.23421	-1.31493
H	7.82840	-1.55369	-2.16094
H	5.53905	-2.43646	-1.89155
C	5.93109	-1.73042	-1.16447
C	4.87769	1.65625	-2.16614
H	4.83438	2.40543	-2.96153
H	5.10718	2.14713	-1.21716
H	5.62111	0.89014	-2.38072
N	-3.03983	0.98171	-0.51780
C	-4.03777	1.59325	-0.73270
S	-5.38660	2.44097	-1.00132

[5]FePh2TIPCysOEtOH
Charge: 0
Energy: -2392428.6065736

Fe	-1.58892	0.42186	-0.43858
S	-0.83822	-1.12242	-2.23168
N	0.12265	1.64786	-1.27974
C	1.19167	0.70339	-1.61802
C	2.50177	1.39787	-1.97765
O	2.63976	2.59188	-2.14280
C	0.70335	-0.24005	-2.73173
O	3.50133	0.49814	-2.04931
H	0.46220	2.36754	-0.64428
H	-0.19038	2.14113	-2.11635
H	1.39711	0.10391	-0.72451
H	1.49632	-0.95485	-2.96222
H	0.51561	0.34680	-3.64035
C	-0.13614	0.08945	2.47802
P	-0.07412	-1.73756	2.44747
N	0.42975	0.74353	3.53364
H	0.75889	2.82544	3.97648
C	0.39009	2.08887	3.28008
N	-0.54786	0.96735	1.56536
C	-0.22341	2.22882	2.05134
H	0.84220	0.29293	4.33902
N	-2.42396	-3.14917	2.13896
C	-1.67003	-2.11459	1.64914
N	-2.35021	-1.47161	0.70296
C	-3.62033	-3.16103	1.47498
N	1.02364	-2.46686	-0.11712
C	-3.57438	-2.10717	0.58233
N	2.46273	-1.78206	1.44633
C	1.18719	-1.99878	1.15803
C	2.27461	-2.50641	-0.67880
C	3.16290	-2.07859	0.29261
H	2.41370	-2.78804	-1.71060
H	0.17095	-2.34829	-0.70345
H	-4.38235	-3.90225	1.65906
H	-2.13452	-3.78571	2.86883
C	-0.44971	3.49864	1.33996
C	0.54836	4.48982	1.38597
H	1.47619	4.29150	1.91667
C	0.37153	5.70510	0.72661
H	1.15514	6.45700	0.76224
C	-0.80062	5.94209	0.00395
H	-0.93522	6.88430	-0.52078
C	-1.79013	4.95793	-0.05151
H	-2.70066	5.12821	-0.61941
C	-1.62760	3.74306	0.61580
H	-2.39857	2.98110	0.53710
C	-4.65721	-1.69159	-0.32531
H	-3.38478	-1.28975	-2.02466
C	-4.40231	-1.30328	-1.65004
H	-5.23773	-0.62317	-3.50636
C	-5.45404	-0.92733	-2.48607
H	-7.58701	-0.65259	-2.67486
C	-6.77116	-0.94694	-2.02024
H	-8.05388	-1.35491	-0.33283
C	-7.03371	-1.34395	-0.70709
H	-6.18729	-1.98774	1.16618
C	-5.98412	-1.71015	0.13505
C	4.60891	-1.86583	0.17177
H	4.72923	-0.67887	1.95638
C	5.28948	-1.08515	1.12052
C	6.65309	-0.82952	0.98432
H	7.16164	-0.21856	1.72593
H	8.42897	-1.15072	-0.20374
C	7.36599	-1.35040	-0.09882
C	6.70035	-2.13797	-1.04299
H	7.24585	-2.55902	-1.88379
H	4.83309	-3.01597	-1.64373
C	5.33663	-2.39454	-0.90822
C	4.81800	1.03074	-2.27795
H	4.87972	1.48195	-3.27276
H	5.05427	1.78951	-1.52707
H	5.49355	0.18085	-2.18687
O	-3.14379	1.43307	-0.54783
H	-3.93657	0.98883	-0.88100

[2]aCDOBr
Charge: 0
Energy: -3360907.5732482

Fe	-0.07384	-0.06524	-0.41227
S	-0.57412	0.84278	-2.39111
C	1.11826	4.10483	3.27266
C	0.82597	3.31988	2.03726
C	0.70993	1.97271	1.80937
N	0.58849	3.90517	0.80339
C	0.33519	2.92925	-0.10347
N	0.40507	1.74287	0.47700
H	2.02492	4.71383	3.16611
H	1.26828	3.42550	4.11604
H	0.29117	4.77805	3.53020
H	0.80648	1.15977	2.50972
H	0.56651	4.89678	0.61085
H	0.09062	3.08342	-1.14353
C	-0.55304	-3.04142	4.40387
C	-0.01082	-2.27956	3.24140
C	-0.61330	-1.47255	2.31372
N	1.32822	-2.29859	2.87583
C	1.48407	-1.53221	1.76698
N	0.32456	-1.01330	1.40525
H	-0.09291	-2.73093	5.35066
H	-0.39292	-4.12065	4.28876
H	-1.63014	-2.87296	4.48196
H	-1.66190	-1.23859	2.22266
H	2.05628	-2.83153	3.32954
H	2.42031	-1.39572	1.25025
C	5.48769	0.48919	-1.38838
C	4.05861	0.05848	-1.39595
C	2.98474	0.41174	-0.61972
N	3.54754	-0.86105	-2.30070
C	2.22452	-1.03040	-2.05365
N	1.85575	-0.27409	-1.03440
N	-1.94362	0.26984	0.14778
C	-2.77706	1.10793	-0.76404
C	-4.30234	0.81903	-0.45366
O	-4.47898	-0.18109	0.29464
C	-2.40981	0.74352	-2.19256
O	-5.09277	1.60133	-1.00409
H	5.65202	1.21449	-0.58671
H	5.77387	0.96734	-2.33376
H	6.17005	-0.35424	-1.22199
H	2.94226	1.11594	0.19658
H	4.06357	-1.31602	-3.04025
H	1.56250	-1.68277	-2.60212
H	-1.96247	0.71776	1.06549
H	-2.55111	-0.56255	0.26612
H	-2.54992	2.16252	-0.58025
H	-2.90245	1.41997	-2.89421
H	-2.71205	-0.28568	-2.41083
Br	-0.73346	-2.38036	-1.16517

[4]aCDOCl
Charge: 0
Energy: -2034378.1096620

Fe	0.09488	-0.48810	-0.38827
S	0.42076	-2.56067	0.97679
C	-2.76185	3.02257	3.44462
C	-1.90346	1.96723	2.82965
C	-1.48916	1.74736	1.53981
N	-1.33005	0.93503	3.55841
C	-0.61464	0.15133	2.70718
N	-0.68871	0.62028	1.47506
H	-3.64866	2.59740	3.93207
H	-3.10703	3.71512	2.67192
H	-2.21729	3.60696	4.19754
H	-1.71185	2.32109	0.65273
H	-1.43224	0.78165	4.55160
H	-0.09319	-0.75305	2.98654
C	1.51020	5.15564	-1.40620
C	1.01603	3.75257	-1.52944
C	0.74731	2.78150	-0.59860
N	0.72525	3.15393	-2.74701
C	0.31312	1.87966	-2.51509
N	0.31001	1.62475	-1.22004
H	0.79125	5.88110	-1.80865
H	2.46153	5.30174	-1.93355
H	1.67467	5.39881	-0.35282
H	0.83098	2.84058	0.47649
H	0.84157	3.57581	-3.65737
H	0.08545	1.15514	-3.28240
C	-5.64859	-1.61086	-0.45333
C	-4.19076	-1.50721	-0.75644
C	-3.19764	-0.70478	-0.25714
N	-3.55328	-2.30512	-1.69745
C	-2.23824	-1.97027	-1.72890
N	-1.99304	-0.99811	-0.86853
N	2.29877	-0.18387	0.16770
C	2.73147	-1.18844	1.08635
C	4.51093	-1.29744	1.05692
O	4.90528	-1.20450	-0.09606

C	2.23458	-2.56573	0.68190
O	4.90935	-1.44793	2.20312
H	-5.91737	-0.88565	0.31996
H	-5.92042	-2.60789	-0.08295
H	-6.26894	-1.40309	-1.33509
H	-3.26719	0.05520	0.50629
H	-3.98623	-3.02954	-2.25204
H	-1.48913	-2.42899	-2.35790
H	2.49550	0.76217	0.48346
H	2.73946	-0.32826	-0.74464
H	2.48877	-0.92249	2.11438
H	2.71041	-3.34206	1.28589
H	2.45437	-2.73435	-0.37626
Cl	0.89830	-1.31080	-2.56882

4aCDOF
Charge: 0
Energy: -1808251.5114419

Fe	0.09989	-0.46706	-0.55551
S	0.44163	-2.84760	0.24200
C	-2.51524	2.07128	4.05819
C	-1.67574	1.18216	3.20179
C	-1.36818	1.20736	1.86445
N	-1.00682	0.06828	3.69142
C	-0.34338	-0.52297	2.66157
N	-0.53961	0.14904	1.54298
H	-3.34246	1.52515	4.52970
H	-2.94846	2.86885	3.44830
H	-1.92987	2.54296	4.85808
H	-1.69173	1.90293	1.10493
H	-1.01818	-0.25731	4.64759
H	0.22752	-1.43656	2.73862
C	1.52559	5.40725	-0.63055
C	1.09376	4.00703	-0.91604
C	0.68092	2.98108	-0.10175
N	1.04143	3.47429	-2.19563
C	0.61754	2.18376	-2.10823
N	0.38467	1.85753	-0.85030
H	0.87365	6.14599	-1.11504
H	2.55226	5.59724	-0.96946
H	1.49343	5.59184	0.44693
H	0.57726	2.98394	0.97397
H	1.30367	3.95150	-3.04619
H	0.52647	1.48360	-2.92562
C	-5.71048	-1.49782	-0.78262
C	-4.27163	-1.20932	-1.05584
C	-3.23244	-0.83587	-0.24102
N	-3.70933	-1.29039	-2.32241
C	-2.38935	-0.97635	-2.22779
N	-2.07529	-0.69319	-0.97810
N	2.28010	-0.33860	-0.01959
C	2.79464	-1.54176	0.58693
C	4.48234	-1.59861	0.38114
O	4.79002	-1.28638	-0.77111
C	2.23453	-2.77499	-0.11992
O	5.03594	-1.94527	1.42406
H	-5.91590	-1.37256	0.28427
H	-5.98138	-2.52663	-1.05361
H	-6.37908	-0.82217	-1.33248
H	-3.24083	-0.66303	0.82505
H	-4.19024	-1.56484	-3.16664
H	-1.67138	-0.97649	-3.03401
H	2.46095	0.49425	0.53650
H	2.73480	-0.21501	-0.92855
H	2.59949	-1.54973	1.65943
H	2.73212	-3.68169	0.23472
H	2.41911	-2.66857	-1.19388
F	0.37496	-0.54192	-2.40839

^{4}aCDON$_{3}$
Charge: 0
Energy: -1848639.0809686

Fe	0.22738	-0.01696	-0.51842
S	1.39540	-1.58371	-2.11264
C	-0.97419	-3.22898	4.25793
C	-0.47397	-2.75285	2.93440
C	-0.55138	-1.53909	2.29945
N	0.22808	-3.56328	2.05324
C	0.54082	-2.83376	0.95005
N	0.08189	-1.60061	1.07123
H	-1.67871	-4.06432	4.15406
H	-1.49533	-2.41552	4.77017
H	-0.15606	-3.56283	4.90899
H	-1.00995	-0.62239	2.63653
H	0.47156	-4.53201	2.20413
H	1.08251	-3.20362	0.09112
C	-0.37868	4.37245	3.33121
C	-0.66553	3.25148	2.38857
C	0.03674	2.12228	2.05364
N	-1.81868	3.18206	1.62117
C	-1.76288	2.05596	0.86248
N	-0.64923	1.38645	1.10266
H	-1.14009	4.45385	4.11773
H	-0.33072	5.33751	2.81110
H	0.58761	4.20992	3.81648
H	0.99396	1.79858	2.43592
H	-2.52543	3.89978	1.54734
H	-2.50926	1.78610	0.13308
C	-5.40539	-1.44160	-1.34763
C	-3.98066	-1.01885	-1.48811
C	-2.93846	-0.96556	-0.59670
N	-3.43897	-0.57048	-2.68513
C	-2.13092	-0.26913	-2.48064
N	-1.79960	-0.49954	-1.22446
N	2.34970	0.40171	0.14124
C	3.27836	-0.46267	-0.53928
C	4.86531	0.24252	-0.48555
O	4.79522	1.45344	-0.67540
C	2.93480	-0.59402	-2.01818
O	5.69826	-0.63363	-0.27796
H	-5.59999	-1.74859	-0.31621
H	-5.64679	-2.29118	-1.99936
H	-6.10069	-0.62769	-1.59066
H	-2.92332	-1.23922	0.44839
H	-3.93640	-0.46183	-3.55742
H	-1.45638	0.10755	-3.23460
H	2.46910	0.36161	1.15052
H	2.50582	1.36538	-0.16661
H	3.35755	-1.42510	-0.03474
H	3.74351	-1.09437	-2.55646
H	2.78147	0.40505	-2.43745
N	0.32451	1.65388	-1.73643
N	-0.61149	2.39323	-1.89249
N	-1.52821	3.09602	-2.04444

^{4}aCDONCS
Charge: 0
Energy: -2053750.3662952

Fe	-0.15013	0.13703	-0.37621
S	-1.09029	0.84411	-2.56456
C	0.70568	4.90716	2.84760
C	0.34130	3.95178	1.75993
C	0.37449	2.58272	1.68545
N	-0.14562	4.36018	0.52475
C	-0.38380	3.25972	-0.23317
N	-0.07801	2.16641	0.44529
H	1.50330	5.59517	2.53898
H	1.06196	4.35325	3.72028
H	-0.15277	5.51306	3.16452
H	0.67805	1.85239	2.41951
H	-0.30449	5.31538	0.23664
H	-0.76863	3.26675	-1.24289
C	-0.92080	-3.79539	3.25252
C	-0.20288	-2.59303	2.73860
C	-0.57122	-1.27886	2.60277
N	1.08880	-2.64633	2.24045
C	1.41875	-1.40895	1.79477
N	0.43732	-0.54413	1.99611
H	-0.40734	-4.24506	4.11177
H	-1.00892	-4.56358	2.47422
H	-1.93118	-3.52071	3.56785
H	-1.50411	-0.82063	2.90065
H	1.57591	-3.49328	1.96887
H	2.34388	-1.19573	1.28185
C	5.57084	1.18556	-0.92198
C	4.17430	0.67940	-1.06909
C	3.00159	1.00198	-0.43319
N	3.81743	-0.30305	-1.98219
C	2.48441	-0.53472	-1.87034
N	1.96384	0.24138	-0.93786
N	-2.32936	0.03474	0.21256
C	-3.14503	0.52784	-0.85810
C	-4.80445	-0.10810	-0.65886
O	-4.74526	-1.26365	-0.26446
C	-2.69218	0.01400	-2.21498
O	-5.59435	0.76705	-0.97599
H	5.60858	1.94273	-0.13397
H	5.93791	1.64786	-1.84727
H	6.27009	0.38475	-0.64938
H	2.82837	1.72848	0.34728
H	4.44314	-0.78331	-2.61331
H	1.93873	-1.26378	-2.44899
H	-2.50961	0.51560	1.09020
H	-2.50088	-0.96473	0.34611
H	-3.24701	1.61105	-0.81639
H	-3.42752	0.26458	-2.98284
H	-2.56638	-1.07171	-2.16841
N	-0.17949	-1.92996	-0.72712
C	0.48291	-2.91296	-0.77414
S	1.44850	-4.23049	-0.80112

^{6}aCDOOH
Charge: 0
Energy: -1793169.5324549

Fe	-0.00047	-0.66483	-0.48007
S	-0.01742	-2.73246	0.69907
C	-2.30168	3.16583	3.46916
C	-1.60742	2.02804	2.79684
C	-1.43569	1.69966	1.47506
N	-0.95974	1.01635	3.49305
C	-0.43876	0.13853	2.59545
N	-0.70666	0.53064	1.36391
H	-3.11193	2.82149	4.12452
H	-2.74003	3.82764	2.71718
H	-1.61188	3.76332	4.07877
H	-1.79103	2.21722	0.59627
H	-0.89195	0.93759	4.49805
H	0.09089	-0.76816	2.84875
C	2.56584	4.64040	-1.24432
C	1.85451	3.34255	-1.43659
C	0.95545	2.65706	-0.65993
N	2.02727	2.54166	-2.55574
C	1.26043	1.43045	-2.41438
N	0.59026	1.47223	-1.27510
H	2.32455	5.36280	-2.03485
H	3.65511	4.50806	-1.23293
H	2.27561	5.08343	-0.28757
H	0.56067	2.93771	0.30484
H	2.67129	2.71575	-3.31432
H	1.24108	0.58957	-3.09159
C	-5.85691	-0.92829	-0.65314
C	-4.39721	-0.85674	-0.95579
C	-3.30525	-0.57899	-0.17558
N	-3.87263	-1.09890	-2.21978
C	-2.52395	-0.97021	-2.16025
N	-2.15276	-0.64890	-0.93335
N	1.97982	-0.45089	0.32238
C	2.53841	-1.59972	1.08102
C	4.08283	-1.71242	0.74157
O	4.41726	-1.03807	-0.27498
C	1.83604	-2.88172	0.64007
O	4.72900	-2.47096	1.47928
H	-6.02569	-0.70580	0.40399
H	-6.26656	-1.92682	-0.85200
H	-6.43515	-0.20592	-1.24378
H	-3.26809	-0.34365	0.87645
H	-4.40297	-1.35224	-3.04117
H	-1.82940	-1.12948	-2.97127
H	2.03367	0.40157	0.87892
H	2.71430	-0.33883	-0.41327
H	2.39261	-1.44747	2.15491
H	2.15613	-3.71166	1.27299
H	2.12597	-3.11079	-0.39154
O	0.37464	-1.23082	-2.24063
H	0.55758	-2.18364	-2.25692

[5]FePhTpBIHQBr
Charge: 0
Energy: -4021099.4361201

Fe	0.54066	-0.25099	-0.39136
S	1.18458	2.01498	0.08051
P	1.12913	-3.56240	1.17645
O	-1.42744	0.38090	0.09596
O	-3.35655	1.47426	0.27898
N	-0.46971	-3.07123	3.42779
N	-0.06421	-1.23579	2.25452
N	-0.46221	-4.46560	-0.93057
N	-0.60493	-2.27717	-0.65731
N	3.77407	-2.77889	1.18408
N	2.48672	-1.18706	0.34631
C	0.19241	-2.52862	2.35481
C	-1.18051	-2.06343	4.03005
C	-0.92604	-0.92120	3.28780
C	0.02890	-3.37467	-0.26565
C	-1.55303	-2.66728	-1.58846
C	-1.45446	-4.03395	-1.77218
C	2.50405	-2.43051	0.81968
C	4.59466	-1.71158	0.93198
C	3.79253	-0.71830	0.40697
C	-1.47061	0.42725	3.49298
C	-2.67116	0.61962	4.19795
H	-3.20731	-0.23676	4.60059
C	-3.20381	1.89905	4.35089
H	-4.13844	2.03210	4.88968
C	-2.55031	3.00251	3.79510
H	-2.97592	3.99700	3.89850
C	-1.35456	2.81780	3.09694
H	-0.84228	3.66169	2.64405
C	-0.81235	1.54191	2.95487
H	0.10059	1.40519	2.38730
C	-2.59128	-1.79306	-2.16566
C	-3.90767	-2.28293	-2.24309
H	-4.12589	-3.28586	-1.88453
C	-4.94105	-1.48230	-2.73033
H	-5.95329	-1.87580	-2.77360
C	-4.67664	-0.17272	-3.13748
H	-5.48219	0.45967	-3.50105
C	-3.37010	0.31804	-3.07460
H	-3.14960	1.33388	-3.39053
C	-2.33296	-0.48595	-2.60405
H	-1.31879	-0.10973	-2.59029
C	4.27550	0.61589	0.00474
C	5.04843	1.35533	0.91449
H	5.21753	0.96240	1.91406
C	5.57205	2.59542	0.55192
H	6.15839	3.16503	1.26818
C	5.33207	3.10529	-0.72651
H	5.73624	4.07383	-1.01016
C	4.56644	2.37151	-1.63414
H	4.36635	2.76591	-2.62646
C	4.03732	1.13276	-1.27526
H	3.42559	0.57394	-1.97366
C	-2.05215	1.44249	-0.02729
C	-1.52655	2.72744	-0.49752
C	-0.13170	3.03288	-0.48651
C	0.23664	4.32839	-0.93187
H	1.29276	4.57985	-0.92322
C	-0.69286	5.25068	-1.38123
H	-0.35575	6.22550	-1.72615
C	-2.06067	4.93244	-1.40127
H	-2.79299	5.64935	-1.76094
C	-2.46142	3.68744	-0.95297
H	-3.51264	3.42323	-0.95330
C	-3.94996	0.22730	0.68140
H	-4.98415	0.47357	0.92479
H	-3.43351	-0.16963	1.55720
H	-3.90726	-0.49417	-0.13630
H	4.05024	-3.67665	1.55610
H	5.65882	-1.73671	1.10650
H	-0.42571	-4.03471	3.72843
H	-1.76355	-2.22613	4.92333
H	-0.13204	-5.41495	-0.82915
H	-1.98992	-4.70139	-2.42920
Br	1.26674	-0.66910	-2.85378

[5]FePhTpBIHQCl
Charge: 0
Energy: -2694571.4074284

Fe	0.59946	-0.26951	-0.60106
S	1.32445	1.94294	0.01675
P	1.11051	-3.64140	0.93424
O	-1.34088	0.39338	-0.04665
O	-3.23337	1.52202	0.25957
N	-0.48393	-3.18900	3.19416
N	-0.01764	-1.32224	2.09441
N	-0.52105	-4.46649	-1.17304
N	-0.60473	-2.27952	-0.86206
N	3.76898	-2.91365	0.94757
N	2.52365	-1.29887	0.09046
C	0.20161	-2.62392	2.14677
C	-1.17114	-2.18506	3.82936
C	-0.87801	-1.02314	3.13302
C	0.00500	-3.39880	-0.49584
C	-1.57137	-2.62980	-1.78942
C	-1.51054	-3.99558	-1.99687
C	2.50725	-2.53409	0.58451
C	4.61974	-1.87646	0.67158
C	3.84359	-0.86914	0.13310
C	-1.38270	0.33287	3.38517
C	-2.57489	0.53733	4.10082
H	-3.13607	-0.31560	4.47574
C	-3.06674	1.82641	4.30095
H	-3.99543	1.96935	4.84749
C	-2.38002	2.92808	3.78290
H	-2.77377	3.93113	3.92323
C	-1.19311	2.73115	3.07338
H	-0.65726	3.57441	2.64763
C	-0.69196	1.44468	2.88271
H	0.21362	1.29805	2.30520
C	-2.59545	-1.71920	-2.33554
C	-3.92551	-2.17291	-2.39730
H	-4.16401	-3.17567	-2.05136
C	-4.94573	-1.33702	-2.85205
H	-5.96880	-1.70267	-2.88337
C	-4.65352	-0.02793	-3.24145
H	-5.44821	0.63191	-3.57929
C	-3.33325	0.42669	-3.19416
H	-3.09208	1.44142	-3.49866
C	-2.30902	-0.41205	-2.75664
H	-1.28432	-0.06491	-2.75479
C	4.36083	0.43472	-0.31688
C	5.25574	1.13145	0.51145
H	5.49484	0.73322	1.49454
C	5.80999	2.34002	0.09340
H	6.49182	2.87699	0.74771
C	5.47703	2.86257	-1.15899
H	5.90444	3.80751	-1.48494
C	4.58784	2.17261	-1.98466
H	4.31423	2.57831	-2.95462
C	4.02901	0.96442	-1.57080

H	3.32242	0.44080	-2.20401
C	-1.93389	1.47920	-0.06901
C	-1.37549	2.78626	-0.42881
C	0.02850	3.04824	-0.41557
C	0.42795	4.37221	-0.73403
H	1.49122	4.59128	-0.72112
C	-0.48019	5.36261	-1.06647
H	-0.11919	6.35800	-1.31527
C	-1.85728	5.08754	-1.09112
H	-2.57368	5.85851	-1.35952
C	-2.28763	3.81484	-0.76495
H	-3.34645	3.58325	-0.76902
C	-3.85457	0.26449	0.57727
H	-4.87249	0.52063	0.87359
H	-3.32574	-0.21950	1.40046
H	-3.85978	-0.38854	-0.29690
H	4.02097	-3.81312	1.33240
H	5.68412	-1.93267	0.83711
H	-0.46925	-4.16393	3.45855
H	-1.76596	-2.36542	4.71144
H	-0.21557	-5.42573	-1.08890
H	-2.07105	-4.63838	-2.65765
Cl	1.15360	-0.57306	-2.88875

^{5}FePhTpBIHQF
Charge: 0
Energy: -2468447.1211414

Fe	0.52971	-0.23877	-0.24053
S	1.39423	1.37989	1.37067
P	0.77499	-3.88344	0.02493
O	-1.36688	0.72581	0.04511
O	-2.84859	2.38547	0.08707
N	-0.83540	-3.93073	2.29416
N	-0.52074	-1.86529	1.55070
N	-0.79368	-3.93893	-2.29622
N	-0.60037	-1.90134	-1.46179
N	3.51823	-3.45151	0.12246
N	2.40259	-1.55471	-0.08669
C	-0.16883	-3.13565	1.39796
C	-1.64991	-3.12346	3.04367
C	-1.46152	-1.83688	2.56680
C	-0.19611	-3.15830	-1.34248
C	-1.49033	-1.85886	-2.51957
C	-1.60834	-3.13169	-3.04954
C	2.28380	-2.87335	0.00774
C	4.45518	-2.45172	0.09102
C	3.75782	-1.26326	-0.03994
C	-2.20102	-0.64280	3.00698
C	-3.54786	-0.76941	3.39052
H	-4.03470	-1.74011	3.33413
C	-4.27613	0.34670	3.80267
H	-5.31935	0.23492	4.08690
C	-3.67093	1.60603	3.82744
H	-4.24116	2.47945	4.13272
C	-2.33257	1.73626	3.44813
H	-1.85286	2.71107	3.45128
C	-1.59797	0.62081	3.04822
H	-0.56527	0.73393	2.73378
C	-2.24172	-0.66244	-2.94082
C	-3.59701	-0.79605	-3.28849
H	-4.07430	-1.77098	-3.22209
C	-4.34218	0.31661	-3.68031
H	-5.39180	0.20022	-3.93786
C	-3.74316	1.57829	-3.71888
H	-4.32539	2.44926	-4.00867
C	-2.39480	1.71415	-3.37760
H	-1.92149	2.69224	-3.39996
C	-1.63905	0.60404	-2.99977
H	-0.58867	0.70324	-2.73756
C	4.35672	0.07838	-0.12850
C	5.52145	0.35474	0.60602
H	5.93252	-0.40233	1.26985
C	6.12990	1.60630	0.52470
H	7.02394	1.81120	1.10803
C	5.57863	2.59680	-0.29183
H	6.04661	3.57647	-0.35047
C	4.41987	2.32541	-1.02297
H	3.97411	3.09535	-1.64663
C	3.80696	1.07501	-0.94900
H	2.89250	0.87678	-1.49978
C	-1.58203	1.94093	0.08319
C	-0.58139	3.02177	0.11467
C	0.73634	2.84138	0.63943
C	1.59519	3.96749	0.59110
H	2.60231	3.84556	0.97675
C	1.19763	5.18284	0.05568
H	1.90171	6.01184	0.03029
C	-0.09808	5.34659	-0.45615
H	-0.41355	6.29515	-0.88114
C	-0.97199	4.27299	-0.41178
H	-1.97914	4.37713	-0.80055
C	-3.86796	1.37021	0.02364
H	-4.81095	1.91812	0.00477
H	-3.81293	0.73051	0.90734
H	-3.75288	0.76951	-0.88049
H	3.69974	-4.44257	0.19601
H	5.51489	-2.64933	0.13032
H	-0.73162	-4.93146	2.38562
H	-2.26374	-3.50213	3.84610
H	-0.64420	-4.92950	-2.42625
H	-2.17557	-3.50196	-3.88938
F	1.07378	0.39421	-1.91016

^{5}FePhTpBIHQN$_3$
Charge: 0
Energy: -2508843.2903090

Fe	1.50130	-0.15461	-0.24075
S	0.56548	-1.39268	1.63342
P	-1.32451	-1.31819	-2.65416
O	1.15117	1.60570	0.96963
O	1.31236	2.91547	2.76882
N	-2.21954	-1.10078	0.06098
N	-3.77371	-0.86497	-1.51478
N	-1.05782	1.26003	-3.48073
N	0.44405	0.88422	-1.90554
N	-0.18999	-3.74360	-2.02540
N	1.13024	-2.11066	-1.34417
C	-2.49427	-1.13110	-1.27841
C	-3.38346	-0.80071	0.70598
C	-4.34951	-0.64898	-0.28236
C	-0.51734	0.32606	-2.64610
C	0.51679	2.22182	-2.28894
C	-0.42859	2.45589	-3.26374
C	-0.02070	-2.38914	-1.95542
C	0.88607	-4.34604	-1.42365
C	1.71151	-3.32706	-1.00438
C	-5.77351	-0.32237	-0.13362
C	-6.62044	-0.33301	-1.25444
H	-6.19949	-0.58652	-2.22187
C	-7.97369	-0.02596	-1.12473
H	-8.61393	-0.04069	-2.00324
C	-8.50913	0.29723	0.12467
H	-9.56457	0.53590	0.22460
C	-7.67466	0.31270	1.24539
H	-8.07843	0.56630	2.22224
C	-6.32083	0.00789	1.11802
H	-5.68309	0.03440	1.99780
C	1.47748	3.22243	-1.79772
C	1.05047	4.54459	-1.58783
H	-0.00141	4.79249	-1.70515
C	1.96269	5.53053	-1.21101
H	1.61936	6.54905	-1.05005
C	3.30860	5.20394	-1.02229
H	4.01722	5.96830	-0.71505
C	3.73763	3.88922	-1.22229
H	4.77665	3.62023	-1.06137
C	2.83116	2.90756	-1.62336
H	3.16335	1.88984	-1.78780
C	2.99436	-3.46897	-0.29925
C	3.09527	-4.35501	0.78482
H	2.20856	-4.88244	1.12545
C	4.31128	-4.52481	1.44441
H	4.37638	-5.20364	2.29036
C	5.43678	-3.80782	1.02992
H	6.38293	-3.93188	1.54993
C	5.34105	-2.92409	-0.04709
H	6.21031	-2.35671	-0.36722
C	4.12794	-2.75739	-0.71316
H	4.04954	-2.06262	-1.54046
C	0.83136	1.84430	2.13718
C	-0.10996	1.05492	2.96002
C	-0.29119	-0.34233	2.77935
C	-1.23170	-0.98039	3.62047
H	-1.36875	-2.05221	3.51071
C	-1.97039	-0.28258	4.56786
H	-2.68872	-0.81603	5.18580
C	-1.78682	1.09576	4.73207
H	-2.35904	1.64891	5.47070
C	-0.85118	1.74536	3.94089
H	-0.68476	2.81019	4.06025
C	2.22735	3.74299	2.01227
H	2.47242	4.57109	2.67746
H	1.74660	4.10161	1.10157
H	3.12122	3.17188	1.75246
H	-0.97231	-4.21489	-2.45879
H	0.99591	-5.41743	-1.36443
H	-1.30399	-1.27139	0.50970
H	-3.41841	-0.73127	1.78255
H	-1.81751	1.08698	-4.12551
H	-0.65487	3.34610	-3.82895
N	3.44299	0.11309	-0.30313
N	4.12926	0.80381	0.40931
N	4.82372	1.46862	1.05436

^{5}FePhTpBIHQNCS

Charge: 0
Energy: -2713942.6489081

Fe	-0.39332	0.40245	-0.18194
S	-1.51139	-0.58069	1.71297
P	0.20344	3.92108	-1.02478
O	1.29234	-0.77275	0.37342
O	2.43967	-2.60886	0.89005
N	2.00282	4.23214	1.07922
N	1.09303	2.20947	1.06418
N	1.53092	2.94255	-3.26915
N	1.02793	1.32870	-1.84220
N	-2.50121	4.24789	-0.49880
N	-1.89807	2.12449	-0.36943
C	1.07732	3.40805	0.49453
C	2.63639	3.51830	2.06174
C	2.07530	2.25184	2.04053
C	0.85581	2.61563	-2.12339
C	1.85537	0.80838	-2.82334
C	2.15794	1.81302	-3.72583
C	-1.47819	3.35388	-0.64787
C	-3.61811	3.55031	-0.11399
C	-3.24312	2.22423	-0.03834
C	2.49187	1.11192	2.87081
C	3.82908	1.01367	3.29516
H	4.55001	1.76814	2.98959
C	4.24989	-0.06799	4.06850
H	5.28888	-0.13539	4.38054
C	3.34319	-1.07198	4.41955
H	3.67352	-1.92393	5.00780
C	2.01345	-0.97760	4.00166
H	1.29929	-1.75540	4.25739
C	1.58617	0.10966	3.24099
H	0.55717	0.15815	2.90125
C	2.41765	-0.55464	-2.83835
C	3.76439	-0.72885	-3.20380
H	4.37258	0.14022	-3.44262
C	4.33482	-2.00181	-3.22784
H	5.37933	-2.11886	-3.50466
C	3.56962	-3.11824	-2.88065
H	4.01529	-4.10935	-2.89040
C	2.23113	-2.95183	-2.51684
H	1.62231	-3.80885	-2.24345
C	1.65686	-1.68155	-2.49935
H	0.62121	-1.55213	-2.21913
C	-4.11583	1.09490	0.32471
C	-4.84914	1.13590	1.51858
H	-4.74588	1.99042	2.18253
C	-5.66497	0.06294	1.87579
H	-6.21682	0.09305	2.81161
C	-5.75488	-1.05510	1.04265
H	-6.38126	-1.89629	1.32889
C	-5.04066	-1.09086	-0.15801
H	-5.09075	-1.95427	-0.81452
C	-4.23284	-0.01523	-0.51901
H	-3.67454	-0.04206	-1.44406
C	1.28010	-1.96361	0.71263
C	0.09463	-2.80586	0.93013
C	-1.16569	-2.26949	1.33251
C	-2.23420	-3.18525	1.46487
H	-3.20359	-2.78955	1.75058
C	-2.08137	-4.53969	1.20904
H	-2.93996	-5.20074	1.29977
C	-0.83722	-5.05688	0.82206
H	-0.71635	-6.11563	0.61286
C	0.23648	-4.19155	0.69701
H	1.20726	-4.56865	0.39396
C	3.63575	-1.84660	0.63671
H	4.45549	-2.54711	0.79944
H	3.69958	-1.01034	1.33560
H	3.64226	-1.47845	-0.39092
H	-2.44199	5.24254	-0.66631
H	-4.57575	4.02186	0.04226
H	2.17478	5.19634	0.83133
H	3.39192	3.95279	2.69756
H	1.54832	3.85527	-3.70219
H	2.73909	1.79785	-4.63467
N	-1.27100	-0.72174	-1.65126
C	-1.88610	-1.59973	-2.16584
S	-2.73670	-2.77998	-2.88357

^{3}FePhTpBIHQOH
Charge: 0
Energy: -2453333.3575574

Fe	0.33395	-0.34655	-0.15624
S	1.04766	1.48100	1.13499
P	1.51697	-3.63348	0.19603
O	-1.74696	0.47732	0.14496
O	-3.38660	1.97409	-0.05259
N	0.09495	-3.61005	2.58462
N	-0.08348	-1.67482	1.51827
N	-0.02504	-4.04117	-2.09512
N	-0.21660	-1.97532	-1.32808
N	4.21620	-2.88699	0.21479
N	2.84069	-1.17186	-0.06903
C	0.51676	-2.86757	1.51804
C	-0.81507	-2.86585	3.28531
C	-0.94071	-1.66394	2.61643
C	0.43652	-3.12897	-1.18536
C	-1.14111	-2.15298	-2.35032
C	-1.00544	-3.43989	-2.83832
C	2.91090	-2.48062	0.08549
C	5.00375	-1.76654	0.12711
C	4.13815	-0.69872	-0.05207
C	-1.93272	-0.63558	2.99190
C	-3.24182	-1.06107	3.27623
H	-3.50002	-2.11022	3.15614
C	-4.21844	-0.14688	3.67445
H	-5.22848	-0.49173	3.88067
C	-3.89978	1.20813	3.78662
H	-4.66112	1.92585	4.08084
C	-2.59791	1.63548	3.51198
H	-2.34035	2.68814	3.58943
C	-1.61713	0.72206	3.12871
H	-0.61468	1.05842	2.88797
C	-2.17783	-1.19656	-2.78579
C	-3.46023	-1.69243	-3.08398
H	-3.67605	-2.74838	-2.93906
C	-4.46674	-0.83752	-3.53399
H	-5.45387	-1.23561	-3.75496
C	-4.20851	0.52779	-3.68017
H	-4.99429	1.19811	-4.01948
C	-2.93922	1.02574	-3.37447
H	-2.73304	2.08856	-3.47215
C	-1.92359	0.17499	-2.93745
H	-0.92877	0.54146	-2.67978
C	4.49139	0.71358	-0.24276
C	5.64624	1.25091	0.34587
H	6.26682	0.62780	0.98608
C	5.98229	2.58920	0.14381
H	6.87364	2.99911	0.61194
C	5.16552	3.40292	-0.64624
H	5.42331	4.44819	-0.79789
C	4.01545	2.86965	-1.23429
H	3.36961	3.50006	-1.83988
C	3.67632	1.53186	-1.03749
H	2.78115	1.10341	-1.47800
C	-2.07779	1.65465	0.03432
C	-1.19459	2.84187	-0.02093
C	0.15803	2.83786	0.44843
C	0.86706	4.06312	0.36130
H	1.89771	4.06963	0.70233
C	0.30308	5.21464	-0.16531
H	0.89649	6.12463	-0.22190
C	-1.01644	5.20313	-0.63880
H	-1.46296	6.09661	-1.06581
C	-1.74619	4.02838	-0.55411
H	-2.76999	4.00484	-0.90918
C	-4.29513	0.85992	-0.03537
H	-5.28488	1.29867	-0.17229
H	-4.23385	0.34127	0.92407
H	-4.06823	0.16597	-0.84689
H	4.53724	-3.83774	0.33119
H	6.08124	-1.81449	0.16306
H	0.40957	-4.54387	2.80546
H	-1.28902	-3.21794	4.18806
H	0.31450	-4.98627	-2.20004
H	-1.51327	-3.94295	-3.64619
O	0.71881	0.56798	-1.73881
H	0.86236	1.50673	-1.54127

^{3}FebBPMENBrOH
Charge: 2+
Energy: -2984226.7935638

Fe	-0.02609	-0.62873	0.22808
C	4.50487	0.80886	0.03009
C	3.74746	0.53586	-1.11367
C	3.90576	0.69968	1.28514
C	2.41547	0.17097	-0.97145
C	1.49524	-0.10539	-2.13334
C	2.56819	0.32476	1.36612
C	-0.65399	3.52191	-0.89126
N	1.84048	0.07800	0.25891
C	-0.05752	2.33084	-0.50479
C	-2.02419	3.53495	-1.16619
N	0.51138	-1.14442	-1.71395
C	1.17111	-2.48721	-1.77034
N	-0.75982	1.18081	-0.38718
C	-0.76816	-1.12765	-2.48177
C	-2.75394	2.35625	-1.01367
C	-2.09760	1.20040	-0.60172
C	-1.83004	-1.83372	-1.65194
N	-1.93913	-1.25040	-0.26062
C	-2.83109	-0.05021	-0.22339
C	-2.49540	-2.29763	0.65496
H	5.54901	1.09207	-0.06101
H	4.18709	0.59781	-2.10400

H	4.45969	0.89394	2.19719
H	2.05177	-0.43471	-3.01743
H	0.94883	0.80189	-2.40581
H	2.05646	0.22352	2.31429
H	-0.05226	4.42078	-0.96977
H	0.99649	2.28129	-0.27093
H	-2.51788	4.45018	-1.47793
H	1.42493	-2.71099	-2.81231
H	2.07296	-2.46909	-1.16001
H	0.51256	-3.25448	-1.37247
H	-0.64436	-1.63300	-3.44696
H	-1.03984	-0.08971	-2.67871
H	-3.82481	2.33351	-1.18860
H	-1.57713	-2.88749	-1.53309
H	-2.80627	-1.78842	-2.14631
H	-3.71724	-0.21885	-0.84508
H	-3.16731	0.07185	0.81130
H	-1.82909	-3.15892	0.65006
H	-2.56121	-1.89463	1.66451
H	-3.49106	-2.59227	0.30450
O	0.42821	-2.19763	0.81891
H	0.37700	-2.29114	1.79174
Br	-0.67151	0.13260	2.48911

^{3}FebBPMENClOH
Charge: 2+
Energy: -1657697.6189457

Fe	-0.06030	-0.62840	0.44854
C	4.43147	0.86716	-0.01124
C	3.59614	0.66587	-1.11452
C	3.92938	0.65094	1.27299
C	2.28423	0.26353	-0.90380
C	1.27423	0.04585	-1.99598
C	2.60868	0.24241	1.42414
C	-0.80688	3.59388	-0.35164
N	1.80688	0.06584	0.35399
C	-0.16713	2.38667	-0.10279
C	-2.19449	3.60264	-0.51129
N	0.34409	-1.03383	-1.55096
C	1.00856	-2.35947	-1.75675
N	-0.84123	1.22095	-0.01140
C	-0.98715	-0.97783	-2.22851
C	-2.89494	2.40333	-0.38386
C	-2.18915	1.23427	-0.11264
C	-1.97881	-1.74863	-1.37823
N	-1.98151	-1.24438	0.04879
C	-2.87541	-0.05413	0.23491
C	-2.44942	-2.35045	0.94667
H	5.46142	1.17871	-0.15563
H	3.95942	0.81064	-2.12686
H	4.54621	0.78950	2.15438
H	1.75043	-0.22339	-2.94477
H	0.69742	0.95998	-2.16057
H	2.16940	0.05992	2.39612
H	-0.22433	4.50645	-0.41544
H	0.90487	2.33868	0.03366
H	-2.72310	4.52854	-0.71542
H	1.17577	-2.50518	-2.82956
H	1.95790	-2.37095	-1.22358
H	0.39480	-3.16254	-1.35947
H	-0.92256	-1.41203	-3.23317
H	-1.27965	0.06770	-2.33043
H	-3.97639	2.37418	-0.47119
H	-1.71034	-2.80434	-1.33920
H	-2.99179	-1.68233	-1.78863
H	-3.80488	-0.19815	-0.32643
H	-3.13085	-0.01253	1.29834
H	-1.77178	-3.19621	0.84417
H	-2.44279	-2.00326	1.97867
H	-3.46504	-2.64014	0.65415
O	0.44277	-2.26793	0.85732
H	0.53979	-2.35725	1.82803
Cl	-0.46598	-0.14239	2.56852

^{3}FebBPMENFOH
Charge: 2+
Energy: -1431573.2716648

Fe	0.04549	-0.63921	-0.53741
C	-4.36720	0.88258	-0.10567
C	-3.58319	0.56575	1.01066
C	-3.81274	0.81027	-1.38600
C	-2.26343	0.18046	0.81543
C	-1.27187	-0.09884	1.92236
C	-2.48721	0.40974	-1.52208
C	0.83152	3.55698	0.43777
N	-1.75123	0.10703	-0.43897
C	0.17393	2.35461	0.21636
C	2.22763	3.58162	0.39635
N	-0.27158	-1.10238	1.43510
C	-0.84265	-2.47437	1.63959
N	0.84019	1.20692	-0.03578
C	1.08711	-0.98656	2.05630
C	2.91465	2.40260	0.10665
C	2.19082	1.23653	-0.12289
C	2.10276	-1.67573	1.14508
N	1.98047	-1.22095	-0.29273
C	2.82652	-0.03040	-0.60763
C	2.36050	-2.32829	-1.22438
H	-5.40276	1.18078	0.02674
H	-3.99239	0.61670	2.01456
H	-4.39451	1.05214	-2.26880
H	-1.76929	-0.45818	2.82854
H	-0.74122	0.82174	2.18194
H	-1.98013	0.32343	-2.47647
H	0.25504	4.45393	0.63621
H	-0.90582	2.30022	0.23043
H	2.77088	4.50453	0.57432
H	-0.95360	-2.65067	2.71453
H	-1.81173	-2.53460	1.14601
H	-0.19359	-3.22770	1.20141
H	1.09753	-1.45506	3.04701
H	1.31892	0.07098	2.18073
H	3.99780	2.38661	0.04094
H	1.94007	-2.75389	1.15004
H	3.12152	-1.49951	1.50570
H	3.83892	-0.17075	-0.21336
H	2.89278	0.03227	-1.69832
H	1.75461	-3.20531	-1.00251
H	2.16593	-1.99883	-2.24571
H	3.42340	-2.56426	-1.10249
O	-0.49952	-2.22798	-0.98557
H	-0.52414	-2.28390	-1.96358
F	0.31082	-0.19484	-2.22129

^{6}FebBPMENMeCNOH
Charge: 2+
Energy: -1452273.3340673

Fe	-0.19932	-0.47438	-0.49573
O	-0.19493	-0.74600	-2.27810
C	-2.74487	3.66183	0.06655
C	-1.94183	3.16484	1.09727
C	-2.80228	2.97777	-1.15054
C	-1.21270	1.99975	0.88227
C	-0.26266	1.41063	1.90324
C	-2.05319	1.81561	-1.29495
C	3.18854	2.43730	-0.74361
N	-1.27685	1.34312	-0.29880
C	1.91784	1.87519	-0.71112
C	4.29451	1.59638	-0.59493
N	-0.22445	-0.06551	1.76552
C	-1.42646	-0.64434	2.42141
N	1.72120	0.55224	-0.54760
C	1.02498	-0.66850	2.29775
C	4.08970	0.22458	-0.43853
C	2.78632	-0.26852	-0.43336
N	-2.02284	-1.71079	-0.34356
C	1.22129	-2.06552	1.70992
N	1.16568	-2.06883	0.21278
C	2.48298	-1.74706	-0.40664
C	0.70648	-3.39508	-0.29007
C	-2.98628	-2.30237	-0.59546
C	-4.19304	-3.05121	-0.91333
H	-3.32186	4.56956	0.21488
H	-1.88435	3.67328	2.05445
H	-3.41573	3.33430	-1.97080
H	-0.54396	1.71348	2.91981
H	0.74300	1.80044	1.71607
H	-2.04835	1.23126	-2.20898
H	3.30570	3.50690	-0.87964
H	1.02376	2.47967	-0.81552
H	5.30156	2.00179	-0.60488
H	-1.41332	-0.44090	3.49980
H	-2.32218	-0.20393	1.98065
H	-1.46582	-1.72047	2.25825
H	1.00002	-0.73409	3.39379
H	1.85936	-0.01938	2.02765
H	4.92817	-0.45629	-0.33149
H	0.43191	-2.73152	2.06302
H	2.17197	-2.48877	2.05673
H	3.28605	-2.30819	0.08698
H	2.43903	-2.09069	-1.44593
H	-0.25323	-3.63589	0.16709
H	0.57395	-3.33504	-1.37178
H	1.43275	-4.17937	-0.04464
H	-4.22635	-3.25376	-1.98936
H	-5.07783	-2.47209	-0.62826
H	-4.19703	-4.00162	-0.36887
H	0.33933	-0.41592	-3.01878

^{3}FebBPMENN$_3$OH
Charge: 2+
Energy: -1471964.1585015

Fe	0.07836	-0.63693	-0.10556
C	-4.44925	0.85435	-0.26750

C	-3.60773	1.14003	0.81152
C	-3.95336	0.11142	-1.34043
C	-2.29630	0.67988	0.78804
C	-1.28319	0.96649	1.86890
C	-2.63310	-0.32406	-1.30182
C	0.76715	3.56272	-1.05233
N	-1.82438	-0.04413	-0.26020
C	0.13648	2.35526	-0.78408
C	2.15859	3.63372	-0.94200
N	-0.31220	-0.16337	1.90155
C	-0.93308	-1.29987	2.65215
N	0.82229	1.25185	-0.41988
C	1.01950	0.18959	2.47785
C	2.87024	2.48431	-0.59713
C	2.17154	1.30278	-0.36329
C	2.02131	-0.85901	2.01894
N	1.99859	-1.02562	0.51781
C	2.86562	-0.01644	-0.16773
C	2.48244	-2.39940	0.18148
H	-5.47744	1.20281	-0.26609
H	-3.96544	1.70803	1.66440
H	-4.57337	-0.13142	-2.19660
H	-1.76155	1.09834	2.84570
H	-0.74229	1.88857	1.63979
H	-2.19702	-0.89432	-2.11249
H	0.17827	4.42596	-1.34247
H	-0.93836	2.25222	-0.86211
H	2.68160	4.56532	-1.13475
H	-1.04372	-1.01612	3.70462
H	-1.91611	-1.51156	2.23167
H	-0.32526	-2.19555	2.56152
H	0.97213	0.21722	3.57294
H	1.29505	1.18506	2.12865
H	3.95337	2.49632	-0.52873
H	1.77718	-1.83061	2.44924
H	3.03448	-0.60346	2.34758
H	3.81558	0.09342	0.36724
H	3.09246	-0.41260	-1.16278
H	1.78809	-3.13056	0.59077
H	2.52190	-2.51486	-0.90127
H	3.48547	-2.54781	0.59693
O	-0.35534	-2.34049	0.15169
H	-1.31020	-2.50873	0.04835
N	0.43212	-0.86839	-1.89267
N	0.35267	-1.99387	-2.40613
N	0.30796	-2.99105	-2.95571

^{3}FebBPMENNCSOH
Charge: 2+
Energy: -1677071.4213481

Fe	-0.03134	-0.05118	-0.68734
C	-4.26576	1.49631	0.80781
C	-3.88807	0.15245	0.86664
C	-3.35594	2.43993	0.32591
C	-2.61229	-0.20945	0.44943
C	-2.07337	-1.61552	0.49864
C	-2.09734	2.01169	-0.07957
C	0.69655	-0.18002	3.64147
N	-1.73335	0.71710	-0.00997
C	0.10610	0.03996	2.40327
C	1.94094	-0.81255	3.69093
N	-1.10800	-1.78337	-0.62876
C	-1.89327	-2.05237	-1.87630
N	0.69077	-0.33378	1.24614
C	-0.11033	-2.86871	-0.38728
C	2.56027	-1.17389	2.49476
C	1.91486	-0.90356	1.29008
C	1.07295	-2.62794	-1.30990
N	1.59572	-1.22131	-1.16011
C	2.58086	-1.10694	-0.04146
C	2.26520	-0.81804	-2.43420
H	-5.25899	1.79951	1.12417
H	-4.57619	-0.60732	1.22283
H	-3.61502	3.49073	0.25580
H	-2.87607	-2.35826	0.44008
H	-1.54319	-1.77726	1.44131
H	-1.35791	2.69805	-0.47238
H	0.18654	0.13627	4.54485
H	-0.85860	0.52423	2.32081
H	2.42428	-1.01154	4.64234
H	-2.43151	-2.99929	-1.75956
H	-2.59575	-1.23656	-2.03826
H	-1.23540	-2.09553	-2.73912
H	-0.55223	-3.85356	-0.57849
H	0.19241	-2.83450	0.66013
H	3.53683	-1.64758	2.49110
H	0.76838	-2.74436	-2.35034
H	1.87509	-3.34982	-1.12141
H	3.25644	-1.96983	-0.03658
H	3.19346	-0.22153	-0.24119
H	1.53482	-0.85446	-3.24020
H	2.63272	0.20379	-2.33670
H	3.10358	-1.49166	-2.64485
O	-0.47183	0.13420	-2.39276
H	-0.33790	1.05332	-2.68940
N	0.94148	1.57919	-0.68477
C	1.59882	2.56860	-0.64254
S	2.48601	3.91623	-0.58788

^{3}FebBPMENOHBr
Charge: 2+
Energy: -2984222.9244220

Fe	0.00366	-0.38087	-0.35695
C	-3.36532	2.93154	0.00164
C	-2.55960	2.58012	1.08939
C	-3.16348	2.30694	-1.23041
C	-1.57356	1.61724	0.91488
C	-0.59651	1.19387	1.98125
C	-2.17008	1.34012	-1.34073
C	2.50929	3.16247	-0.45801
N	-1.39726	1.01452	-0.28789
C	1.39770	2.33421	-0.38684
C	3.78236	2.58594	-0.42757
N	-0.24241	-0.24193	1.74807
C	-1.31952	-1.08031	2.37436
N	1.51301	0.99372	-0.28535
C	1.09690	-0.63239	2.29386
C	3.89628	1.19719	-0.36027
C	2.73780	0.42586	-0.31394
C	1.54611	-1.89751	1.57980
N	1.51687	-1.72399	0.08012
C	2.76211	-1.06877	-0.43868
C	1.41415	-3.06902	-0.57105
H	-4.14420	3.67863	0.11910
H	-2.69653	3.04326	2.06128
H	-3.76900	2.55152	-2.09632
H	-1.01019	1.33005	2.98565
H	0.31429	1.79469	1.91633
H	-1.97223	0.81145	-2.26373
H	2.37574	4.23584	-0.53748
H	0.39337	2.73581	-0.41429
H	4.67151	3.20737	-0.47131
H	-1.31252	-0.90293	3.45556
H	-2.28571	-0.79853	1.95851
H	-1.15469	-2.13538	2.17281
H	1.03226	-0.80911	3.37359
H	1.79411	0.18922	2.13013
H	4.86808	0.71386	-0.36612
H	0.87468	-2.72399	1.81478
H	2.55180	-2.19306	1.89840
H	3.64233	-1.50904	0.04279
H	2.81640	-1.29894	-1.50731
H	0.55459	-3.60672	-0.17854
H	1.29026	-2.93217	-1.64516
H	2.33100	-3.63586	-0.37249
O	0.32021	-0.39397	-2.07853
H	-0.21701	-1.03807	-2.58102
Br	-1.76299	-2.04328	-0.64620

^{3}FebBPMENOHCl
Charge: 2+
Energy: -1657695.0933519

Fe	0.05696	-0.53563	-0.48429
C	-4.27219	1.32810	-0.01298
C	-3.41818	1.16918	1.08335
C	-3.83519	0.94844	-1.28323
C	-2.14994	0.64109	0.87834
C	-1.11316	0.45777	1.95687
C	-2.55867	0.41454	-1.42465
C	1.18125	3.61514	-0.07501
N	-1.74288	0.27747	-0.36378
C	0.42371	2.45571	-0.16246
C	2.57363	3.50826	-0.01079
N	-0.28115	-0.73279	1.59748
C	-1.03052	-1.96073	2.02816
N	0.99400	1.23222	-0.18207
C	1.09075	-0.72211	2.19576
C	3.16002	2.24381	-0.07033
C	2.34099	1.12339	-0.18026
C	1.96269	-1.66987	1.38662
N	1.91919	-1.33618	-0.08559
C	2.88411	-0.24861	-0.44854
C	2.27874	-2.55272	-0.88114
H	-5.26887	1.73496	0.12728
H	-3.73400	1.44415	2.08457
H	-4.47053	1.05213	-2.15609
H	-1.57286	0.32321	2.94138
H	-0.46446	1.33579	2.01320
H	-2.16476	0.09160	-2.37925
H	0.68637	4.58009	-0.06048
H	-0.65567	2.49079	-0.22297
H	3.19291	4.39651	0.06790
H	-1.13081	-1.94085	3.11895
H	-2.01484	-1.96466	1.56268
H	-0.50580	-2.86082	1.72006

H	1.05362	-1.04167	3.24356
H	1.47497	0.29784	2.16954
H	4.23876	2.12514	-0.05546
H	1.60483	-2.69468	1.48830
H	2.99945	-1.64943	1.73979
H	3.84484	-0.41859	0.04980
H	3.05072	-0.32104	-1.52791
H	1.61943	-3.37540	-0.61543
H	2.15990	-2.32793	-1.94090
H	3.32026	-2.82344	-0.67332
O	0.40419	-0.22944	-2.17343
H	0.12408	-0.96869	-2.75000
Cl	-0.90790	-2.48921	-0.97687

^{3}FebBPMENOHF
Charge: 2+
Energy: -1431574.5165181

Fe	0.06140	-0.56771	-0.57101
C	-4.40355	0.92105	-0.03837
C	-3.56807	0.69503	1.06087
C	-3.90489	0.73486	-1.32859
C	-2.25761	0.29341	0.83780
C	-1.23662	0.04688	1.91975
C	-2.58450	0.32558	-1.48784
C	0.99528	3.54772	0.29715
N	-1.78913	0.11862	-0.42362
C	0.28689	2.37580	0.07147
C	2.39141	3.49403	0.34206
N	-0.30147	-1.01018	1.42862
C	-0.96465	-2.34741	1.58260
N	0.90931	1.19016	-0.10121
C	1.04190	-0.99008	2.08312
C	3.03237	2.27200	0.13123
C	2.26221	1.13865	-0.10890
C	2.00477	-1.77629	1.20404
N	1.92982	-1.31945	-0.23706
C	2.85583	-0.17842	-0.52186
C	2.24898	-2.46596	-1.14221
H	-5.43274	1.23093	0.11437
H	-3.93112	0.82062	2.07586
H	-4.52368	0.89754	-2.20434
H	-1.70464	-0.25894	2.86140
H	-0.66229	0.95718	2.11494
H	-2.13712	0.16833	-2.46087
H	0.46077	4.48180	0.43125
H	-0.79373	2.36867	0.01889
H	2.97265	4.39256	0.52508
H	-1.09926	-2.54981	2.65043
H	-1.92871	-2.32845	1.07751
H	-0.36513	-3.12686	1.12207
H	0.98947	-1.43326	3.08447
H	1.35640	0.04872	2.18981
H	4.11527	2.20010	0.13270
H	1.75220	-2.83672	1.21528
H	3.03320	-1.68360	1.56777
H	3.83272	-0.35733	-0.06004
H	2.99706	-0.14499	-1.60659
H	1.50109	-3.24410	-1.00303
H	2.21426	-2.11889	-2.17474
H	3.25031	-2.84689	-0.91315
O	0.37278	-0.13609	-2.23569
H	0.10774	-0.88699	-2.80706
F	-0.55793	-2.14175	-1.03349

^{6}FebBPMENOHMeCN
Charge: 2+
Energy: -1452273.9123612

Fe	0.06995	0.11983	-0.83815
O	-0.26589	0.21108	-2.60003
C	-4.57281	0.43130	0.74351
C	-3.81627	-0.73363	0.89543
C	-3.98364	1.56010	0.16908
C	-2.48885	-0.73332	0.47909
C	-1.56699	-1.92208	0.62941
C	-2.65463	1.48351	-0.23267
C	0.68390	0.49975	3.59127
N	-1.92417	0.36493	-0.07050
C	0.17190	0.58991	2.30308
C	1.96693	-0.02692	3.76430
N	-0.60428	-1.95731	-0.50177
C	-1.29180	-2.43794	-1.73585
N	0.86693	0.19532	1.21607
C	0.61202	-2.75917	-0.19591
C	2.69403	-0.42035	2.64100
C	2.11828	-0.28136	1.37841
N	0.68696	2.29177	-0.82725
C	1.74710	-2.36083	-1.13327
N	2.04819	-0.89681	-1.05349
C	2.90190	-0.55494	0.11631
C	2.71213	-0.44565	-2.30890
C	1.01144	3.40334	-0.87475
C	1.41700	4.80117	-0.93621
H	-5.61158	0.45256	1.05841
H	-4.25209	-1.63079	1.32321
H	-4.54370	2.47739	0.02397
H	-2.13532	-2.85821	0.69083
H	-0.99827	-1.81856	1.55908
H	-2.14498	2.31991	-0.69895
H	0.08933	0.82871	4.43662
H	-0.82118	0.98001	2.11337
H	2.39525	-0.12552	4.75704
H	-1.60995	-3.47953	-1.60755
H	-2.15886	-1.80614	-1.92905
H	-0.62747	-2.34884	-2.59276
H	0.40512	-3.83237	-0.29563
H	0.89029	-2.57102	0.84334
H	3.69764	-0.82232	2.73871
H	1.47107	-2.57648	-2.16674
H	2.64654	-2.94813	-0.90954
H	3.65967	-1.33049	0.28318
H	3.44380	0.36428	-0.13284
H	2.06247	-0.67644	-3.15224
H	2.85494	0.63629	-2.26452
H	3.68453	-0.93650	-2.43722
H	1.33420	5.25805	0.05556
H	0.77536	5.34433	-1.63827
H	2.45567	4.87131	-1.27696
H	-0.13914	0.88170	-3.29039

^{3}FebBPMENOHN$_3$
Charge: 2+
Energy: -1471963.5882147

Fe	0.03796	-0.54941	-0.43988
C	-3.80764	2.18037	0.13561
C	-2.97475	1.84452	1.20766
C	-3.49304	1.72255	-1.14521
C	-1.85526	1.05561	0.97274
C	-0.82959	0.70368	2.02186
C	-2.36492	0.92753	-1.31563
C	1.91642	3.37055	-0.20481
N	-1.57524	0.59825	-0.27489
C	0.95940	2.36482	-0.22286
C	3.26772	3.01501	-0.21531
N	-0.21794	-0.60768	1.65724
C	-1.13387	-1.69314	2.13151
N	1.29260	1.05764	-0.24802
C	1.16293	-0.80984	2.19387
C	3.61073	1.66424	-0.27504
C	2.59657	0.71088	-0.31231
C	1.83140	-1.91029	1.38149
N	1.75823	-1.63021	-0.10099
C	2.87149	-0.74286	-0.56536
C	1.84317	-2.92055	-0.85145
H	-4.68925	2.79199	0.30077
H	-3.19087	2.18978	2.21366
H	-4.10899	1.96954	-2.00303
H	-1.27069	0.66444	3.02366
H	-0.04400	1.46412	2.03764
H	-2.05944	0.54988	-2.28369
H	1.60489	4.40915	-0.18492
H	-0.09726	2.59707	-0.22289
H	4.04053	3.77707	-0.19179
H	-1.16353	-1.68649	3.22660
H	-2.13797	-1.51010	1.74747
H	-0.79660	-2.66330	1.77542
H	1.12853	-1.08942	3.25347
H	1.70643	0.13145	2.11230
H	4.64929	1.35140	-0.31323
H	1.32867	-2.86338	1.54870
H	2.87675	-2.03780	1.68301
H	3.81982	-1.06784	-0.12307
H	2.94657	-0.87080	-1.64957
H	1.02955	-3.57418	-0.54432
H	1.75246	-2.71529	-1.91825
H	2.80837	-3.39837	-0.64922
O	0.33351	-0.31961	-2.16129
H	-0.01558	-1.06246	-2.68977
N	-0.91679	-2.12280	-0.67146
N	-2.13604	-2.12699	-0.87701
N	-3.25871	-2.22726	-1.06233

^{3}FebBPMENOHNCS
Charge: 2+
Energy: -1677070.5790797

Fe	-0.08874	-0.34984	-0.30769
C	-1.58547	4.14459	0.00974
C	-1.02180	3.47598	1.10033
C	-1.68642	3.48698	-1.21814
C	-0.57637	2.16944	0.93402
C	0.14229	1.37453	1.99563
C	-1.23356	2.17552	-1.31701
C	3.68707	1.71206	-0.67565
N	-0.69731	1.53879	-0.25962
C	2.32937	1.45639	-0.52897

C	4.57771	0.63750	-0.70069
N	-0.13668	-0.07449	1.77815
C	-1.44615	-0.39967	2.41619
N	1.84012	0.20604	-0.40683
C	0.94267	-0.96834	2.29341
C	4.06995	-0.65783	-0.60612
C	2.69534	-0.83763	-0.48059
C	0.80550	-2.32598	1.61720
N	0.70470	-2.18850	0.11601
C	2.04827	-2.18825	-0.54410
C	-0.08295	-3.32979	-0.43839
H	-1.93864	5.16535	0.11863
H	-0.92448	3.96192	2.06584
H	-2.10924	3.97617	-2.08888
H	-0.14830	1.68753	3.00462
H	1.21960	1.53873	1.89911
H	-1.26867	1.61071	-2.24032
H	4.03259	2.73565	-0.77013
H	1.60952	2.26300	-0.51527
H	5.64529	0.80385	-0.80481
H	-1.37432	-0.26709	3.50172
H	-2.21252	0.26725	2.02007
H	-1.73548	-1.42522	2.19541
H	0.87587	-1.07970	3.38261
H	1.90527	-0.51243	2.06129
H	4.72592	-1.52140	-0.64709
H	-0.10313	-2.82585	1.95559
H	1.64604	-2.97799	1.87755
H	2.68063	-2.97637	-0.12052
H	1.88082	-2.41622	-1.60087
H	-1.05947	-3.36354	0.04356
H	-0.21126	-3.17807	-1.51019
H	0.44355	-4.27386	-0.25839
O	0.06751	-0.53350	-2.06753
H	-0.76443	-0.84776	-2.46768
N	-1.89746	-0.92233	-0.37676
C	-3.03881	-1.19766	-0.55467
S	-4.59384	-1.57902	-0.77071

^{3}FebBPMENOHOOtBu
Charge: 2+
Energy: -1562403.4358534

Fe	0.21577	-0.30353	-0.16504
O	-1.58726	-0.82745	0.14861
H	-0.81923	-0.81236	-2.16374
O	0.10203	-0.62061	-1.90494
O	-2.43664	-0.39863	-0.78977
C	-1.01374	4.27279	0.07844
C	-0.33841	3.63034	1.12049
C	-1.31465	3.55929	-1.08298
C	0.01526	2.29436	0.97152
C	0.83237	1.51690	1.97477
C	-0.94456	2.22054	-1.16430
C	4.04140	1.43951	-1.14651
N	-0.30080	1.60760	-0.15426
C	2.70171	1.29757	-0.80624
C	4.84009	0.29734	-1.22923
N	0.45730	0.07738	1.88180
C	-0.78309	-0.13857	2.68203
N	2.14792	0.09629	-0.55044
C	-3.90745	-2.35481	-0.51667
C	1.54274	-0.85069	2.31339
C	4.25972	-0.94892	-0.99414
C	2.90601	-1.01429	-0.67590
C	-4.30272	-0.20170	0.79044
C	-3.87881	-0.83195	-0.53055
C	1.24414	-2.23470	1.74823
C	-4.58415	-0.22823	-1.73847
N	0.93025	-2.17274	0.27238
C	2.15817	-2.31142	-0.57054
C	-0.01730	-3.26612	-0.08784
H	-1.29638	5.31668	0.17313
H	-0.08503	4.15917	2.03367
H	-1.82507	4.02749	-1.91753
H	0.69633	1.89844	2.99303
H	1.89360	1.61427	1.72711
H	-1.13538	1.61255	-2.03870
H	4.44426	2.42686	-1.34366
H	2.04651	2.15601	-0.74115
H	5.89241	0.37434	-1.48408
H	-0.57956	0.04067	3.74397
H	-1.55375	0.55076	2.33619
H	-1.15255	-1.15360	2.54868
H	-3.50187	-2.76582	-1.44631
H	-4.94613	-2.68633	-0.42517
H	-3.34978	-2.75466	0.33442
H	1.61357	-0.89497	3.40726
H	2.48936	-0.46904	1.93047
H	4.84137	-1.86174	-1.07281
H	-4.17872	0.88545	0.76336
H	-3.73131	-0.61450	1.62612
H	-5.36100	-0.41926	0.96284
H	0.37344	-2.66493	2.24546
H	2.08276	-2.91600	1.92705
H	-4.47529	0.86037	-1.75871
H	-5.65135	-0.46067	-1.67456
H	-4.20284	-0.64741	-2.67453
H	2.78786	-3.12765	-0.19903
H	1.82098	-2.57026	-1.57837
H	-0.92264	-3.16832	0.51046
H	-0.27382	-3.16877	-1.14293
H	0.44114	-4.24450	0.09566

^{3}FebBPMENOOtBuOH
Charge: 2+
Energy: -1562401.9281050

Fe	-0.37294	-0.17046	-0.66817
O	-0.60008	0.13187	-2.40672
O	1.12844	1.04113	-0.72820
O	2.27851	0.60569	-0.23168
C	-3.53296	3.10555	0.68231
C	-3.77492	1.73230	0.77252
C	-2.29841	3.55182	0.20560
C	-2.77608	0.84437	0.38899
C	-2.89984	-0.65799	0.47556
C	-1.34429	2.61067	-0.16471
C	0.18569	-0.37694	3.66010
N	-1.57871	1.28928	-0.06874
C	-0.21725	0.01576	2.39104
C	0.98508	-1.51598	3.78935
N	-2.10005	-1.25412	-0.63409
C	-2.90490	-1.15118	-1.89285
C	2.99449	2.85490	0.44610
N	0.13461	-0.65948	1.27519
C	-1.68066	-2.66370	-0.38825
C	1.37341	-2.19832	2.63817
C	0.94442	-1.73333	1.39561
C	3.40770	1.63354	-0.36563
C	4.57218	0.86875	0.24950
C	3.58745	1.91804	-1.85136
C	-0.49018	-2.95222	-1.29066
N	0.60723	-1.94714	-1.06526
C	1.45278	-2.32047	0.10955
C	1.47048	-1.88871	-2.28230
H	-4.30131	3.81581	0.97162
H	-4.72823	1.35442	1.12752
H	-2.07756	4.60958	0.11358
H	-3.94618	-0.97828	0.42378
H	-2.49308	-1.00899	1.42827
H	-0.37104	2.89585	-0.54636
H	-0.12636	0.19639	4.52622
H	-0.84089	0.88843	2.24653
H	1.30604	-1.85996	4.76770
H	-3.81183	-1.75693	-1.78695
H	-3.16640	-0.10831	-2.06422
H	-2.32249	-1.48612	-2.74582
H	3.81667	3.57673	0.44036
H	2.78468	2.58390	1.48536
H	2.11606	3.33941	0.01115
H	-2.50074	-3.36062	-0.59723
H	-1.41164	-2.76773	0.66475
H	2.01026	-3.07544	2.69569
H	4.79741	-0.03938	-0.31851
H	4.36901	0.60513	1.29200
H	5.46171	1.50547	0.22880
H	-0.18131	0.96775	-2.68208
H	3.81865	1.00278	-2.40523
H	4.42565	2.60988	-1.97786
H	2.69462	2.38380	-2.27663
H	-0.78517	-2.87123	-2.33722
H	-0.11242	-3.96893	-1.13438
H	1.56220	-3.40911	0.17439
H	2.45116	-1.90806	-0.05985
H	0.85725	-1.59397	-3.13136
H	2.24413	-1.13631	-2.12744
H	1.93591	-2.86459	-2.46307

^{2}FeTMCOHNCOCH3
Charge: 2+
Energy: -1455364.0322644

Fe	-0.01425	0.02924	-0.20703
N	-1.53381	1.57465	-0.42373
N	1.39375	1.73333	-0.10769
N	1.63598	-1.47072	-0.27140
N	-1.30247	-1.68938	-0.59993
C	-0.74997	2.69027	-1.05485
C	0.54509	2.96303	-0.30724
C	2.38120	1.57756	-1.23243
C	3.24505	0.30881	-1.19654
C	2.56085	-1.05360	-1.38096
C	0.95139	-2.77444	-0.59098
C	-0.36626	-2.61062	-1.33004
C	-2.47913	-1.37606	-1.47541
C	-3.31018	-0.16533	-1.04666
C	-2.66384	1.19115	-1.33285

C	-2.09115	1.99742	0.89090
C	2.11098	1.89535	1.18591
C	2.41550	-1.68995	0.98152
C	-1.79873	-2.33609	0.65088
H	-1.36132	3.60170	-1.07451
H	-0.53547	2.39672	-2.08049
H	0.33300	3.38173	0.67781
H	1.12168	3.71964	-0.85146
H	3.04810	2.44942	-1.19623
H	1.81552	1.61614	-2.16113
H	3.93480	0.40554	-2.04366
H	3.89227	0.30340	-0.31469
H	1.98682	-1.05979	-2.30498
H	3.34113	-1.82311	-1.45142
H	1.62485	-3.39879	-1.18968
H	0.79091	-3.29684	0.35275
H	-0.84070	-3.59310	-1.44975
H	-0.19440	-2.19449	-2.32134
H	-3.11575	-2.26922	-1.50381
H	-2.11881	-1.23187	-2.49886
H	-3.62446	-0.24772	-0.00200
H	-4.23780	-0.19861	-1.62948
H	-2.28757	1.21075	-2.35925
H	-3.42156	1.98239	-1.26795
H	-2.77060	2.84786	0.75950
H	-1.28611	2.28665	1.56313
H	-2.63735	1.16783	1.33871
H	2.73491	2.79684	1.15713
H	2.74511	1.03881	1.38794
H	1.38689	1.98966	1.99444
H	3.14598	-2.49143	0.81647
H	1.74501	-1.97310	1.78878
H	2.95487	-0.79190	1.26488
H	-2.35028	-3.25013	0.40213
H	-2.46350	-1.65051	1.17568
H	-0.97145	-2.57752	1.31138
C	-0.24477	-0.36069	2.87544
N	-0.15573	-0.05845	1.53201
C	-0.65197	0.68863	3.86820
H	-0.42692	0.31939	4.87182
H	-0.13323	1.63727	3.69870
H	-1.73055	0.87257	3.79530
O	0.01881	-1.53249	3.14705
O	0.17043	0.15219	-1.98314
H	-0.62572	0.00723	-2.51847

^{6}FeTPABrOH
Charge: 1+
Energy: -3030802.4739052

Fe	0.23486	0.57709	-0.65249
N	0.16709	-1.67759	-0.87024
N	-0.31507	-0.18510	1.46437
N	2.24769	-0.08258	-0.18477
N	-1.89464	0.15670	-0.86118
C	-0.69174	0.60126	2.48762
C	-1.30491	0.10037	3.63266
C	-1.55259	-1.26999	3.71084
C	-1.16268	-2.08652	2.64979
C	-0.53582	-1.50856	1.54568
C	0.00747	-2.37681	0.42822
C	3.16049	0.62667	0.49609
C	4.45770	0.15938	0.69209
C	4.80559	-1.08470	0.16605
C	3.84914	-1.82071	-0.53744
C	2.57557	-1.28398	-0.70300
C	1.48107	-1.96982	-1.49351
C	-2.88884	0.98215	-0.50429
C	-4.22708	0.61156	-0.61332
C	-4.52908	-0.66082	-1.09823
C	-3.48792	-1.51719	-1.46428
C	-2.17512	-1.07113	-1.34022
C	-0.97784	-1.88213	-1.78727
H	-0.49649	1.66023	2.36007
H	-1.58728	0.77441	4.43414
H	-2.04184	-1.69712	4.58101
H	-1.33608	-3.15813	2.67731
H	-0.61608	-3.27118	0.30540
H	0.99605	-2.72784	0.74435
H	2.82374	1.58617	0.87419
H	5.17171	0.76005	1.24477
H	5.80671	-1.48155	0.30414
H	4.08696	-2.79406	-0.95477
H	1.46468	-1.53759	-2.49779
H	1.66486	-3.04936	-1.57402
H	-2.58170	1.95248	-0.12781
H	-5.00713	1.30595	-0.32087
H	-5.56104	-0.98578	-1.18937
H	-3.69010	-2.51321	-1.84525
H	-1.23290	-2.94575	-1.88482
H	-0.67144	-1.50386	-2.76710
O	0.52232	0.65094	-2.46222
H	0.62408	1.53166	-2.86046
Br	0.27550	2.94596	0.02049

^{6}FeTPAClOH
Charge: 1+
Energy: -1704274.7988465

Fe	-0.00200	-0.73525	0.83732
N	-0.00197	-0.86165	-1.44556
N	0.00248	1.44824	0.13806
N	-2.09363	-0.56449	0.29101
N	2.09040	-0.57051	0.29186
C	0.00572	2.50565	0.97162
C	0.01071	3.81824	0.51401
C	0.01258	4.04377	-0.86401
C	0.00927	2.94927	-1.72476
C	0.00413	1.66035	-1.18533
C	-0.00070	0.46119	-2.11822
C	-3.05079	-0.05382	1.07824
C	-4.37627	0.03231	0.65905
C	-4.70166	-0.42050	-0.61965
C	-3.69735	-0.94776	-1.43542
C	-2.39707	-1.01383	-0.94287
C	-1.24326	-1.62924	-1.70553
C	3.04871	-0.06269	1.07953
C	4.37441	0.02067	0.66048
C	4.69878	-0.43184	-0.61859
C	3.69327	-0.95610	-1.43482
C	2.39282	-1.01954	-0.94237
C	1.23768	-1.63189	-1.70545
H	0.00428	2.26448	2.02855
H	0.01315	4.63927	1.22274
H	0.01657	5.05441	-1.26102
H	0.01058	3.08640	-2.80235
H	0.87339	0.53084	-2.77627
H	-0.87817	0.53463	-2.77132
H	-2.72328	0.28098	2.05724
H	-5.12868	0.44653	1.32122
H	-5.72380	-0.36237	-0.98122
H	-3.91915	-1.30697	-2.43537
H	-1.08431	-2.63819	-1.31431
H	-1.46534	-1.69629	-2.77877
H	2.72192	0.27216	2.05875
H	5.12776	0.43259	1.32300
H	5.72106	-0.37580	-0.98008
H	3.91429	-1.31504	-2.43505
H	1.45981	-1.69911	-2.77867
H	1.07635	-2.64061	-1.31459
O	-0.00460	-2.57236	0.82827
H	-0.00537	-3.00883	1.69665
Cl	-0.00171	-0.17119	3.03538

^{6}FeTPAFOH
Charge: 1+
Energy: -1478150.2815607

Fe	0.00198	-0.69084	-1.02524
N	0.00201	-0.92553	1.29085
N	-0.00210	1.41644	-0.19384
N	2.08868	-0.56275	-0.45281
N	-2.08546	-0.56833	-0.45365
C	-0.00524	2.47955	-1.01723
C	-0.01026	3.78448	-0.53830
C	-0.01223	3.98462	0.84483
C	-0.00903	2.87822	1.69173
C	-0.00386	1.59846	1.13092
C	0.00075	0.36565	2.02152
C	3.03676	-0.01458	-1.22404
C	4.36358	0.06522	-0.80812
C	4.69540	-0.43443	0.45190
C	3.69809	-0.99877	1.25161
C	2.39585	-1.05549	0.76192
C	1.24426	-1.70354	1.50377
C	-3.03477	-0.02280	-1.22524
C	-4.36179	0.05421	-0.80944
C	-4.69251	-0.44539	0.45088
C	-3.69394	-1.00693	1.25099
C	-2.39155	-1.06098	0.76138
C	-1.23860	-1.70612	1.50364
H	-0.00369	2.23555	-2.07406
H	-0.01266	4.61973	-1.23031
H	-0.01626	4.98906	1.25742
H	-0.01048	3.00092	2.77104
H	-0.87357	0.40936	2.68192
H	0.87828	0.41320	2.67736
H	2.69725	0.35845	-2.18560
H	5.11150	0.51041	-1.45511
H	5.71841	-0.38275	0.81203
H	3.92690	-1.39258	2.23686
H	1.08203	-2.69191	1.06368
H	1.47832	-1.82503	2.57005
H	-2.69609	0.35049	-2.18699
H	-5.11069	0.49728	-1.45675
H	-5.71565	-0.39583	0.81094
H	-3.92189	-1.40065	2.23647
H	-1.47262	-1.82784	2.56991

H	-1.07412	-2.69428	1.06388
O	0.00428	-2.53195	-1.11532
H	0.00544	-2.94320	-1.99501
F	0.00185	0.03332	-2.65990

^{6}FeTPAN$_3$OH
Charge: 1+
Energy: -1518534.4816001

Fe	0.00264	0.98613	-0.11865
N	0.00176	-0.80562	-1.57989
N	-0.00323	-0.85892	1.21540
N	2.10362	0.41997	-0.31694
N	-2.09976	0.42663	-0.32184
C	-0.00702	-0.78377	2.55838
C	-0.01359	-1.91385	3.36784
C	-0.01656	-3.16957	2.75567
C	-0.01272	-3.24336	1.36497
C	-0.00591	-2.05963	0.62222
C	-0.00028	-2.12194	-0.89758
C	3.06663	0.73890	0.55850
C	4.38845	0.33820	0.38008
C	4.70495	-0.42624	-0.74333
C	3.69526	-0.76215	-1.64817
C	2.39893	-0.31348	-1.40761
C	1.24145	-0.56277	-2.35168
C	-3.06379	0.74872	0.55131
C	-4.38622	0.35112	0.37051
C	-4.70226	-0.41363	-0.75283
C	-3.69153	-0.75284	-1.65526
C	-2.39460	-0.30710	-1.41243
C	-1.23586	-0.55984	-2.35401
H	-0.00470	0.22315	2.96274
H	-0.01643	-1.81052	4.44755
H	-0.02185	-4.07656	3.35267
H	-0.01489	-4.20360	0.85708
H	-0.87427	-2.69874	-1.22312
H	0.87720	-2.69729	-1.21613
H	2.74662	1.32652	1.41319
H	5.14435	0.61721	1.10604
H	5.72359	-0.76189	-0.91240
H	3.90927	-1.35929	-2.52899
H	1.08258	0.35072	-2.93213
H	1.46491	-1.38698	-3.04276
H	-2.74410	1.33629	1.40616
H	-5.14294	0.63266	1.09463
H	-5.72136	-0.74695	-0.92369
H	-3.90517	-1.35025	-2.53599
H	-1.46010	-1.38372	-3.04523
H	-1.07352	0.35302	-2.93452
O	0.00603	2.07218	-1.60381
H	0.00782	3.03958	-1.52854
N	0.00268	2.11742	1.43917
N	0.00471	3.32928	1.57358
N	0.00656	4.46539	1.74184

^{6}FeTPANCSOH
Charge: 1+
Energy: -1723642.1248868

Fe	0.24122	0.33265	-0.86656
N	0.43368	-1.90542	-0.43806
N	-0.25975	0.09884	1.39535
N	2.30181	0.04973	-0.25174
N	-1.81941	-0.39123	-0.91996
C	-0.74933	1.09394	2.15276
C	-1.34326	0.87056	3.39184
C	-1.44658	-0.44281	3.85177
C	-0.93991	-1.47640	3.06444
C	-0.34298	-1.16423	1.84240
C	0.32150	-2.23830	1.00359
C	3.10670	1.02445	0.19429
C	4.44311	0.78993	0.50756
C	4.94491	-0.50294	0.35425
C	4.09931	-1.51547	-0.10526
C	2.77726	-1.20146	-0.40926
C	1.78733	-2.20449	-0.96535
C	-2.90573	0.38182	-0.78966
C	-4.19215	-0.15171	-0.77458
C	-4.33928	-1.53445	-0.88744
C	-3.20189	-2.33502	-1.01660
C	-1.94969	-1.72631	-1.03725
C	-0.65780	-2.48591	-1.25328
H	-0.66273	2.09044	1.73458
H	-1.72152	1.70576	3.97136
H	-1.91557	-0.66020	4.80666
H	-1.00174	-2.50974	3.39251
H	-0.19481	-3.19747	1.13610
H	1.33490	-2.37405	1.39764
H	2.64951	2.00409	0.29018
H	5.06846	1.60129	0.86360
H	5.98057	-0.72383	0.59393
H	4.45915	-2.53198	-0.22940
H	1.74629	-2.07319	-2.05011
H	2.09780	-3.23414	-0.74273
H	-2.71746	1.44650	-0.69454
H	-5.05095	0.50274	-0.67277
H	-5.32627	-1.98665	-0.87200
H	-3.28402	-3.41376	-1.10451
H	-0.79027	-3.55752	-1.05188
H	-0.37345	-2.35800	-2.30193
O	0.56199	-0.09355	-2.62862
H	0.55930	0.62738	-3.27912
N	-0.00046	2.23418	-0.74850
C	-0.29015	3.39087	-0.60032
S	-0.68402	4.91917	-0.37693

^{6}FeTPAOHBr
Charge: 1+
Energy: -3030804.0865543

Fe	0.20108	-0.37882	-0.73187
O	0.13467	-0.18441	-2.55267
N	0.14870	0.00289	1.58150
N	-0.56985	1.69351	-0.52652
N	2.15217	0.33914	-0.21088
N	-1.82998	-0.81419	-0.15495
Br	0.86368	-2.77146	-0.48547
C	-1.02951	2.36038	-1.59887
C	-1.74929	3.54509	-1.47758
C	-2.01160	4.03745	-0.19795
C	-1.53421	3.33829	0.91080
C	-0.80414	2.16766	0.70646
C	-0.16203	1.42740	1.86238
C	2.99919	0.81059	-1.13978
C	4.28514	1.22974	-0.81301
C	4.68969	1.15888	0.52094
C	3.80021	0.67346	1.48214
C	2.53306	0.26081	1.07952
C	1.51811	-0.34706	2.02546
C	-2.81994	-0.89076	-1.05702
C	-4.14249	-1.10054	-0.67830
C	-4.43407	-1.21922	0.68139
C	-3.39846	-1.13008	1.61400
C	-2.09719	-0.93361	1.15890
C	-0.89301	-0.92356	2.07664
H	-0.80825	1.89776	-2.55485
H	-2.10198	4.05962	-2.36487
H	-2.58184	4.95169	-0.06361
H	-1.71968	3.69596	1.91912
H	-0.78431	1.51550	2.76204
H	0.78046	1.93983	2.08615
H	2.60916	0.83521	-2.15199
H	4.94788	1.60279	-1.58608
H	5.68466	1.48123	0.81230
H	4.08551	0.60976	2.52745
H	1.61640	-1.43567	1.96998
H	1.70942	-0.03680	3.06163
H	-2.51521	-0.77477	-2.09195
H	-4.92009	-1.16429	-1.43155
H	-5.45553	-1.37690	1.01385
H	-3.59456	-1.21830	2.67790
H	-1.18828	-0.69271	3.10922
H	-0.46567	-1.93176	2.06153
H	0.36361	-0.97149	-3.07551

^{6}FeTPAOHCl
Charge: 1+
Energy: -1704275.9518324

Fe	0.19658	-0.57256	-0.86414
O	0.13807	-0.11253	-2.63894
N	0.19862	-0.49998	1.47819
N	-0.31923	1.53361	-0.36183
N	2.21862	-0.12042	-0.29380
N	-1.87572	-0.83082	-0.30919
Cl	0.56712	-2.83569	-0.88859
C	-0.68606	2.39627	-1.32524
C	-1.24082	3.63806	-1.03194
C	-1.43403	3.98220	0.30717
C	-1.05438	3.08116	1.30169
C	-0.48811	1.86236	0.92762
C	0.04184	0.89264	1.96550
C	3.10429	0.39413	-1.16083
C	4.42692	0.63468	-0.80062
C	4.82694	0.33408	0.50226
C	3.89728	-0.19575	1.39996
C	2.59401	-0.42084	0.96485
C	1.52578	-1.05473	1.83222
C	-2.87680	-0.65713	-1.18432
C	-4.21107	-0.76665	-0.80333
C	-4.49973	-1.05265	0.53176
C	-3.45084	-1.22457	1.43777
C	-2.14043	-1.11416	0.97971
C	-0.93241	-1.37605	1.85466
H	-0.52829	2.04384	-2.33894
H	-1.52174	4.31085	-1.83496
H	-1.87619	4.93727	0.57441

H	-1.18990	3.31911	2.35249
H	-0.59037	0.91749	2.86216
H	1.02835	1.25783	2.27313
H	2.71491	0.60246	-2.15200
H	5.12072	1.04839	-1.52418
H	5.84985	0.51318	0.81911
H	4.17860	-0.43625	2.42033
H	1.50544	-2.12598	1.61102
H	1.75679	-0.92666	2.89843
H	-2.57145	-0.42359	-2.19910
H	-4.99898	-0.62672	-1.53528
H	-5.52904	-1.13864	0.86633
H	-3.64469	-1.44722	2.48227
H	-1.18957	-1.27745	2.91814
H	-0.61765	-2.40874	1.67322
H	0.27618	-0.84052	-3.26854

^{6}FeTPAOHF
Charge: 1+
Energy: -1478151.3603373

Fe	-0.00504	-0.66218	1.03114
O	-0.00365	0.05959	2.72322
N	-0.00545	-0.93361	-1.29387
N	0.00608	1.41854	0.18071
N	-2.09145	-0.56762	0.46111
N	2.08293	-0.58298	0.46344
F	-0.01164	-2.45384	1.11273
C	0.01433	2.49220	0.99202
C	0.02706	3.79138	0.49767
C	0.03185	3.97678	-0.88718
C	0.02345	2.86075	-1.72093
C	0.01024	1.58688	-1.14761
C	-0.00218	0.34915	-2.03231
C	-3.04167	-0.01797	1.22927
C	-4.36730	0.06264	0.80998
C	-4.69724	-0.43876	-0.44970
C	-3.69873	-1.00571	-1.24608
C	-2.39775	-1.06197	-0.75348
C	-1.24648	-1.71491	-1.49062
C	3.03634	-0.04050	1.23269
C	4.36240	0.03340	0.81344
C	4.68929	-0.46706	-0.44739
C	3.68745	-1.02653	-1.24490
C	2.38623	-1.07639	-0.75227
C	1.23128	-1.72164	-1.49042
H	0.01072	2.26215	2.05226
H	0.03332	4.63377	1.18089
H	0.04210	4.97641	-1.31117
H	0.02694	2.97085	-2.80157
H	0.86936	0.38745	-2.69705
H	-0.88254	0.39785	-2.68460
H	-2.70184	0.35718	2.18943
H	-5.11617	0.50974	1.45457
H	-5.71948	-0.38697	-0.81201
H	-3.92591	-1.40215	-2.23062
H	-1.08075	-2.69628	-1.03719
H	-1.48548	-1.85405	-2.55373
H	2.69871	0.33478	2.19357
H	5.11390	0.47473	1.45893
H	5.71177	-0.42030	-0.80973
H	3.91227	-1.42213	-2.23032
H	1.46991	-1.86138	-2.55354
H	1.05968	-2.70240	-1.03782
H	-0.00763	-0.56567	3.46682

^{2}FeTPAOHN$_3$
Charge: 1+
Energy: -1518529.3175862

Fe	0.14895	-0.45155	-0.47799
N	0.27680	-0.18638	1.57808
N	-0.07645	1.56249	-0.45584
N	2.12918	-0.37484	-0.32360
N	-1.79930	-0.51969	-0.15987
C	-0.37766	2.28079	-1.55004
C	-0.70262	3.63132	-1.46842
C	-0.72824	4.24223	-0.21337
C	-0.41540	3.48718	0.91759
C	-0.08428	2.14389	0.75528
C	0.36796	1.26934	1.90067
C	2.98231	-0.12225	-1.32523
C	4.35943	-0.08682	-1.12215
C	4.85227	-0.30847	0.16375
C	3.95549	-0.55607	1.20598
C	2.59322	-0.59135	0.92669
C	1.52832	-0.90573	1.95572
C	-2.74748	-0.45347	-1.10386
C	-4.09955	-0.43876	-0.77034
C	-4.45917	-0.48652	0.57634
C	-3.46089	-0.56344	1.55153
C	-2.13071	-0.59143	1.14717
C	-0.97113	-0.81932	2.09539
H	-0.35279	1.72187	-2.47936
H	-0.93858	4.18531	-2.37045
H	-0.98946	5.29141	-0.11469
H	-0.42309	3.93118	1.90825
H	-0.18937	1.49599	2.81663
H	1.41851	1.50324	2.10495
H	2.52147	0.05161	-2.29132
H	5.02389	0.11344	-1.95548
H	5.92018	-0.28254	0.35714
H	4.30656	-0.72423	2.21910
H	1.31469	-1.97573	1.90354
H	1.85411	-0.65337	2.97208
H	-2.37425	-0.41785	-2.12152
H	-4.84832	-0.39175	-1.55326
H	-5.50472	-0.46995	0.86807
H	-3.71092	-0.61569	2.60636
H	-1.20521	-0.47588	3.11006
H	-0.78768	-1.89672	2.13259
O	0.03025	-0.46341	-2.28028
H	0.53819	-1.21078	-2.63932
N	0.29993	-2.36755	-0.26409
N	-0.60623	-3.04149	-0.73599
N	-1.43237	-3.71809	-1.16149

^{4}FeTPAOHNCS
Charge: 1+
Energy: -1723633.7318786

Fe	-0.00618	0.44234	-0.48746
N	-0.00162	-0.22102	1.58048
N	0.01984	-1.56212	-0.85237
N	-2.18273	0.14553	-0.00594
N	2.17533	0.19461	-0.00158
C	0.03186	-2.08793	-2.08972
C	0.05427	-3.46147	-2.29904
C	0.06486	-4.30636	-1.18684
C	0.05241	-3.75119	0.09205
C	0.02949	-2.36336	0.22817
C	0.01267	-1.71759	1.60010
C	-3.18099	0.01486	-0.88844
C	-4.49842	-0.19067	-0.48312
C	-4.76907	-0.27103	0.88378
C	-3.72198	-0.13775	1.79921
C	-2.43573	0.08090	1.31185
C	-1.23643	0.33274	2.19884
C	3.17780	0.08633	-0.88230
C	4.49815	-0.09444	-0.47472
C	4.76738	-0.17375	0.89252
C	3.71591	-0.06398	1.80606
C	2.42665	0.13076	1.31653
C	1.22073	0.35684	2.20146
H	0.02297	-1.35613	-2.89093
H	0.06343	-3.85592	-3.30915
H	0.08271	-5.38466	-1.31299
H	0.06022	-4.38333	0.97486
H	0.88805	-2.06251	2.16168
H	-0.86591	-2.07854	2.14636
H	-2.89370	0.08304	-1.93332
H	-5.28740	-0.28693	-1.22113
H	-5.78288	-0.43689	1.23524
H	-3.90145	-0.19410	2.86838
H	-1.09287	1.41505	2.27201
H	-1.38985	-0.06764	3.20947
H	2.89132	0.15199	-1.92757
H	5.29047	-0.17277	-1.21127
H	5.78351	-0.32065	1.24570
H	3.89420	-0.12006	2.87545
H	1.38035	-0.04149	3.21194
H	1.05519	1.43596	2.27563
O	-0.00688	0.76067	-2.25384
H	-0.01831	1.71339	-2.45535
N	-0.02788	2.27337	0.02256
C	-0.03905	3.38204	-0.44765
S	-0.05424	4.87335	-1.01156

^{5}FeTPAOCCPhBr
Charge: 1+
Energy: -3224811.3144803

Fe	0.63005	-0.28122	-0.27729
O	-0.91994	-1.67472	0.30223
N	2.21169	1.31472	-0.33821
N	0.25147	0.83818	1.62216
N	-0.50588	1.50660	-1.02267
N	2.37286	-1.23373	0.66478
Br	0.95785	-1.27474	-2.57344
C	-0.84393	0.67472	2.38117
C	-1.22792	1.59783	3.34908
C	-0.44711	2.74169	3.52210
C	0.68561	2.91467	2.72731
C	1.00953	1.93571	1.78708
C	2.27611	2.03607	0.95433
C	-1.82934	1.71744	-1.00696
C	-2.40226	2.92614	-1.39545
C	-1.55827	3.96010	-1.79985

C	-0.17891	3.74685	-1.80219
C	0.31399	2.50211	-1.41321
C	1.79335	2.16945	-1.47019
C	2.38414	-2.32691	1.44047
C	3.56250	-2.90368	1.90618
C	4.77415	-2.30563	1.55764
C	4.76312	-1.15984	0.76081
C	3.54054	-0.65424	0.32188
C	3.44490	0.54180	-0.60776
H	-1.42481	-0.21813	2.17609
H	-2.12115	1.42717	3.94042
H	-0.71893	3.49151	4.25898
H	1.31062	3.79646	2.83190
H	3.08668	1.59420	1.54475
H	2.54144	3.09004	0.79791
H	-2.44183	0.88880	-0.66530
H	-3.47976	3.04942	-1.37213
H	-1.96473	4.92014	-2.10346
H	0.50652	4.53199	-2.10601
H	1.96038	1.58964	-2.38460
H	2.39432	3.08817	-1.52843
H	1.40938	-2.73907	1.68436
H	3.52827	-3.79222	2.52735
H	5.71507	-2.72119	1.90536
H	5.68835	-0.66775	0.47730
H	4.34753	1.16481	-0.53450
H	3.37019	0.16115	-1.63193
C	-1.15353	-3.02140	-0.19669
H	-1.49273	-3.71249	0.57176
H	-0.38931	-3.37181	-0.88692
C	-2.04043	-1.92956	-0.62665
H	-1.83434	-1.52849	-1.61783
C	-3.39384	-1.66748	-0.07502
C	-3.69308	-1.89626	1.27640
C	-4.96827	-1.62414	1.76760
C	-5.95774	-1.12409	0.91441
C	-5.66561	-0.89371	-0.43093
C	-4.38582	-1.15849	-0.92327
H	-2.92460	-2.28160	1.94127
H	-5.19412	-1.80595	2.81441
H	-6.95226	-0.91719	1.29848
H	-6.43114	-0.50837	-1.09793
H	-4.15782	-0.97906	-1.97148

[5]FeTPAOCCPhCl
Charge: 1+
Energy: -1898282.6581725

Fe	0.65759	-0.31203	-0.54862
O	-0.91835	-1.73832	-0.10736
N	2.27531	1.24183	-0.46241
N	0.44533	0.48415	1.53038
N	-0.48377	1.60534	-0.90580
N	2.43154	-1.44291	0.12095
Cl	0.80343	-0.87574	-2.80048
C	-0.59420	0.20944	2.33478
C	-0.87895	0.95977	3.47149
C	-0.05585	2.04609	3.77271
C	1.01854	2.33519	2.93225
C	1.24408	1.52612	1.81771
C	2.44744	1.75125	0.91694
C	-1.79177	1.84969	-0.74876
C	-2.33986	3.12392	-0.88044
C	-1.48473	4.18621	-1.17146
C	-0.11972	3.93542	-1.32161
C	0.34660	2.62826	-1.18876
C	1.80314	2.26699	-1.41746
C	2.46852	-2.64052	0.72102
C	3.66157	-3.29394	1.01885
C	4.86116	-2.66344	0.68670
C	4.82423	-1.41094	0.07177
C	3.58719	-0.83165	-0.20678
C	3.45873	0.49233	-0.93921
H	-1.21220	-0.62790	2.02833
H	-1.72929	0.70402	4.09451
H	-0.25083	2.66339	4.64453
H	1.67383	3.17707	3.13474
H	3.29354	1.22111	1.36874
H	2.71504	2.81623	0.90773
H	-2.41266	0.99299	-0.50504
H	-3.40643	3.27327	-0.75030
H	-1.87091	5.19580	-1.27493
H	0.57418	4.74032	-1.54352
H	1.87584	1.82545	-2.41719
H	2.43283	3.16792	-1.38993
H	1.50250	-3.07441	0.96253
H	3.64766	-4.26553	1.50092
H	5.81316	-3.13660	0.90763
H	5.74009	-0.89218	-0.19407
H	4.38449	1.07810	-0.84790
H	3.29298	0.27080	-1.99870
C	-1.19744	-2.95898	-0.84734
H	-1.53742	-3.77767	-0.21690
H	-0.45811	-3.18477	-1.61236
C	-2.06535	-1.78581	-1.03513
H	-1.87339	-1.20715	-1.93724
C	-3.39866	-1.60855	-0.40562
C	-3.66215	-2.06458	0.89453
C	-4.91922	-1.87104	1.46362
C	-5.92569	-1.22283	0.74003
C	-5.66851	-0.76492	-0.55332
C	-4.40693	-0.95119	-1.12243
H	-2.87927	-2.56406	1.45899
H	-5.11747	-2.22853	2.47001
H	-6.90600	-1.07700	1.18405
H	-6.44708	-0.26265	-1.11988
H	-4.20585	-0.59373	-2.12976

[5]FeTPAOCCPhF
Charge: 1+
Energy: -1672154.0800658

Fe	0.61822	-0.41427	-0.60653
O	-1.01939	-1.72500	0.07438
N	2.24604	1.12299	-0.81165
N	0.68811	0.51200	1.44278
N	-0.56023	1.51959	-0.92259
N	2.47494	-1.53745	-0.07532
F	0.44885	-1.05027	-2.30360
C	-0.24220	0.30439	2.38819
C	-0.36726	1.12277	3.50693
C	0.50206	2.20744	3.63475
C	1.46136	2.42788	2.64684
C	1.53006	1.55269	1.56189
C	2.60784	1.70501	0.49837
C	-1.82329	1.80761	-0.58449
C	-2.34167	3.10082	-0.64273
C	-1.50135	4.13318	-1.05660
C	-0.18052	3.83597	-1.40021
C	0.25418	2.51356	-1.32778
C	1.65335	2.09748	-1.75013
C	2.60625	-2.67412	0.61985
C	3.84030	-3.28347	0.83831
C	4.98041	-2.67233	0.31648
C	4.84646	-1.48183	-0.40094
C	3.57283	-0.94580	-0.58564
C	3.33049	0.31150	-1.40470
H	-0.90407	-0.53744	2.21082
H	-1.13160	0.91972	4.24941
H	0.43027	2.87646	4.48708
H	2.14721	3.26722	2.71354
H	3.50157	1.18669	0.86393
H	2.88185	2.76352	0.39347
H	-2.43220	0.97064	-0.25595
H	-3.37373	3.28637	-0.36461
H	-1.86386	5.15551	-1.10818
H	0.50088	4.61697	-1.72341
H	1.56967	1.59348	-2.71907
H	2.29494	2.98159	-1.87952
H	1.68385	-3.09687	1.00800
H	3.90222	-4.20668	1.40450
H	5.96166	-3.11139	0.46964
H	5.71504	-0.97848	-0.81435
H	4.26335	0.88162	-1.52334
H	2.98766	0.00313	-2.39842
C	-1.26856	-2.96006	-0.65004
H	-1.65403	-3.76282	-0.02520
H	-0.49117	-3.20475	-1.36966
C	-2.10812	-1.78264	-0.92017
H	-1.85027	-1.23762	-1.82589
C	-3.47710	-1.57877	-0.38312
C	-3.82380	-1.98004	0.91522
C	-5.11602	-1.76953	1.39229
C	-6.07461	-1.15743	0.57811
C	-5.73369	-0.75081	-0.71314
C	-4.43727	-0.95443	-1.18992
H	-3.07593	-2.44625	1.55080
H	-5.37825	-2.08391	2.39847
H	-7.08223	-0.99796	0.95074
H	-6.47394	-0.27415	-1.34909
H	-4.17012	-0.63524	-2.19472

[4]FeTMCOHCN
Charge: 1+
Energy: -1383318.3839161

Fe	0.04761	-0.00253	0.02278
O	-0.00844	-0.08637	-1.80513
C	0.08903	-0.00668	1.97561
N	0.11206	0.00306	3.14306
N	1.67990	-1.51629	-0.08803
N	-1.27748	-1.75843	0.02849
N	-1.69758	1.46505	0.04334
N	1.23453	1.81159	-0.10571
C	0.97031	-2.58984	-0.83986
C	-0.37419	-2.93635	-0.20156
C	-2.22215	-1.57820	-1.12145
C	-3.15659	-0.35901	-1.03396

C	-2.55113	1.05293	-1.11601
C	-1.06613	2.79717	-0.20650
C	0.31549	2.72002	-0.85473
C	2.49487	1.59617	-0.88436
C	3.33900	0.38936	-0.45229
C	2.81569	-0.98484	-0.89458
C	2.18160	-2.02095	1.21453
C	-2.04073	-2.03033	1.27723
C	-2.51365	1.58574	1.27876
C	1.58776	2.41032	1.21176
H	1.58653	-3.49969	-0.87925
H	0.81184	-2.22494	-1.85278
H	-0.88461	-3.67540	-0.83151
H	-0.20733	-3.41074	0.76661
H	-1.61667	-1.50764	-2.02328
H	-2.84689	-2.48135	-1.18715
H	-3.81984	-0.44080	-1.90413
H	-3.82125	-0.44354	-0.16892
H	-3.37741	1.77488	-1.20482
H	-1.92984	1.12083	-2.00807
H	-1.71893	3.41268	-0.83945
H	-0.98873	3.31071	0.75313
H	0.74333	3.73125	-0.90632
H	0.22481	2.34081	-1.87218
H	2.23129	1.49126	-1.94179
H	3.09943	2.51085	-0.81186
H	4.32307	0.51833	-0.91802
H	3.52139	0.40979	0.62623
H	3.63794	-1.71395	-0.86233
H	2.48261	-0.92764	-1.93389
H	2.89706	-2.83977	1.05641
H	2.66465	-1.21351	1.76314
H	1.35433	-2.36777	1.82992
H	-2.63866	-2.94441	1.16095
H	-1.35188	-2.13816	2.11274
H	-2.70419	-1.20281	1.50726
H	-3.25149	2.39313	1.17274
H	-3.04392	0.65923	1.47974
H	-1.86199	1.78342	2.12935
H	2.08073	3.38046	1.06282
H	0.69799	2.53593	1.82281
H	2.25089	1.73923	1.75403
H	0.71011	0.36813	-2.26707

^{6}FeTMCOHNCO
Charge: 1+
Energy: -1430577.2843560

Fe	0.00697	0.01091	-0.10001
O	-0.13075	0.09850	-1.97964
N	0.28490	-0.03012	1.81950
C	0.73483	-0.04662	2.94059
O	1.17438	-0.06161	4.04178
N	1.40992	-1.70433	-0.44965
N	-1.53812	-1.65957	0.02029
N	-1.56505	1.63423	0.05894
N	1.37543	1.73666	-0.41934
C	0.50594	-2.68023	-1.11710
C	-0.78882	-2.91151	-0.33487
C	-2.59756	-1.35246	-0.98523
C	-3.34446	-0.01732	-0.80268
C	-2.59143	1.31544	-0.97933
C	-0.83641	2.90513	-0.27622
C	0.45169	2.70731	-1.07586
C	2.46918	1.34228	-1.35673
C	3.20305	0.04023	-0.99222
C	2.48728	-1.26348	-1.38581
C	2.00182	-2.28552	0.77627
C	-2.14119	-1.86064	1.36139
C	-2.18900	1.81299	1.39151
C	1.94509	2.29803	0.82648
H	1.01224	-3.64834	-1.24783
H	0.28397	-2.28989	-2.10897
H	-1.43657	-3.58672	-0.90951
H	-0.55718	-3.42621	0.59894
H	-2.13000	-1.37926	-1.97028
H	-3.34436	-2.16109	-0.96195
H	-4.12365	-0.01521	-1.57520
H	-3.89395	-0.02314	0.14325
H	-3.34072	2.12195	-0.98422
H	-2.07369	1.31929	-1.93844
H	-1.50061	3.57816	-0.83415
H	-0.60947	3.40478	0.66720
H	0.94601	3.68282	-1.19441
H	0.22065	2.30672	-2.06071
H	2.01894	1.22865	-2.34331
H	3.19474	2.16703	-1.40451
H	4.14884	0.05276	-1.54635
H	3.48749	0.02960	0.06517
H	3.22547	-2.07435	-1.46850
H	2.02637	-1.12427	-2.36458
H	2.58960	-3.18221	0.53497
H	2.64666	-1.55059	1.25676
H	1.21875	-2.54016	1.48838
H	-2.81451	-2.72912	1.35622
H	-1.34626	-2.00599	2.09115
H	-2.70433	-0.98194	1.66309
H	-2.86312	2.68085	1.39155
H	-2.75826	0.93070	1.67166
H	-1.40531	1.94745	2.13638
H	2.50316	3.22014	0.61304
H	1.15255	2.50537	1.54318
H	2.61325	1.57073	1.28668
H	-0.54662	-0.46709	-2.64088

^{6}FeTMCOHO2CCF3
Charge: 1+
Energy: -1655402.5761050

Fe	0.68518	0.24614	0.09236
O	2.27651	1.11170	0.56103
N	-0.15016	1.36698	1.80687
N	1.02045	-1.32903	1.66516
N	1.70620	-0.94501	-1.56228
N	0.49345	1.74865	-1.52291
C	0.70704	0.86442	2.91873
C	0.71803	-0.66408	2.98097
C	2.47039	-1.68280	1.57814
C	2.94804	-2.28722	0.24517
C	3.01683	-1.40069	-1.01184
C	1.89328	0.02440	-2.69706
C	1.73517	1.49477	-2.30598
C	0.53753	3.12231	-0.93575
C	-0.41923	3.36522	0.24171
C	0.06354	2.82981	1.60023
C	-1.58103	1.08949	2.06734
C	0.16764	-2.53764	1.54275
C	0.94717	-2.11013	-2.08753
C	-0.71772	1.57686	-2.35799
H	0.34877	1.25580	3.88201
H	1.71263	1.23884	2.73727
H	1.44583	-0.98356	3.73703
H	-0.25514	-1.02731	3.31432
H	3.02727	-0.77040	1.79502
H	2.69228	-2.41267	2.37121
H	3.97911	-2.61502	0.42700
H	2.39682	-3.20610	0.02662
H	3.54382	-1.96648	-1.79497
H	3.61641	-0.51130	-0.80902
H	2.88125	-0.11727	-3.15298
H	1.16114	-0.22844	-3.46531
H	1.74179	2.10466	-3.22140
H	2.57041	1.81150	-1.68375
H	1.56011	3.29008	-0.59356
H	0.32411	3.84370	-1.73731
H	-0.50875	4.45246	0.34854
H	-1.42862	3.01032	0.01000
H	-0.44858	3.36888	2.40989
H	1.13487	3.01400	1.69455
H	-1.89919	1.57369	3.00071
H	-2.18561	1.45350	1.24066
H	-1.75356	0.01878	2.13362
H	0.43163	-3.27714	2.31115
H	-0.87737	-2.25498	1.65899
H	0.26405	-2.98473	0.55804
H	1.50967	-2.59410	-2.89812
H	0.75254	-2.83550	-1.30455
H	-0.02227	-1.78182	-2.45266
H	-0.71872	2.29648	-3.18797
H	-0.75453	0.56307	-2.75417
H	-1.60822	1.70991	-1.74751
O	-1.06125	-0.46035	-0.34743
C	-2.00944	-1.30641	-0.61506
O	-1.89991	-2.46296	-0.97231
C	-3.42321	-0.71649	-0.36381
F	-4.35506	-1.32843	-1.08671
F	-3.72592	-0.86177	0.94923
F	-3.47312	0.61273	-0.64120
H	3.20174	0.98954	0.31508

^{4}FeTMCOHOH
Charge: 1+
Energy: -1372652.7864201

Fe	-0.06215	0.00313	0.13022
O	-0.07491	0.10435	-1.68818
O	-0.15705	-0.02674	1.91454
H	0.67935	0.20130	2.34843
N	-1.01056	1.92948	-0.01259
N	1.88442	1.29016	0.11474
N	1.03600	-1.90131	0.08890
N	-1.86025	-1.32907	-0.00141
C	-0.01095	2.73123	-0.77285
C	1.38748	2.67306	-0.15455
C	2.65369	0.75392	-1.04592
C	3.08829	-0.72015	-0.93887
C	2.03270	-1.83911	-1.02470
C	0.01900	-2.98222	-0.13691

C	-1.31669	-2.50306	-0.71971
C	-2.93579	-0.67006	-0.79082
C	-3.26901	0.76254	-0.35037
C	-2.27426	1.84030	-0.80393
C	-1.27786	2.52400	1.31552
C	2.73481	1.34768	1.32145
C	1.72224	-2.20276	1.36950
C	-2.36096	-1.71680	1.33458
H	-0.32836	3.78326	-0.82200
H	0.01202	2.32938	-1.78414
H	2.08419	3.20730	-0.81558
H	1.38773	3.21399	0.79421
H	2.02279	0.87599	-1.92535
H	3.56189	1.36406	-1.17932
H	3.75297	-0.89202	-1.79498
H	3.72634	-0.87247	-0.06270
H	2.56539	-2.80194	-1.06364
H	1.47826	-1.73853	-1.95784
H	0.43488	-3.75927	-0.79074
H	-0.17135	-3.45654	0.82691
H	-2.02226	-3.34804	-0.69578
H	-1.19984	-2.23389	-1.77211
H	-2.60757	-0.64138	-1.83261
H	-3.84418	-1.29045	-0.74682
H	-4.23013	1.01490	-0.81432
H	-3.44635	0.81220	0.72830
H	-2.76460	2.82461	-0.77479
H	-1.98454	1.63905	-1.83595
H	-1.68539	3.53878	1.20584
H	-1.97968	1.89759	1.86247
H	-0.36221	2.55527	1.90214
H	3.57902	2.04025	1.18703
H	2.14316	1.69372	2.17400
H	3.14081	0.36631	1.56162
H	2.20525	-3.18875	1.32794
H	2.48276	-1.45473	1.57776
H	0.99184	-2.17616	2.17682
H	-3.18492	-2.44010	1.24700
H	-1.55265	-2.13937	1.92789
H	-2.70368	-0.83112	1.86697
H	-0.21264	-0.71154	-2.18539

^{6}FeTMCSBr
Charge: 1+
Energy: -3166970.2207669

Fe	0.03037	0.05374	0.30894
N	1.06041	-1.87516	0.75953
N	-1.73926	-1.04176	1.10050
N	-1.23053	1.85574	-0.33105
N	1.69788	1.15805	-0.63158
C	-0.03711	-2.87344	0.58718
C	-1.29831	-2.46277	1.35023
C	-2.82961	-1.00765	0.06320
C	-3.32908	0.37950	-0.38367
C	-2.38938	1.34258	-1.13630
C	-0.27930	2.68479	-1.15810
C	0.98398	1.97277	-1.66757
C	2.67237	0.21552	-1.28877
C	3.14778	-0.95652	-0.41041
C	2.17563	-2.13129	-0.20975
C	1.59438	-1.95771	2.14352
C	-2.24515	-0.48988	2.38554
C	-1.78188	2.75038	0.72466
C	2.46149	2.00405	0.34015
S	0.67827	1.14596	2.29350
C	1.66169	2.49914	1.54060
H	0.28640	-3.86020	0.94857
H	-0.25013	-2.95127	-0.47645
H	-1.13227	-2.56696	2.42386
H	-2.11059	-3.15148	1.09046
H	-3.69273	-1.54969	0.47749
H	-2.46287	-1.56122	-0.79872
H	-4.14401	0.16742	-1.08700
H	-3.81272	0.89157	0.45399
H	-1.98913	0.85482	-2.02128
H	-2.98686	2.20693	-1.46294
H	-0.80896	3.09065	-2.02900
H	0.01210	3.54106	-0.54869
H	1.66261	2.73660	-2.07296
H	0.71743	1.29498	-2.47432
H	3.54582	0.80380	-1.60286
H	2.19706	-0.17953	-2.18477
H	3.52462	-0.60060	0.55456
H	4.02260	-1.37442	-0.92298
H	1.72921	-2.39747	-1.16675
H	2.74292	-3.00088	0.15111
H	1.96160	-2.97298	2.34640
H	0.82187	-1.70345	2.86854
H	2.40562	-1.24395	2.27255
H	-3.11102	-1.06737	2.73618
H	-2.53522	0.54977	2.26459
H	-1.45836	-0.52833	3.13965
H	-2.27674	3.61558	0.26275
H	-0.99500	3.09457	1.38961
H	-2.51285	2.22295	1.33055
H	2.91296	2.85059	-0.19624
H	3.27899	1.39334	0.72290
H	2.35489	2.87721	2.29810
H	0.99776	3.32703	1.28240
Br	-0.34576	-1.05819	-2.23607

^{6}FeTMCSCl
Charge: 1+
Energy: -1840445.8518486

Fe	0.00217	0.07036	0.08110
N	-1.14766	1.99044	0.12484
N	1.72385	1.43068	0.47825
N	1.36844	-1.75671	-0.18353
N	-1.61896	-1.34157	-0.45992
C	-0.13020	2.97322	-0.35253
C	1.18667	2.83734	0.41481
C	2.74984	1.21530	-0.60076
C	3.33224	-0.20408	-0.74116
C	2.43152	-1.37892	-1.17245
C	0.44251	-2.81904	-0.71791
C	-0.88640	-2.33057	-1.31372
C	-2.67968	-0.64218	-1.26666
C	-3.20092	0.67697	-0.66670
C	-2.31109	1.92286	-0.81725
C	-1.63193	2.38177	1.47219
C	2.33870	1.23507	1.81686
C	2.04179	-2.32891	1.01405
C	-2.27274	-1.97303	0.72827
S	-0.47945	-0.54018	2.30382
C	-1.38702	-2.09879	1.96473
H	-0.50453	3.99974	-0.22844
H	0.03211	2.79322	-1.41274
H	1.05261	3.18017	1.44224
H	1.93415	3.49790	-0.04049
H	3.58980	1.89557	-0.39478
H	2.28932	1.51741	-1.53906
H	4.08924	-0.11754	-1.53066
H	3.89938	-0.46612	0.15746
H	1.94048	-1.14416	-2.11341
H	3.07761	-2.25562	-1.33128
H	0.96115	-3.40445	-1.48790
H	0.23597	-3.50658	0.10309
H	-1.52050	-3.21070	-1.49248
H	-0.70013	-1.84765	-2.26934
H	-3.52240	-1.33738	-1.38696
H	-2.26646	-0.44547	-2.25443
H	-3.50180	0.54425	0.37803
H	-4.12883	0.90216	-1.20613
H	-1.91886	1.96456	-1.83245
H	-2.92802	2.81857	-0.65701
H	-2.06617	3.39058	1.44130
H	-0.81499	2.36314	2.19291
H	-2.38086	1.67188	1.81789
H	3.17761	1.92929	1.96100
H	2.69600	0.21507	1.92413
H	1.59213	1.40598	2.59328
H	2.56729	-3.25564	0.74530
H	1.31935	-2.53370	1.79939
H	2.76948	-1.62966	1.41585
H	-2.67472	-2.95542	0.44199
H	-3.12171	-1.34490	0.99814
H	-2.01724	-2.32092	2.83115
H	-0.67213	-2.92013	1.87849
Cl	0.15948	0.49164	-2.36482

^{6}FeTMCSF
Charge: 1+
Energy: -1614334.1082271

Fe	0.00832	0.08934	0.05061
N	-1.01120	2.08216	-0.07279
N	1.83822	1.34909	0.31944
N	1.28062	-1.81290	-0.21552
N	-1.66837	-1.25734	-0.52462
C	0.09800	2.92666	-0.59550
C	1.35781	2.76753	0.24845
C	2.72131	1.06085	-0.85850
C	3.24843	-0.37527	-0.99471
C	2.24330	-1.49331	-1.31379
C	0.28789	-2.84342	-0.66087
C	-0.94804	-2.27190	-1.34783
C	-2.63456	-0.52179	-1.40088
C	-3.09769	0.84486	-0.87448
C	-2.10690	2.00032	-1.08326
C	-1.53291	2.61948	1.20463
C	2.56074	1.17020	1.60134
C	1.99850	-2.37210	0.95540
C	-2.38218	-1.82926	0.65469
S	-0.57822	-0.39378	2.25895
C	-1.54715	-1.92535	1.93568
H	-0.19666	3.98596	-0.61313

H	0.29001	2.60316	-1.61783
H	1.16937	3.10159	1.27041
H	2.15278	3.40998	-0.15291
H	3.58666	1.73818	-0.80219
H	2.14304	1.30657	-1.74837
H	3.93880	-0.34741	-1.84694
H	3.87516	-0.64119	-0.13812
H	1.65247	-1.20071	-2.18057
H	2.80674	-2.40629	-1.56027
H	0.77296	-3.55267	-1.34614
H	-0.00896	-3.41641	0.21759
H	-1.62328	-3.09978	-1.60843
H	-0.64936	-1.76764	-2.26496
H	-3.50821	-1.16836	-1.56596
H	-2.14202	-0.37273	-2.36173
H	-3.41273	0.78277	0.17235
H	-4.00268	1.10140	-1.43761
H	-1.63365	1.88567	-2.05873
H	-2.65158	2.95553	-1.07688
H	-1.88962	3.65069	1.07184
H	-0.75916	2.59747	1.97163
H	-2.34753	1.99212	1.56218
H	3.40438	1.87050	1.67423
H	2.93632	0.15478	1.68879
H	1.87177	1.34022	2.43046
H	2.43169	-3.35220	0.71044
H	1.31211	-2.46876	1.79558
H	2.80472	-1.71307	1.26571
H	-2.79494	-2.81484	0.39343
H	-3.22735	-1.17222	0.86403
H	-2.22450	-2.08171	2.78043
H	-0.86550	-2.77894	1.92004
F	0.12776	0.30932	-1.80391

^{6}FeTMCSN$_{3}$
Charge: 1+
Energy: -1654707.8022770

Fe	-0.05297	0.04265	-0.20298
N	1.19275	1.89160	-0.52387
N	-1.74412	1.47782	-0.52553
N	-1.48654	-1.66786	0.37170
N	1.53798	-1.44313	0.30360
C	0.27157	2.94811	-0.01813
C	-1.11481	2.83712	-0.65530
C	-2.60660	1.42367	0.70154
C	-3.25029	0.06767	1.04706
C	-2.36768	-1.12876	1.45446
C	-0.56825	-2.74334	0.88091
C	0.83241	-2.28898	1.31264
C	2.70958	-0.74509	0.92988
C	3.22431	0.49360	0.17286
C	2.42683	1.80278	0.31596
C	1.57176	2.17306	-1.92955
C	-2.55130	1.22563	-1.74542
C	-2.33934	-2.27879	-0.68058
C	2.01685	-2.22254	-0.87933
S	0.19035	-0.75676	-2.39365
C	1.00350	-2.35932	-2.01448
H	0.67766	3.94816	-0.22936
H	0.19583	2.83580	1.06199
H	-1.04712	3.06399	-1.72063
H	-1.77381	3.59618	-0.21500
H	-3.42153	2.15150	0.56983
H	-1.98724	1.75378	1.53453
H	-3.88454	0.27055	1.91916
H	-3.95094	-0.22604	0.25966
H	-1.72690	-0.84554	2.28737
H	-3.03315	-1.93681	1.79515
H	-1.03558	-3.25795	1.73135
H	-0.47134	-3.48640	0.08897
H	1.42521	-3.18888	1.53253
H	0.76443	-1.71460	2.23380
H	3.53090	-1.47053	1.01659
H	2.44085	-0.46057	1.94701
H	3.38445	0.26178	-0.88509
H	4.22139	0.69907	0.58010
H	2.14454	1.94567	1.35960
H	3.08353	2.64281	0.04741
H	2.05506	3.15728	-2.00610
H	0.69334	2.14884	-2.57351
H	2.24938	1.40215	-2.29142
H	-3.34028	1.98274	-1.85323
H	-3.00702	0.24045	-1.70210
H	-1.90314	1.24820	-2.62239
H	-2.86429	-3.15968	-0.28513
H	-1.73351	-2.56298	-1.53775
H	-3.08302	-1.56858	-1.03120
H	2.36297	-3.21269	-0.54858
H	2.88431	-1.69603	-1.27840
H	1.52821	-2.69754	-2.91305
H	0.24201	-3.11158	-1.79606
N	0.00379	0.54972	1.71727
N	0.50938	0.72816	2.79559
N	1.00959	0.89482	3.82482

^{6}FeTMCSNCS
Charge: 1+
Energy: -1859818.5389532

Fe	0.33351	-0.01125	0.23887
N	-0.87416	-1.00034	1.86165
N	0.01895	1.80376	1.50930
N	1.27414	1.22028	-1.46801
N	0.52259	-1.70169	-1.19805
C	-1.71608	0.13568	2.33366
C	-0.87120	1.37278	2.64197
C	-0.68485	2.82256	0.65970
C	0.04260	3.30079	-0.61082
C	0.30676	2.32163	-1.77158
C	1.37495	0.23711	-2.60035
C	0.45333	-0.98431	-2.50773
C	-0.64695	-2.63352	-1.06031
C	-0.97088	-3.08382	0.37564
C	-1.72073	-2.08454	1.27346
C	-0.07813	-1.54991	2.98577
C	1.26144	2.37302	2.08842
C	2.62479	1.80896	-1.27548
C	1.78745	-2.47840	-1.02050
S	2.42213	-0.69594	1.03877
C	2.94989	-1.69461	-0.40976
H	-2.27003	-0.14721	3.24068
H	-2.44240	0.36024	1.55510
H	-0.22988	1.17568	3.50269
H	-1.53491	2.19846	2.92812
H	-0.86730	3.70840	1.28661
H	-1.65074	2.39858	0.39076
H	-0.60721	4.07878	-1.03078
H	0.96286	3.82679	-0.33901
H	-0.62693	1.86316	-2.08962
H	0.70172	2.90461	-2.61771
H	1.17233	0.74616	-3.55228
H	2.41157	-0.09803	-2.64585
H	0.71268	-1.66986	-3.32743
H	-0.57910	-0.67427	-2.65010
H	-0.44694	-3.52177	-1.67604
H	-1.52026	-2.13850	-1.48392
H	-0.07396	-3.45564	0.88200
H	-1.62892	-3.95509	0.27461
H	-2.52123	-1.61573	0.70137
H	-2.19091	-2.63603	2.10022
H	-0.74054	-1.89126	3.79359
H	0.60684	-0.79614	3.37286
H	0.53063	-2.38124	2.63492
H	1.03405	3.24501	2.71701
H	1.94521	2.67178	1.29883
H	1.76467	1.61426	2.68931
H	2.98409	2.25776	-2.21216
H	3.32452	1.04607	-0.94156
H	2.60067	2.58375	-0.51403
H	2.08653	-2.91666	-1.98360
H	1.56256	-3.30638	-0.34760
H	3.71346	-2.40304	-0.07499
H	3.43148	-1.03817	-1.13832
N	-1.46809	0.27659	-0.64196
C	-2.56623	0.28373	-1.11756
S	-4.03944	0.26999	-1.74515

^{6}FeTMCSOH
Charge: 1+
Energy: -1599235.5284897

Fe	-0.00445	0.10415	-0.02356
O	0.07177	0.41641	-1.89731
N	-1.12007	2.03912	-0.05331
N	1.76333	1.44543	0.31363
N	1.36733	-1.76792	-0.22146
N	-1.62537	-1.34565	-0.50181
C	-0.07015	2.95199	-0.58641
C	1.22356	2.84413	0.21999
C	2.69482	1.18229	-0.83043
C	3.28892	-0.23384	-0.94033
C	2.37269	-1.42812	-1.26882
C	0.42008	-2.83844	-0.67756
C	-0.87918	-2.34228	-1.32031
C	-2.64533	-0.65023	-1.35182
C	-3.16110	0.69266	-0.80370
C	-2.25126	1.91424	-1.02117
C	-1.62218	2.52119	1.25363
C	2.45643	1.30271	1.61590
C	2.07484	-2.28585	0.97705
C	-2.28646	-1.93644	0.69837
S	-0.48854	-0.42668	2.22506
C	-1.41061	-1.99231	1.95195
H	-0.41774	3.99539	-0.56412
H	0.10859	2.66145	-1.62007
H	1.05627	3.19608	1.23944
H	1.98030	3.50650	-0.22056

H	3.53729	1.88616	-0.74848
H	2.13733	1.41254	-1.73761
H	4.00727	-0.17932	-1.76809
H	3.89910	-0.45776	-0.06045
H	1.83477	-1.23514	-2.19629
H	3.01197	-2.30757	-1.44488
H	0.92480	-3.50512	-1.39099
H	0.17730	-3.44848	0.19245
H	-1.51231	-3.21736	-1.52957
H	-0.65745	-1.86303	-2.27206
H	-3.49465	-1.33336	-1.49703
H	-2.18479	-0.47064	-2.32284
H	-3.44903	0.60564	0.24903
H	-4.09226	0.90203	-1.34362
H	-1.81519	1.85800	-2.01807
H	-2.85785	2.82951	-0.95988
H	-2.03620	3.53475	1.15460
H	-0.82118	2.52516	1.99213
H	-2.38891	1.84495	1.62698
H	3.28634	2.01862	1.69818
H	2.84328	0.29425	1.73222
H	1.74543	1.47430	2.42526
H	2.56187	-3.24533	0.75126
H	1.37304	-2.40780	1.79897
H	2.83797	-1.58513	1.30487
H	-2.67209	-2.93682	0.45122
H	-3.14774	-1.30844	0.92815
H	-2.05530	-2.16616	2.81890
H	-0.70532	-2.82695	1.91918
H	0.41640	-0.07032	-2.65550

^{4}FeBnTPENBr
Charge: 0
Energy: -3237127.6008415

Fe	-0.84504	0.12276	0.39833
N	-0.98759	-2.13039	-0.05740
N	-0.25522	2.26093	0.62918
N	-2.80661	0.29145	-0.14966
N	-0.76223	1.01638	-1.80297
N	1.26129	-0.58996	-0.42617
C	0.54454	0.74268	-2.41243
H	1.20041	1.58450	-2.16945
H	0.48143	0.70169	-3.51337
C	1.17063	-0.55658	-1.89743
H	0.54675	-1.40176	-2.19944
H	2.15417	-0.69937	-2.37128
C	-1.02878	2.45222	-1.66382
H	-2.10070	2.57241	-1.47898
H	-0.79232	3.01142	-2.58426
C	-0.28854	3.03735	-0.47792
C	0.27518	4.30860	-0.51341
H	0.23992	4.88866	-1.43147
C	0.87431	4.82345	0.64280
H	1.32137	5.81338	0.63927
C	0.88105	4.03573	1.79269
H	1.32754	4.38877	2.71712
C	0.31105	2.76413	1.74339
H	0.30537	2.09381	2.59794
C	-1.88705	0.27246	-2.39696
H	-1.56192	-0.77182	-2.47882
H	-2.13556	0.62814	-3.41194
C	-3.09630	0.34815	-1.49209
C	-4.39063	0.45907	-1.96927
H	-4.55791	0.51747	-3.04226
C	-5.47086	0.49017	-1.07086
H	-6.49261	0.57006	-1.42666
C	-5.17700	0.41905	0.30395
H	-5.96928	0.43721	1.04686
C	-3.86133	0.32495	0.71955
H	-3.58772	0.25921	1.76876
C	1.42408	-1.96694	0.07279
H	1.57155	-1.89208	1.15664
H	2.30108	-2.46723	-0.36438
C	0.17848	-2.79333	-0.14561
C	0.23589	-4.17114	-0.36006
H	1.19952	-4.66646	-0.43839
C	-0.95485	-4.89046	-0.46079
H	-0.93783	-5.96476	-0.62172
C	-2.16460	-4.20359	-0.35138
H	-3.11697	-4.72003	-0.41924
C	-2.13101	-2.82470	-0.15530
H	-3.04054	-2.23957	-0.06737
C	2.28706	0.32307	0.15037
H	2.12144	0.30186	1.23213
H	2.04526	1.33445	-0.18106
C	3.72377	-0.01081	-0.19432
C	4.33441	0.53785	-1.33105
H	3.78044	1.24599	-1.94424
C	5.64505	0.20185	-1.67545
H	6.10242	0.63933	-2.55908
C	6.36883	-0.68827	-0.87927
H	7.39031	-0.94945	-1.14244
C	5.77761	-1.23169	0.26409
H	6.33996	-1.91373	0.89634
C	4.46678	-0.89319	0.60287
H	4.01407	-1.30833	1.49998
Br	-0.33180	-0.54242	2.90037

^{4}FeBnTPENCl
Charge: 0
Energy: -1910597.1901992

Fe	0.86176	-0.09496	0.62379
N	0.99222	2.17613	0.28850
N	0.30136	-2.25741	0.72489
N	2.82610	-0.22624	0.08908
N	0.81644	-0.88130	-1.63380
N	-1.23808	0.63364	-0.21091
C	-0.48207	-0.58767	-2.25048
H	-1.13458	-1.44602	-2.06257
H	-0.40097	-0.48936	-3.34673
C	-1.12790	0.67836	-1.67962
H	-0.50776	1.54336	-1.92890
H	-2.10596	0.83674	-2.16009
C	1.09751	-2.31948	-1.56747
H	2.17010	-2.43754	-1.38472
H	0.87145	-2.83272	-2.51687
C	0.35907	-2.97607	-0.41770
C	-0.18005	-4.25515	-0.51874
H	-0.12717	-4.79043	-1.46278
C	-0.77838	-4.83437	0.60663
H	-1.20595	-5.83148	0.55224
C	-0.81223	-4.10271	1.79250
H	-1.26162	-4.50797	2.69382
C	-0.26673	-2.81920	1.80841
H	-0.28514	-2.18398	2.68918
C	1.94269	-0.09420	-2.16773
H	1.60758	0.95009	-2.19154
H	2.20725	-0.38720	-3.19858
C	3.13846	-0.21441	-1.25212
C	4.43905	-0.29870	-1.71476
H	4.62067	-0.30246	-2.78714
C	5.50871	-0.37128	-0.80447
H	6.53556	-0.43041	-1.14904
C	5.19305	-0.36916	0.56892
H	5.97447	-0.42244	1.32180
C	3.87256	-0.30009	0.96987
H	3.58672	-0.29074	2.01786
C	-1.41944	1.97926	0.36175
H	-1.57501	1.84112	1.43763
H	-2.29719	2.49472	-0.05601
C	-0.18012	2.82852	0.19945
C	-0.24886	4.21164	0.02701
H	-1.21632	4.69890	-0.05475
C	0.93564	4.94672	-0.02934
H	0.90935	6.02522	-0.15775
C	2.15101	4.26972	0.08004
H	3.09855	4.79818	0.04443
C	2.12956	2.88486	0.23226
H	3.04359	2.30555	0.31441
C	-2.25945	-0.31983	0.30385
H	-2.10439	-0.35459	1.38645
H	-2.00289	-1.30939	-0.07877
C	-3.69567	0.01691	-0.04053
C	-4.28704	-0.47605	-1.21248
H	-3.71825	-1.14445	-1.85596
C	-5.59712	-0.13557	-1.55467
H	-6.03914	-0.52971	-2.46610
C	-6.34002	0.70316	-0.72119
H	-7.36108	0.96764	-0.98272
C	-5.76820	1.19059	0.45674
H	-6.34532	1.83215	1.11746
C	-4.45789	0.84770	0.79314
H	-4.02019	1.21882	1.71659
Cl	0.21144	0.35486	2.93592

^{4}FeBnTPENF
Charge: 0
Energy: -1684465.6027956

Fe	0.80288	0.05609	-0.82818
N	1.01475	-2.14043	-0.63862
N	0.32702	2.29693	-0.68004
N	2.80479	0.21092	-0.25956
N	0.84118	0.75633	1.55387
N	-1.24454	-0.64907	0.08797
C	-0.45070	0.44478	2.17492
H	-1.09394	1.32070	2.04361
H	-0.35310	0.28707	3.26323
C	-1.12706	-0.77898	1.54751
H	-0.52668	-1.67157	1.74372
H	-2.10378	-0.94151	2.02963
C	1.15815	2.18856	1.59456
H	2.23794	2.29184	1.43985
H	0.93172	2.63763	2.57597
C	0.44738	2.94600	0.49025
C	-0.02955	4.24772	0.65905

H	0.06571	4.74059	1.62263
C	-0.62686	4.89414	-0.42476
H	-1.00360	5.90787	-0.31835
C	-0.74153	4.21605	-1.63871
H	-1.20505	4.68010	-2.50357
C	-0.25836	2.90968	-1.71872
H	-0.34469	2.28462	-2.60267
C	1.95956	-0.09598	1.99125
H	1.60835	-1.13257	1.91397
H	2.24603	0.08985	3.04093
C	3.13918	0.09243	1.06994
C	4.44850	0.11498	1.51548
H	4.64519	0.03329	2.58208
C	5.50686	0.22842	0.59508
H	6.54005	0.24033	0.92480
C	5.16794	0.32718	-0.77214
H	5.93784	0.41587	-1.53366
C	3.84012	0.32110	-1.14962
H	3.54384	0.39993	-2.19238
C	-1.39296	-1.95579	-0.58806
H	-1.49404	-1.72328	-1.65410
H	-2.28837	-2.50045	-0.25483
C	-0.15459	-2.79653	-0.40269
C	-0.20044	-4.13655	-0.04017
H	-1.16170	-4.60556	0.15284
C	0.99155	-4.86668	0.06044
H	0.98038	-5.91625	0.33764
C	2.19570	-4.19859	-0.20554
H	3.15000	-4.71382	-0.14794
C	2.16208	-2.85298	-0.54309
H	3.07202	-2.29550	-0.73822
C	-2.26020	0.33221	-0.37547
H	-2.07927	0.43345	-1.44878
H	-2.01037	1.29581	0.07432
C	-3.69813	-0.02938	-0.06866
C	-4.30513	0.38797	1.12446
H	-3.74682	1.01867	1.81361
C	-5.61651	0.01976	1.43137
H	-6.07041	0.35507	2.36039
C	-6.34520	-0.77186	0.54119
H	-7.36695	-1.05831	0.77563
C	-5.75753	-1.18475	-0.65729
H	-6.32286	-1.79061	-1.36062
C	-4.44622	-0.81384	-0.95812
H	-3.99441	-1.12869	-1.89559
F	-0.05629	0.12555	-2.49684

^{4}FeBnTPENN$_3$
Charge: 0
Energy: -1724856.3355474

Fe	0.88824	-0.09680	0.57289
N	0.95291	2.14046	0.07353
N	0.36224	-2.22757	0.88942
N	2.85860	-0.24278	0.06371
N	0.87545	-1.11247	-1.59597
N	-1.22882	0.51385	-0.36734
C	-0.41980	-0.90803	-2.25396
H	-1.06196	-1.75189	-1.98272
H	-0.32671	-0.92627	-3.35352
C	-1.09139	0.40071	-1.82998
H	-0.47743	1.24439	-2.15725
H	-2.06272	0.49429	-2.34098
C	1.17811	-2.53136	-1.37361
H	2.25093	-2.61164	-1.17266
H	0.96672	-3.14738	-2.26319
C	0.44087	-3.07031	-0.16289
C	-0.07837	-4.36062	-0.11904
H	-0.00932	-5.00117	-0.99394
C	-0.67938	-4.81414	1.06176
H	-1.09150	-5.81740	1.12038
C	-0.73781	-3.95001	2.15475
H	-1.19238	-4.25571	3.09205
C	-0.21061	-2.66568	2.02607
H	-0.24843	-1.92753	2.82224
C	1.99408	-0.36598	-2.20067
H	1.64175	0.66423	-2.33554
H	2.27233	-0.75984	-3.19353
C	3.18324	-0.36806	-1.26976
C	4.48809	-0.47924	-1.71233
H	4.67775	-0.59407	-2.77714
C	5.55303	-0.43617	-0.79339
H	6.58325	-0.51338	-1.12371
C	5.22591	-0.29523	0.57012
H	6.00186	-0.25639	1.32959
C	3.90159	-0.20688	0.95317
H	3.60976	-0.09512	1.99368
C	-1.46320	1.91188	0.03290
H	-1.73297	1.92122	1.09347
H	-2.30372	2.36166	-0.51720
C	-0.22247	2.76333	-0.11989
C	-0.30308	4.13026	-0.38995
H	-1.27286	4.59297	-0.54836
C	0.86980	4.88203	-0.43574
H	0.83298	5.94913	-0.63576
C	2.08894	4.23692	-0.22033
H	3.02862	4.77974	-0.24426
C	2.08141	2.86675	0.02538
H	2.99892	2.31110	0.19049
C	-2.23434	-0.40300	0.23453
H	-2.08309	-0.33117	1.31586
H	-1.95784	-1.42080	-0.04675
C	-3.67549	-0.12895	-0.14293
C	-4.24750	-0.73532	-1.27045
H	-3.66049	-1.44562	-1.84942
C	-5.56161	-0.45368	-1.64850
H	-5.98873	-0.93534	-2.52425
C	-6.32751	0.43905	-0.89580
H	-7.35177	0.65813	-1.18519
C	-5.77460	1.03989	0.23793
H	-6.36908	1.72514	0.83631
C	-4.46007	0.75574	0.61064
H	-4.03798	1.21762	1.49998
N	0.27078	0.34598	2.51680
N	-0.11724	1.41462	2.91830
N	-0.52207	2.43425	3.30841

^{4}FeBnTPENNCS
Charge: 0
Energy: -1929969.5735642

Fe	0.98323	-0.05990	0.50086
N	0.98874	2.17144	-0.05713
N	0.48291	-2.18545	0.83312
N	3.00022	-0.12424	0.17196
N	1.18997	-1.09838	-1.62435
N	-1.08105	0.43952	-0.59434
C	-0.04947	-0.94543	-2.39802
H	-0.68024	-1.81332	-2.18301
H	0.14495	-0.96066	-3.48373
C	-0.80451	0.33674	-2.03927
H	-0.19294	1.20162	-2.31024
H	-1.72735	0.39766	-2.63659
C	1.50874	-2.50345	-1.34062
H	2.55636	-2.54695	-1.02700
H	1.40799	-3.14252	-2.23309
C	0.66139	-3.03676	-0.20212
C	0.13499	-4.32413	-0.20272
H	0.28803	-4.96971	-1.06305
C	-0.58497	-4.76866	0.91352
H	-1.00782	-5.76879	0.93458
C	-0.74689	-3.89893	1.99077
H	-1.29609	-4.19404	2.87920
C	-0.20015	-2.61910	1.90902
H	-0.31437	-1.89064	2.70458
C	2.33459	-0.33567	-2.15334
H	1.96568	0.67768	-2.35424
H	2.71173	-0.75070	-3.10392
C	3.43873	-0.26821	-1.12356
C	4.78087	-0.34012	-1.45150
H	5.06604	-0.47210	-2.49253
C	5.75845	-0.23830	-0.44634
H	6.81536	-0.28493	-0.68597
C	5.31345	-0.07974	0.87919
H	6.01974	0.00388	1.70025
C	3.95737	-0.03007	1.14490
H	3.57359	0.09561	2.15334
C	-1.41328	1.82644	-0.22304
H	-1.77385	1.81762	0.81083
H	-2.22765	2.23172	-0.84231
C	-0.20778	2.73750	-0.29085
C	-0.34425	4.10614	-0.53388
H	-1.32788	4.52424	-0.72749
C	0.79076	4.91515	-0.51352
H	0.70871	5.98352	-0.69260
C	2.03130	4.32619	-0.26273
H	2.94307	4.91463	-0.23742
C	2.08048	2.95162	-0.04516
H	3.01659	2.43826	0.15090
C	-2.11328	-0.51726	-0.09768
H	-2.07281	-0.46631	0.99270
H	-1.78759	-1.52073	-0.37814
C	-3.52563	-0.26449	-0.58182
C	-3.98550	-0.80940	-1.78913
H	-3.33306	-1.46382	-2.36424
C	-5.27542	-0.54030	-2.25084
H	-5.61744	-0.97261	-3.18770
C	-6.12703	0.27508	-1.50218
H	-7.13295	0.48359	-1.85693
C	-5.68573	0.80872	-0.28848
H	-6.35003	1.42916	0.30728
C	-4.39522	0.53938	0.16995
H	-4.05736	0.93775	1.12442
N	0.25478	0.53394	2.38294
C	-0.75908	0.80986	2.93599
S	-2.19806	1.17524	3.62844

^{5}FeLBrCO2CH2CH3
Charge: 0
Energy: -3387550.3337306

Fe	0.01366	-0.21322	-0.05632
P	2.25316	1.57632	-1.33064
C	3.24655	0.05505	-1.24025
C	3.34449	-0.55789	0.16750
O	2.06324	-0.48120	0.82443
C	3.83298	-2.00245	0.11452
O	2.76549	2.64208	-0.33730
O	0.75312	1.16534	-1.11422
O	2.45744	2.29779	-2.69042
H	4.25180	0.29914	-1.59928
H	4.80888	-2.05931	-0.38044
H	3.93555	-2.41636	1.12417
H	3.11559	-2.61446	-0.44140
H	4.03793	0.05330	0.76005
C	-4.46875	2.05358	-2.92923
H	-4.70952	1.59057	-3.89475
H	-3.94479	2.99111	-3.13343
N	-3.99595	-0.09774	-1.67675
H	-4.86733	-0.55204	-1.90907
C	-3.60628	1.17067	-2.09001
C	-2.98470	-0.64225	-0.94970
H	-2.99012	-1.63532	-0.52756
N	-1.98172	0.20678	-0.86743
C	-2.34752	1.33493	-1.57000
H	-1.66137	2.16231	-1.67058
C	0.05885	4.20221	3.47148
H	0.87498	4.71367	2.95480
H	0.36910	4.04211	4.51199
N	-1.23144	2.03688	3.19606
H	-1.83409	2.16301	3.99648
C	-0.23922	2.91606	2.77644
C	-1.24636	0.96973	2.36301
H	-1.90232	0.11861	2.44470
N	-0.31744	1.12293	1.43643
C	0.31813	2.32599	1.67300
H	1.11695	2.67806	1.03764
C	-2.49584	-2.97340	2.82947
H	-3.00571	-2.39662	2.05153
H	-2.32387	-2.30963	3.68596
C	-1.17397	-3.54321	2.30238
H	-0.65964	-4.13579	3.06385
H	-1.36952	-4.20432	1.44695
C	-0.20197	-2.47763	1.80766
O	1.00094	-2.54803	2.08110
O	-0.77046	-1.54373	1.09387
H	2.79565	-0.66134	-1.93395
H	1.88646	-1.29107	1.37694
H	-5.41545	2.30015	-2.43094
H	-0.80839	4.87493	3.47860
H	-3.16363	-3.77635	3.15951
Br	0.33199	-2.00468	-1.75953

^{5}FeLClCO2CH2CH3
Charge: 0
Energy: -2061015.1151923

Fe	-0.14266	0.07730	-0.36329
P	-2.51699	-1.83105	0.40442
C	-3.48864	-0.61561	-0.53673
C	-3.36525	0.83236	-0.03365
O	-1.99095	1.14403	0.29689
C	-3.89316	1.82279	-1.06728
O	-2.84743	-1.76578	1.91300
O	-1.00533	-1.57361	0.09486
O	-2.93875	-3.28357	0.04787
H	-4.53874	-0.92247	-0.48591
H	-4.93632	1.59643	-1.31395
H	-3.84390	2.84935	-0.68736
H	-3.29044	1.76009	-1.97909
H	-3.93092	0.92195	0.90227
C	3.75969	-4.10937	-1.27712
H	3.94466	-4.39196	-2.32140
H	3.12995	-4.88370	-0.83106
N	3.62743	-1.60868	-1.66395
H	4.51356	-1.52649	-2.14119
C	3.07600	-2.78682	-1.17251
C	2.75658	-0.59381	-1.42526
H	2.90321	0.43437	-1.71792
N	1.69007	-1.05601	-0.80639
C	1.86763	-2.41279	-0.64273
H	1.09783	-3.00966	-0.17760
C	2.53093	1.39409	4.42489
H	3.22286	2.08625	3.93754
H	3.12786	0.62393	4.92996
N	0.61097	-0.10835	3.73098
H	0.39914	-0.45665	4.65531
C	1.60811	0.80643	3.41012
C	-0.05411	-0.45388	2.60517
H	-0.88926	-1.13897	2.56432
N	0.46615	0.19762	1.57646
C	1.49635	0.98218	2.05758
H	2.06322	1.61148	1.39141
C	2.69308	3.84544	-0.92757
H	3.14488	2.84930	-0.88878
H	2.58003	4.20355	0.10267
C	1.33853	3.80186	-1.64560
H	0.88571	4.79533	-1.70298
H	1.47267	3.43706	-2.67300
C	0.33052	2.87053	-0.98436
O	-0.83044	3.24264	-0.77498
O	0.82333	1.70370	-0.66931
H	-3.15553	-0.68212	-1.57679
H	-1.73388	2.04403	-0.05824
H	4.72377	-4.11759	-0.75205
H	1.98621	1.95413	5.19559
H	3.38565	4.51957	-1.44294
Cl	-0.77538	0.05217	-2.55209

^{5}FeLFCO2CH2CH3
Charge: 0
Energy: -1834903.0129680

Fe	-0.08348	0.06645	-0.68207
P	-2.68005	-1.61233	-0.18507
C	-3.26112	-0.31483	-1.33536
C	-3.02857	1.12690	-0.85279
O	-1.77136	1.19223	-0.13025
C	-3.01140	2.11709	-2.01305
O	-3.27842	-1.43150	1.22819
O	-1.12030	-1.54446	-0.24258
O	-3.23985	-2.99608	-0.60083
H	-4.32820	-0.46815	-1.52283
H	-3.95605	2.07361	-2.56669
H	-2.86445	3.14132	-1.65364
H	-2.18772	1.85698	-2.68492
H	-3.80619	1.38749	-0.12487
C	3.73876	-4.18334	-0.96260
H	4.10287	-4.47260	-1.95665
H	3.02138	-4.94146	-0.63792
N	3.74043	-1.67930	-1.35280
H	4.70349	-1.61830	-1.65082
C	3.07815	-2.84531	-0.98141
C	2.86954	-0.64236	-1.27535
H	3.09110	0.38771	-1.50852
N	1.69402	-1.08268	-0.87196
C	1.80129	-2.44453	-0.68520
H	0.94423	-3.01600	-0.36244
C	-0.25690	-0.43482	5.14011
H	-1.16306	-1.04578	5.11740
H	-0.47353	0.46200	5.73497
N	1.25875	0.68431	3.44364
H	1.88806	1.10065	4.11454
C	0.14633	-0.09384	3.74445
C	1.33684	0.81416	2.09436
H	2.09301	1.38047	1.57426
N	0.34596	0.16163	1.51748
C	-0.40229	-0.40962	2.52869
H	-1.28425	-0.99252	2.31018
C	3.12151	3.69217	-0.04244
H	3.49456	2.69071	-0.28098
H	2.93071	3.73595	1.03720
C	1.84447	3.99544	-0.83667
H	1.46076	4.99228	-0.60381
H	2.06504	3.96311	-1.91190
C	0.73505	2.98238	-0.57052
O	-0.39804	3.38401	-0.23966
O	1.07947	1.74500	-0.71205
H	-2.71254	-0.47616	-2.26930
H	-1.40029	2.13612	-0.10056
H	4.59115	-4.21064	-0.27170
H	0.51981	-1.00567	5.66578
H	3.91023	4.41730	-0.27002
F	-0.44279	0.16007	-2.43968

^{5}FeLN$_3$CO2CH2CH3
Charge: 0
Energy: -1875287.5311170

Fe	-0.12346	0.06089	-0.24250
P	-2.67827	-1.77439	-0.29646
C	-3.28207	-0.44443	-1.38887
C	-3.27768	0.95605	-0.75016
O	-2.09590	1.12291	0.06178
C	-3.35881	2.05292	-1.80802
O	-3.40360	-1.74868	1.06794
O	-1.12854	-1.61131	-0.19652
O	-3.08403	-3.16962	-0.85006
H	-4.30239	-0.69741	-1.69490
H	-4.25919	1.92921	-2.42009
H	-3.39083	3.04465	-1.34332
H	-2.47846	2.00321	-2.45670
H	-4.13521	1.02500	-0.06817
C	3.80122	-4.13834	-0.95951
H	4.23321	-4.25032	-1.96219
H	3.06166	-4.93227	-0.82607

N	3.83101	-1.60562	-0.90365
H	4.80717	-1.50314	-1.14121
C	3.14624	-2.80896	-0.78248
C	2.95567	-0.58754	-0.69894
H	3.20083	0.46139	-0.75606
N	1.75583	-1.07363	-0.44631
C	1.85429	-2.44907	-0.49622
H	0.97989	-3.06222	-0.33795
C	1.36488	0.76630	5.13861
H	2.25465	1.35439	4.89809
H	1.68726	-0.10385	5.72471
N	-0.49708	-0.39065	3.86628
H	-0.98891	-0.73873	4.67707
C	0.67135	0.36335	3.88031
C	-0.88413	-0.58811	2.58518
H	-1.75980	-1.14451	2.27872
N	-0.02024	0.00356	1.77550
C	0.94937	0.59643	2.56064
H	1.75248	1.15576	2.10899
C	2.98745	3.42873	-0.84434
H	2.92110	2.82637	-1.75631
H	3.38119	2.79151	-0.04475
C	1.61587	3.98888	-0.46794
H	1.67038	4.57285	0.46080
H	1.24646	4.68152	-1.23245
C	0.51745	2.94633	-0.26478
O	-0.66097	3.32190	-0.17539
O	0.93093	1.71697	-0.17948
H	-2.64133	-0.45377	-2.27626
H	-1.74768	2.05877	0.00948
H	4.60393	-4.30172	-0.22879
H	0.72119	1.38183	5.77979
H	3.70368	4.23986	-1.01651
N	-0.28704	0.26085	-2.15274
N	0.72040	0.60558	-2.74345
N	1.64471	0.93444	-3.34863

[5]FeLNCSCO2CH2CH3
Charge: 0
Energy: -2080387.5718441

Fe	0.14082	-0.11641	0.02494
P	2.61025	-0.32976	-1.90352
C	2.59381	-2.04471	-1.29174
C	2.73390	-2.17803	0.23403
O	1.91962	-1.18977	0.90868
C	2.35839	-3.58072	0.70278
O	3.83052	0.44807	-1.36023
O	1.24182	0.31416	-1.50603
O	2.85036	-0.28177	-3.43719
H	3.41841	-2.57982	-1.77423
H	2.98295	-4.32930	0.20313
H	2.49573	-3.68332	1.78475
H	1.30825	-3.78259	0.46799
H	3.77289	-1.95333	0.50547
C	-3.24106	2.71912	-3.73673
H	-3.92824	2.08894	-4.31550
H	-2.40442	2.98337	-4.38888
N	-3.56073	1.53513	-1.52004
H	-4.56956	1.58176	-1.51607
C	-2.72889	2.01260	-2.52602
C	-2.79521	0.93276	-0.57504
H	-3.17386	0.43811	0.30520
N	-1.52280	1.00973	-0.91535
C	-1.46289	1.67226	-2.12395
H	-0.51416	1.82378	-2.61596
C	0.87956	4.36863	3.31627
H	-0.04289	4.20683	3.88026
H	0.82842	5.37014	2.87051
N	2.11264	3.24351	1.40868
H	2.89563	3.88170	1.38863
C	1.02919	3.30618	2.27934
C	1.96617	2.17873	0.59007
H	2.66674	1.88347	-0.17824
N	0.83927	1.55121	0.89499
C	0.24767	2.23601	1.93954
H	-0.68323	1.89289	2.36009
C	-3.38028	-0.97685	2.82429
H	-3.61827	-1.42928	1.85556
H	-3.31482	0.10839	2.69182
C	-2.06838	-1.53938	3.37114
H	-1.82612	-1.08953	4.34403
H	-2.14101	-2.61757	3.54792
C	-0.84507	-1.33244	2.48224
O	0.17147	-2.01210	2.68152
O	-0.96240	-0.39145	1.58846
H	1.64919	-2.48870	-1.62131
H	1.41914	-1.60353	1.67184
H	-3.77151	3.64506	-3.47925
H	1.71316	4.36139	4.02984
H	-4.20634	-1.18766	3.51244
N	-0.53827	-1.76456	-0.72558
C	-1.62951	-2.25318	-0.75074
S	-3.08983	-2.92476	-0.81495

[6]FeTMCCH2CNMe2OBr
Charge: 2+
Energy: -3047854.7339175

Fe	-0.35406	-0.03103	0.05052
N	0.92688	1.12217	-1.35614
C	0.79918	0.38569	-2.67956
H	0.64368	1.11441	-3.48169
H	1.75877	-0.09554	-2.87620
C	-0.31978	-0.66843	-2.75839
H	-1.28789	-0.18594	-2.86646
H	-0.14710	-1.27858	-3.65528
N	-0.37446	-1.54402	-1.54323
C	-1.66308	-2.32198	-1.48211
H	-1.62403	-3.10664	-2.24879
H	-2.47027	-1.64156	-1.74819
C	-1.96739	-2.97636	-0.12386
H	-1.21010	-3.72468	0.12814
H	-2.88620	-3.55391	-0.28146
C	-2.26387	-2.06974	1.08628
H	-3.02766	-1.33511	0.83062
H	-2.65781	-2.70011	1.89450
N	-1.08262	-1.31069	1.64610
C	-1.49320	-0.38987	2.77897
H	-2.48213	-0.68172	3.14615
H	-0.79307	-0.55448	3.59933
C	-1.53060	1.10214	2.41476
H	-2.42354	1.32809	1.83636
H	-1.57432	1.68751	3.34280
N	-0.34372	1.52516	1.59877
C	-0.56241	2.89528	1.01801
H	-0.48672	3.62634	1.83406
H	-1.58261	2.92936	0.64012
C	0.41028	3.31702	-0.09709
H	1.42392	3.42525	0.30445
H	0.11822	4.33987	-0.36450
C	0.42440	2.54375	-1.43111
H	-0.58060	2.49647	-1.84932
H	1.05954	3.09226	-2.13989
C	2.34487	1.09938	-0.91384
H	2.57035	2.00450	-0.34624
H	3.01775	1.10162	-1.77589
C	2.58643	-0.08712	0.00908
O	1.56596	-0.62847	0.53392
N	3.81397	-0.50633	0.27453
C	5.03695	0.12604	-0.25131
H	4.85716	1.15174	-0.57100
H	5.43509	-0.45911	-1.08644
H	5.78117	0.14869	0.54830
C	4.03933	-1.66456	1.15669
H	4.77743	-2.32120	0.68876
H	3.10659	-2.20445	1.30433
H	4.42715	-1.32260	2.12135
C	0.77166	-2.49110	-1.55343
H	0.66141	-3.20358	-2.37984
H	0.81965	-3.03737	-0.61384
H	1.71056	-1.95508	-1.67612
C	-0.07508	-2.27540	2.17219
H	-0.52773	-2.90392	2.94843
H	0.77134	-1.73156	2.58623
H	0.29608	-2.90889	1.37077
C	0.87885	1.51672	2.44262
H	0.74973	2.18078	3.30605
H	1.73438	1.86275	1.86408
H	1.09334	0.50705	2.78758
Br	-2.55581	0.87117	-0.79353

[6]FeTMCCH2CNMe2OCl
Charge: 2+
Energy: -1721330.2111025

Fe	-0.53548	0.12008	-0.10024
N	1.07340	0.72632	-1.50798
C	0.95871	-0.26054	-2.65572
H	1.07020	0.27587	-3.60399
H	1.80629	-0.94415	-2.58087
C	-0.34418	-1.07407	-2.70343
H	-1.17286	-0.44579	-3.02176
H	-0.22020	-1.87148	-3.44862
N	-0.69882	-1.66418	-1.37200
C	-2.12239	-2.15435	-1.35220
H	-2.17543	-3.07146	-1.95333
H	-2.73467	-1.40020	-1.84415
C	-2.69336	-2.44721	0.04524
H	-2.14171	-3.25631	0.53315
H	-3.69321	-2.86122	-0.13213
C	-2.90977	-1.27062	1.01562
H	-3.46598	-0.47219	0.52335
H	-3.51135	-1.63238	1.86010
N	-1.65779	-0.65228	1.59160
C	-1.97983	0.54173	2.46596
H	-3.02601	0.49042	2.78476
H	-1.37241	0.45602	3.36812

C	-1.73664	1.90015	1.79730
H	-2.50906	2.10245	1.05801
H	-1.78932	2.68440	2.56422
N	-0.41160	1.95894	1.09477
C	-0.33553	3.17749	0.21803
H	-0.23070	4.05739	0.86697
H	-1.28820	3.26216	-0.30194
C	0.80861	3.19667	-0.80975
H	1.77799	3.24372	-0.30127
H	0.72621	4.16495	-1.31829
C	0.82789	2.14985	-1.94122
H	-0.12473	2.15191	-2.47077
H	1.61377	2.42868	-2.65629
C	2.40650	0.58939	-0.87124
H	2.72166	1.55032	-0.45945
H	3.16143	0.30802	-1.61109
C	2.32832	-0.40033	0.28471
O	1.17501	-0.66074	0.74746
N	3.42361	-0.93561	0.80022
C	4.79073	-0.61976	0.34925
H	4.83340	0.33293	-0.17717
H	5.16889	-1.41866	-0.29661
H	5.43282	-0.54626	1.23016
C	3.33853	-1.90490	1.90664
H	4.00197	-2.74507	1.68578
H	2.31554	-2.26017	2.00973
H	3.66262	-1.42980	2.83786
C	0.21954	-2.78610	-1.04839
H	0.07083	-3.61063	-1.75631
H	0.03334	-3.14603	-0.03857
H	1.25641	-2.46012	-1.09904
C	-0.92888	-1.65511	2.41738
H	-1.57296	-2.01358	3.22936
H	-0.03085	-1.20134	2.83216
H	-0.62348	-2.49957	1.80470
C	0.69486	1.96089	2.08432
H	0.58676	2.80367	2.77818
H	1.65182	2.05493	1.57235
H	0.70435	1.02639	2.64270
Cl	-2.26064	1.08028	-1.29087

^{6}FeTMCCH2CNMe2OF
Charge: 2+
Energy: -1495217.3209333

Fe	0.54027	0.14342	0.15047
N	-1.15707	0.33450	1.56747
C	-0.98464	-0.85215	2.48375
H	-1.33002	-0.58973	3.49067
H	-1.63889	-1.64756	2.12100
C	0.45518	-1.36031	2.55808
H	1.10530	-0.58797	2.96826
H	0.49222	-2.23137	3.22568
N	0.98988	-1.71956	1.20558
C	2.48324	-1.87107	1.26526
H	2.71451	-2.79833	1.80601
H	2.86030	-1.03152	1.84918
C	3.19155	-1.88891	-0.09613
H	2.85805	-2.72860	-0.71308
H	4.24444	-2.10417	0.12159
C	3.19862	-0.57866	-0.89977
H	3.51224	0.24391	-0.25338
H	3.92705	-0.67200	-1.71610
N	1.88332	-0.17252	-1.51450
C	2.00842	1.17171	-2.18543
H	3.02488	1.29617	-2.57610
H	1.33694	1.17367	-3.04548
C	1.68005	2.33221	-1.24862
H	2.39833	2.37035	-0.42900
H	1.74212	3.27787	-1.80312
N	0.32147	2.17986	-0.63309
C	0.17479	3.14534	0.50574
H	0.10078	4.15933	0.09008
H	1.09321	3.08152	1.08847
C	-1.02016	2.90159	1.43731
H	-1.96833	3.00316	0.89788
H	-1.02061	3.73922	2.14504
C	-0.99989	1.63336	2.30616
H	-0.04328	1.56812	2.82767
H	-1.79760	1.70298	3.05798
C	-2.44671	0.23165	0.85218
H	-2.81476	1.22909	0.60174
H	-3.20851	-0.23307	1.48636
C	-2.24014	-0.53431	-0.45563
O	-1.04855	-0.65024	-0.88583
N	-3.27039	-1.03021	-1.12055
C	-4.67539	-0.87569	-0.70340
H	-4.80750	-0.02753	-0.03272
H	-5.02788	-1.79161	-0.21836
H	-5.27883	-0.69602	-1.59621
C	-3.06789	-1.79081	-2.36648
H	-3.68415	-2.69279	-2.32745
H	-2.01982	-2.06441	-2.46712
H	-3.37815	-1.18326	-3.22230
C	0.35290	-2.95461	0.68859
H	0.52943	-3.79459	1.37222
H	0.76534	-3.20518	-0.28735
H	-0.71867	-2.80645	0.56388
C	1.42054	-1.17092	-2.51405
H	2.14748	-1.26120	-3.33042
H	0.45539	-0.85618	-2.91002
H	1.29089	-2.14367	-2.04441
C	-0.74748	2.36093	-1.64275
H	-0.65928	3.33791	-2.13454
H	-1.72384	2.30283	-1.16215
H	-0.69702	1.56903	-2.38987
F	1.72126	0.89160	1.29741

^{6}FeTMCCH2CNMe2ON$_3$
Charge: 2+
Energy: -1535594.0867300

Fe	-0.45627	-0.02066	0.04595
N	0.81083	1.24195	-1.27909
C	0.66277	0.60488	-2.64303
H	0.58842	1.38732	-3.40683
H	1.58258	0.05446	-2.84870
C	-0.53402	-0.34514	-2.78781
H	-1.46670	0.21690	-2.77474
H	-0.46352	-0.83940	-3.76657
N	-0.59179	-1.36194	-1.69162
C	-1.93283	-2.03811	-1.65341
H	-2.00358	-2.71851	-2.51253
H	-2.69013	-1.26513	-1.78504
C	-2.23671	-2.82835	-0.36984
H	-1.52782	-3.65120	-0.23956
H	-3.20053	-3.31907	-0.55115
C	-2.41596	-2.04863	0.94651
H	-3.12631	-1.23192	0.80318
H	-2.83633	-2.73441	1.69457
N	-1.16460	-1.44637	1.52944
C	-1.47011	-0.63471	2.76614
H	-2.40972	-0.97755	3.21330
H	-0.68478	-0.84015	3.49513
C	-1.56455	0.87310	2.51207
H	-2.46487	1.10008	1.94186
H	-1.63682	1.39285	3.47699
N	-0.39578	1.39120	1.72896
C	-0.67275	2.78237	1.24335
H	-0.62522	3.46649	2.10168
H	-1.69922	2.79901	0.87736
C	0.26535	3.31846	0.14852
H	1.28408	3.42053	0.53746
H	-0.05645	4.35089	-0.03450
C	0.27316	2.64417	-1.23768
H	-0.74041	2.60030	-1.63972
H	0.86775	3.26722	-1.92003
C	2.23155	1.19291	-0.86089
H	2.45714	2.03884	-0.20836
H	2.89456	1.28452	-1.72655
C	2.48892	-0.08440	-0.06527
O	1.48152	-0.68951	0.40774
N	3.72526	-0.51602	0.14133
C	4.93677	0.18168	-0.32183
H	4.74256	1.23168	-0.53717
H	5.33997	-0.31068	-1.21267
H	5.68452	0.13497	0.47364
C	3.96856	-1.75958	0.89192
H	4.72004	-2.34789	0.35892
H	3.04502	-2.32885	0.97323
H	4.34626	-1.52049	1.89112
C	0.48052	-2.37228	-1.86625
H	0.33339	-2.93089	-2.79930
H	0.47542	-3.06997	-1.03095
H	1.45739	-1.89295	-1.88719
C	-0.19921	-2.51769	1.89638
H	-0.64634	-3.20045	2.62939
H	0.69955	-2.06566	2.31237
H	0.09252	-3.08224	1.01397
C	0.83850	1.35473	2.54899
H	0.71017	1.93168	3.47363
H	1.66924	1.78107	1.98711
H	1.09658	0.32482	2.79177
N	-2.11944	0.72891	-0.44812
N	-3.02604	1.36708	-0.93756
N	-3.88377	1.97472	-1.40176

^{6}FeTMCCH2CNMe2ONCS
Charge: 2+
Energy: -1740704.1145778

Fe	0.24129	0.13730	0.09240
N	-0.71244	-1.40783	-1.18751
C	-0.55766	-0.86696	-2.59158
H	-0.31776	-1.68903	-3.27551
H	-1.52872	-0.47590	-2.90076
C	0.50234	0.23127	-2.74473
H	1.49843	-0.18551	-2.60514

H	0.44572	0.62552	-3.76867
N	0.32451	1.33536	-1.74979
C	1.54629	2.20744	-1.69023
H	1.57900	2.82058	-2.60080
H	2.41525	1.55044	-1.70637
C	1.63461	3.13451	-0.46678
H	0.80777	3.85068	-0.45638
H	2.52970	3.74688	-0.62946
C	1.82228	2.49842	0.92343
H	2.64997	1.78707	0.90094
H	2.08383	3.29689	1.63110
N	0.62828	1.76866	1.48090
C	0.95529	1.11404	2.80196
H	1.79425	1.63474	3.27685
H	0.09315	1.24938	3.45674
C	1.29716	-0.37481	2.68869
H	2.26039	-0.50246	2.19626
H	1.37745	-0.79876	3.69885
N	0.27979	-1.13083	1.88842
C	0.79662	-2.49699	1.54888
H	0.78700	-3.10820	2.46173
H	1.83652	-2.38252	1.24556
C	0.03150	-3.25478	0.45100
H	-0.98758	-3.48204	0.78207
H	0.51580	-4.23626	0.38009
C	0.03331	-2.69737	-0.98581
H	1.05790	-2.51263	-1.31202
H	-0.39790	-3.45705	-1.65222
C	-2.15111	-1.54919	-0.86545
H	-2.29552	-2.36584	-0.15510
H	-2.72588	-1.81080	-1.75909
C	-2.65775	-0.26861	-0.20524
O	-1.79197	0.52338	0.27398
N	-3.95704	-0.02177	-0.11610
C	-5.00914	-0.93534	-0.59345
H	-4.64562	-1.95791	-0.68771
H	-5.40175	-0.59131	-1.55582
H	-5.82132	-0.93403	0.13746
C	-4.44326	1.22431	0.50023
H	-5.22390	1.64784	-0.13717
H	-3.62325	1.93245	0.59816
H	-4.86679	1.00795	1.48611
C	-0.86648	2.15322	-2.08681
H	-0.73545	2.63678	-3.06321
H	-1.01850	2.92056	-1.32987
H	-1.76146	1.53442	-2.11135
C	-0.50469	2.71058	1.68743
H	-0.21629	3.50933	2.38188
H	-1.35840	2.16471	2.08569
H	-0.80628	3.15214	0.74041
C	-1.00295	-1.22004	2.62612
H	-0.85615	-1.68891	3.60744
H	-1.71536	-1.81916	2.05940
H	-1.43207	-0.22715	2.75398
N	2.04863	-0.39964	-0.23994
C	3.16957	-0.78245	-0.47327
S	4.63802	-1.28568	-0.77792

^{6}FeTMCCH2CNMe2OOH
Charge: 2+
Energy: -1480125.3795496

Fe	0.59144	0.18744	0.21217
O	1.84024	0.91375	1.32175
N	-1.16814	0.39397	1.56816
C	-1.01070	-0.76049	2.53038
H	-1.30659	-0.44222	3.53681
H	-1.71465	-1.53805	2.22809
C	0.40311	-1.34793	2.58595
H	1.09667	-0.61799	3.00105
H	0.39167	-2.22320	3.24991
N	0.91420	-1.72546	1.23154
C	2.39673	-1.96534	1.27818
H	2.57769	-2.91455	1.80017
H	2.82629	-1.15982	1.87292
C	3.09954	-2.00252	-0.08740
H	2.71882	-2.81817	-0.70929
H	4.13930	-2.27797	0.12605
C	3.18010	-0.69016	-0.88794
H	3.54897	0.11143	-0.24547
H	3.89313	-0.83075	-1.71148
N	1.88429	-0.20663	-1.48585
C	2.06694	1.12524	-2.17123
H	3.10739	1.23539	-2.49681
H	1.45500	1.11679	-3.07453
C	1.69227	2.31983	-1.29204
H	2.39569	2.40484	-0.46442
H	1.74816	3.23884	-1.89100
N	0.32510	2.17124	-0.69436
C	0.12538	3.18838	0.38599
H	0.01346	4.17699	-0.08028
H	1.04299	3.20751	0.97366
C	-1.07003	2.95565	1.32408
H	-2.01149	3.01793	0.76813
H	-1.09550	3.82415	1.99339
C	-1.05741	1.72499	2.25062
H	-0.12584	1.69689	2.81903
H	-1.88165	1.82177	2.97078
C	-2.44199	0.25489	0.82751
H	-2.82246	1.23989	0.54906
H	-3.20903	-0.20783	1.45618
C	-2.19689	-0.52894	-0.46059
O	-1.00098	-0.62024	-0.86793
N	-3.20812	-1.06330	-1.13087
C	-4.62286	-0.93096	-0.74405
H	-4.78282	-0.08631	-0.07502
H	-4.97296	-1.85230	-0.26740
H	-5.21105	-0.75856	-1.64872
C	-2.96574	-1.83895	-2.35909
H	-3.57084	-2.74860	-2.32261
H	-1.91198	-2.10043	-2.42892
H	-3.26075	-1.24965	-3.23311
C	0.21108	-2.92467	0.71783
H	0.38159	-3.78413	1.37870
H	0.57348	-3.17006	-0.27887
H	-0.85854	-2.73709	0.64077
C	1.36607	-1.18490	-2.47857
H	2.09459	-1.33284	-3.28531
H	0.42798	-0.81590	-2.89009
H	1.16608	-2.14025	-1.99891
C	-0.72258	2.28514	-1.73518
H	-0.64161	3.24047	-2.26938
H	-1.70943	2.22769	-1.27599
H	-0.63849	1.46090	-2.44241
H	2.08562	1.49923	2.05143

^{3}FeSSPDPBrOH
Charge: 2+
Energy: -3081443.0561566

Fe	-0.00520	-0.48289	-0.49097
N	1.99071	-0.68367	-0.29694
C	2.66223	-1.68659	0.30868
H	2.06439	-2.43527	0.81031
C	4.04990	-1.75690	0.28161
H	4.54966	-2.58096	0.77906
C	4.76689	-0.76619	-0.39060
H	5.85143	-0.79678	-0.42874
C	4.06816	0.26998	-1.01344
H	4.59089	1.05941	-1.54376
C	2.67929	0.27982	-0.95792
C	1.83639	1.31094	-1.64809
H	2.35710	2.27125	-1.71866
H	1.59973	0.96878	-2.65936
N	0.54617	1.46107	-0.91140
C	-0.42290	2.30396	-1.68774
H	-1.41614	2.13374	-1.27151
H	-0.42995	1.98684	-2.73122
C	0.04059	3.74689	-1.43952
H	-0.78987	4.44886	-1.54155
H	0.79934	4.04108	-2.16974
C	0.62997	3.72445	-0.00152
H	-0.02227	4.23864	0.71019
H	1.59962	4.22475	0.04316
C	0.75545	2.22286	0.37741
H	1.74761	1.96838	0.75743
C	-0.29933	1.78157	1.38696
H	-1.27867	2.13274	1.05359
C	0.02740	2.23409	2.83756
H	0.86587	2.93671	2.82901
H	-0.81700	2.75779	3.29054
C	0.38407	0.93863	3.61476
H	1.27124	1.05711	4.24079
H	-0.43394	0.63485	4.27371
C	0.61811	-0.10591	2.51790
H	0.46068	-1.14437	2.81218
H	1.62129	-0.01335	2.10189
N	-0.35764	0.26230	1.43091
C	-1.74862	-0.15651	1.80884
H	-2.12949	0.46777	2.62275
H	-1.70904	-1.19052	2.16141
C	-2.62765	-0.07751	0.59746
C	-4.00948	0.06890	0.64860
H	-4.50293	0.19184	1.60728
C	-4.73959	0.03673	-0.54103
H	-5.82029	0.13754	-0.52256
C	-4.06229	-0.13025	-1.75059
H	-4.59171	-0.16753	-2.69641
C	-2.67858	-0.25637	-1.73669
H	-2.09369	-0.39083	-2.63756
N	-1.98399	-0.21979	-0.58263
O	0.08599	-0.82781	-2.20637
H	0.15079	-1.78457	-2.39897
Br	-0.48555	-2.78889	0.16822

^{3}FeSSPDPClOH
Charge: 2+

Energy: -1754914.8138733

Fe	-0.00605	-0.75159	-0.40659
N	1.98925	-0.83827	-0.20895
C	2.69783	-1.76009	0.47650
H	2.12660	-2.49176	1.03178
C	4.08763	-1.76752	0.45862
H	4.62224	-2.52543	1.02079
C	4.76254	-0.80036	-0.28793
H	5.84761	-0.78325	-0.31890
C	4.02246	0.14816	-0.99744
H	4.51277	0.91326	-1.59064
C	2.63448	0.09714	-0.94778
C	1.74272	1.01412	-1.73087
H	2.20837	1.99223	-1.88626
H	1.53434	0.56892	-2.70773
N	0.43764	1.15691	-1.01495
C	-0.57312	1.85794	-1.87713
H	-1.55719	1.67779	-1.44425
H	-0.55611	1.43135	-2.88063
C	-0.19198	3.34186	-1.78224
H	-1.05793	3.98168	-1.96556
H	0.55964	3.59842	-2.53374
C	0.37679	3.50521	-0.34530
H	-0.31843	4.04497	0.30409
H	1.31099	4.07069	-0.34429
C	0.59252	2.06230	0.18845
H	1.59728	1.91009	0.58952
C	-0.43598	1.66143	1.24115
H	-1.43507	1.91525	0.87917
C	-0.13945	2.27330	2.63854
H	0.64027	3.03600	2.55483
H	-1.02108	2.76910	3.05006
C	0.32046	1.08733	3.52935
H	1.20507	1.32828	4.12297
H	-0.46481	0.79297	4.23094
C	0.61490	-0.04124	2.53422
H	0.52962	-1.05463	2.92823
H	1.60621	0.07610	2.09667
N	-0.39286	0.15588	1.43267
C	-1.74600	-0.32648	1.86608
H	-2.16272	0.33679	2.63010
H	-1.62661	-1.32134	2.30257
C	-2.64018	-0.41529	0.66624
C	-4.02865	-0.36630	0.72564
H	-4.52179	-0.19891	1.67772
C	-4.76432	-0.55215	-0.44638
H	-5.84932	-0.52899	-0.42057
C	-4.08717	-0.77168	-1.64768
H	-4.62060	-0.92798	-2.57894
C	-2.69776	-0.79528	-1.64336
H	-2.11235	-0.96325	-2.53844
N	-1.99873	-0.60839	-0.50713
O	0.09510	-1.25026	-2.08314
H	0.17883	-2.22194	-2.16501
Cl	-0.31252	-2.80355	0.44520

^{3}FeSSPDPFOH

Charge: 2+

Energy: -1528792.2415594

Fe	0.00361	-0.88771	-0.27130
N	1.95291	-0.95982	-0.05187
C	2.59187	-1.82467	0.75901
H	1.95840	-2.48223	1.34129
C	3.98040	-1.85113	0.81563
H	4.47649	-2.55561	1.47426
C	4.70721	-0.96586	0.01497
H	5.79249	-0.96313	0.04475
C	4.02743	-0.08694	-0.83359
H	4.56602	0.60045	-1.47778
C	2.63798	-0.11766	-0.85736
C	1.77991	0.67881	-1.79899
H	2.24404	1.63373	-2.06275
H	1.63275	0.09915	-2.71517
N	0.42896	0.89065	-1.18332
C	-0.55762	1.38350	-2.20615
H	-1.55533	1.24374	-1.78833
H	-0.47618	0.78289	-3.11268
C	-0.23179	2.87226	-2.36303
H	-1.09236	3.42904	-2.74041
H	0.58288	3.01836	-3.07806
C	0.18702	3.31842	-0.93729
H	-0.61753	3.87028	-0.44204
H	1.05638	3.97883	-0.95769
C	0.48736	2.00816	-0.15697
H	1.49202	2.00373	0.27276
C	-0.53125	1.72244	0.94606
H	-1.54026	1.82633	0.54026
C	-0.30285	2.58912	2.21282
H	0.34908	3.43565	1.97936
H	-1.24289	3.00873	2.57733
C	0.34053	1.63727	3.26025
H	1.23031	2.06650	3.72604
H	-0.36212	1.40839	4.06586
C	0.69407	0.37031	2.46744
H	0.70149	-0.55540	3.04428
H	1.66085	0.47363	1.97524
N	-0.35977	0.28858	1.39540
C	-1.63668	-0.25740	1.96068
H	-2.06361	0.43454	2.69289
H	-1.39236	-1.19628	2.46378
C	-2.58914	-0.53585	0.83571
C	-3.97346	-0.55640	0.96441
H	-4.43211	-0.31400	1.91752
C	-4.74960	-0.90450	-0.14344
H	-5.83181	-0.93583	-0.06402
C	-4.11818	-1.21288	-1.35039
H	-4.68558	-1.49382	-2.23092
C	-2.73057	-1.16211	-1.41552
H	-2.17684	-1.39590	-2.31674
N	-1.99393	-0.81914	-0.34225
O	0.08706	-1.65848	-1.84034
H	0.13781	-2.63028	-1.72833
F	-0.16391	-2.31936	0.73382

^{5}FeSSPDPN$_{3}$OH

Charge: 2+

Energy: -1569175.8476359

Fe	0.02355	0.80519	-0.28169
N	-2.20542	0.89809	-0.02236
C	-2.90342	1.72016	0.78291
H	-2.31560	2.36117	1.43183
C	-4.29444	1.73971	0.78216
H	-4.82797	2.41570	1.44157
C	-4.97535	0.87472	-0.07864
H	-6.06071	0.86096	-0.09965
C	-4.24597	0.02462	-0.91402
H	-4.74743	-0.65559	-1.59522
C	-2.85538	0.07190	-0.86555
C	-1.96600	-0.72741	-1.78432
H	-2.45566	-1.65361	-2.10338
H	-1.74481	-0.13349	-2.67654
N	-0.65417	-1.02945	-1.13488
C	0.30319	-1.63142	-2.12464
H	1.30698	-1.52698	-1.71299
H	0.26071	-1.07219	-3.05974
C	-0.11414	-3.10903	-2.21842
H	0.74269	-3.74004	-2.46451
H	-0.85462	-3.25224	-3.00975
C	-0.71962	-3.44231	-0.82473
H	-0.10078	-4.15352	-0.27069
H	-1.70919	-3.89506	-0.91812
C	-0.79709	-2.08957	-0.06650
H	-1.76161	-1.93823	0.42334
C	0.32580	-1.93562	0.96270
H	1.27805	-2.20920	0.50274
C	0.04437	-2.73291	2.26570
H	-0.73500	-3.47995	2.09147
H	0.93289	-3.27786	2.59191
C	-0.39376	-1.67713	3.31996
H	-1.32525	-1.94784	3.82194
H	0.36667	-1.56168	4.09686
C	-0.55854	-0.37321	2.52240
H	-0.37073	0.54365	3.08264
H	-1.55186	-0.30314	2.07881
N	0.42939	-0.48835	1.39587
C	1.81258	-0.17213	1.86885
H	2.15552	-0.93315	2.57782
H	1.75773	0.78245	2.40205
C	2.76921	-0.03562	0.71053
C	4.13701	-0.27314	0.81259
H	4.56203	-0.64263	1.74053
C	4.94590	-0.01285	-0.29717
H	6.01651	-0.18469	-0.24329
C	4.36510	0.47147	-1.47231
H	4.96452	0.69107	-2.34916
C	2.98804	0.66971	-1.50318
H	2.46794	1.04051	-2.38015
N	2.21590	0.41110	-0.43252
O	0.04564	1.56869	-1.88399
H	-0.44414	2.40515	-2.00306
N	0.27480	2.29726	0.79687
N	0.84946	3.31688	0.40023
N	1.37728	4.28251	0.10089

^{3}FeSSPDPNCSOH

Charge: 2+

Energy: -1774287.7274901

Fe	0.06156	0.36091	-0.53936
N	-1.72748	1.20039	-0.34108
C	-1.99229	2.41170	0.18932
H	-1.14987	2.94522	0.60894
C	-3.27636	2.94010	0.19647
H	-3.45285	3.91783	0.63117
C	-4.31619	2.19254	-0.36256
H	-5.33076	2.57867	-0.37002

C	-4.03543	0.94072	-0.91207
H	-4.81858	0.33486	-1.35607
C	-2.72464	0.47437	-0.89612
C	-2.28758	-0.81588	-1.52424
H	-3.08346	-1.56616	-1.49385
H	-2.02048	-0.62822	-2.56738
N	-1.05425	-1.30595	-0.82957
C	-0.44416	-2.44652	-1.59347
H	0.56881	-2.58755	-1.21606
H	-0.38227	-2.18537	-2.65019
C	-1.32386	-3.65638	-1.25765
H	-0.77339	-4.59219	-1.37710
H	-2.18861	-3.70786	-1.92513
C	-1.76465	-3.40892	0.21033
H	-1.22418	-4.05921	0.90456
H	-2.82806	-3.61266	0.35299
C	-1.42840	-1.92004	0.50314
H	-2.28990	-1.37025	0.89053
C	-0.25889	-1.75623	1.47083
H	0.56889	-2.38655	1.13699
C	-0.65540	-2.03553	2.94693
H	-1.64343	-2.50293	2.98902
H	0.04059	-2.73070	3.42131
C	-0.65115	-0.65204	3.65154
H	-1.53564	-0.49514	4.27292
H	0.22006	-0.54500	4.30385
C	-0.59770	0.35663	2.49722
H	-0.15408	1.32310	2.74454
H	-1.59299	0.53398	2.08939
N	0.21623	-0.31827	1.42894
C	1.67295	-0.26082	1.76570
H	1.89977	-0.86613	2.64924
H	1.91952	0.77869	2.00205
C	2.47265	-0.71077	0.57591
C	3.75122	-1.25264	0.65734
H	4.21049	-1.41406	1.62728
C	4.42499	-1.57383	-0.52300
H	5.42560	-1.99309	-0.48501
C	3.79463	-1.35013	-1.74880
H	4.28482	-1.58343	-2.68769
C	2.51019	-0.81771	-1.75819
H	1.95900	-0.62060	-2.66952
N	1.86704	-0.51476	-0.61462
O	0.02169	0.55270	-2.30831
H	0.34429	1.42807	-2.58817
N	0.96345	1.97561	-0.19200
C	1.68227	2.91234	-0.03710
S	2.63029	4.19478	0.17377

^{5}FeTMCAcOH
Charge: 0
Energy: -1443159.0149347

Fe	0.10016	0.01827	-0.31828
O	0.43247	0.10813	-2.04483
N	-2.31664	0.19171	-0.23293
C	-2.61539	1.54736	-0.69250
C	-1.38625	2.35732	-1.15784
N	-0.24040	2.24738	-0.25515
C	1.00322	2.74732	-0.86300
C	2.31601	2.35201	-0.16584
C	2.88728	0.94608	-0.42733
N	2.41527	-0.15400	0.41665
C	2.83439	-1.47834	-0.03493
C	1.79918	-2.21213	-0.91044
N	0.45697	-2.20882	-0.33005
C	-0.58097	-2.63421	-1.27999
C	-2.03176	-2.28120	-0.89924
C	-2.56610	-0.87208	-1.21792
C	-2.65643	-0.09897	1.12306
C	-1.37754	-0.20198	2.07491
O	-0.27025	-0.08568	1.44908
C	-0.49898	2.89397	1.02319
C	2.64476	0.05323	1.82948
C	0.40943	-2.97380	0.90673
O	-1.55081	-0.37245	3.24421
H	-3.31241	1.50929	-1.53553
H	-3.11764	2.09152	0.10805
H	-1.07415	2.00990	-2.14322
H	-1.70660	3.40305	-1.25913
H	0.96468	3.84446	-0.88109
H	1.04650	2.39975	-1.89619
H	2.26274	2.55868	0.90089
H	3.06201	3.04328	-0.56734
H	2.70870	0.67585	-1.46941
H	3.97613	1.02609	-0.28699
H	3.75015	-1.40592	-0.63045
H	3.06038	-2.08975	0.83763
H	1.75017	-1.73029	-1.88757
H	2.16098	-3.23933	-1.05200
H	-0.53135	-3.72706	-1.38016
H	-0.35262	-2.20745	-2.25778
H	-2.21297	-2.53204	0.14247
H	-2.65369	-2.96091	-1.48377
H	-2.16298	-0.54090	-2.17688
H	-3.65557	-0.96636	-1.33743
H	-3.17733	-1.05262	1.23075
H	-3.28477	0.66893	1.58269
H	-0.60358	3.97712	0.90056
H	0.31372	2.70521	1.71721
H	-1.40871	2.51228	1.47393
H	3.71700	0.09408	2.05810
H	2.20289	-0.75104	2.41102
H	2.19085	0.98035	2.16297
H	0.81619	-3.98019	0.76110
H	-0.60997	-3.07330	1.26606
H	0.98132	-2.47619	1.68393
H	0.11297	0.15692	-2.94420

^{5}FeTMCBrOPr
Charge: 0
Energy: -3061059.2086270

Fe	0.34024	0.00888	0.06415
O	2.23942	0.04445	0.52084
C	3.37489	-0.03665	-0.11896
O	3.49691	-0.29878	-1.31827
C	4.59296	0.22365	0.76678
H	4.48763	1.23904	1.17436
H	4.51773	-0.44698	1.63316
C	5.92755	0.05545	0.04422
H	6.76670	0.25878	0.71889
H	5.99353	0.73512	-0.81060
H	6.03227	-0.96248	-0.34399
N	0.20006	-1.92815	-1.07268
N	-0.47144	-0.89341	1.94133
N	-0.02491	1.95841	1.17273
N	-0.24677	0.89480	-1.87343
C	-0.99704	-2.71397	-0.65677
C	-1.03241	-3.12521	0.82199
C	-1.43515	-2.02406	1.80600
C	-1.16355	0.24345	2.60757
C	-0.34025	1.52743	2.56190
C	-1.17169	2.72180	0.60210
C	-1.02818	3.11752	-0.87325
C	-1.25647	1.99265	-1.88591
C	-0.78825	-0.25497	-2.65061
C	0.07125	-1.50638	-2.49408
C	0.70585	-1.32913	2.72538
C	1.19968	2.78457	1.19876
C	1.02943	1.37334	-2.45705
C	1.43293	-2.73222	-0.92068
H	-1.88695	-2.11384	-0.86687
H	-1.04007	-3.62350	-1.27994
H	-0.10318	-3.62225	1.12122
H	-1.81121	-3.89378	0.90560
H	-1.59504	-2.46722	2.80311
H	-2.38062	-1.59763	1.46541
H	-2.11307	0.38466	2.08448
H	-1.38379	-0.00519	3.65873
H	0.60922	1.38484	3.08403
H	-0.88232	2.32259	3.09691
H	-2.06886	2.10439	0.70416
H	-1.31100	3.63491	1.20600
H	-1.81741	3.85462	-1.06813
H	-0.08733	3.64802	-1.05656
H	-1.28761	2.42089	-2.90139
H	-2.22609	1.53803	-1.67366
H	-0.85381	0.00694	-3.71891
H	-1.80065	-0.43632	-2.28022
H	1.07987	-1.32043	-2.86909
H	-0.35864	-2.31860	-3.10049
H	0.41168	-1.59809	3.75198
H	1.15850	-2.19801	2.24654
H	1.46509	-0.54873	2.74302
H	1.05483	3.69183	1.80681
H	2.01804	2.18715	1.59983
H	1.47757	3.07960	0.18698
H	0.89292	1.63987	-3.51677
H	1.36339	2.25967	-1.91564
H	1.81531	0.62396	-2.35689
H	2.28012	-2.15823	-1.29376
H	1.61233	-2.94746	0.13289
H	1.35001	-3.68384	-1.46955
Br	-3.62983	-0.03982	-0.18657

^{5}FeTMCClOPr
Charge: 0
Energy: -1734527.9953248

Fe	-0.01998	0.00115	0.03949
O	1.87795	0.02228	0.54172
C	3.04022	-0.03043	-0.04724
O	3.22271	-0.26278	-1.24556
C	4.21512	0.22260	0.89863
H	4.08056	1.22746	1.32354
H	4.10917	-0.46840	1.74561
C	5.58272	0.08530	0.23354

H	6.38883	0.28244	0.94927
H	5.67838	0.78460	-0.60246
H	5.71650	-0.92233	-0.17223
N	-0.08366	-1.91333	-1.13651
N	-0.82966	-0.94208	1.89635
N	-0.37065	1.92858	1.18446
N	-0.50097	0.93125	-1.90476
C	-1.28051	-2.71855	-0.76111
C	-1.34459	-3.15218	0.71182
C	-1.78144	-2.07528	1.71033
C	-1.54252	0.18168	2.56240
C	-0.72613	1.47237	2.55624
C	-1.49207	2.71179	0.59197
C	-1.29713	3.13391	-0.87178
C	-1.50295	2.03566	-1.92011
C	-1.02559	-0.20426	-2.71344
C	-0.17835	-1.46494	-2.55291
C	0.33074	-1.38433	2.69920
C	0.86036	2.74122	1.25838
C	0.79390	1.41097	-2.44131
C	1.15432	-2.70508	-0.96627
H	-2.16905	-2.12203	-0.98246
H	-1.29720	-3.62086	-1.39654
H	-0.41624	-3.64343	1.02308
H	-2.11480	-3.93233	0.76534
H	-1.96259	-2.54430	2.69222
H	-2.71759	-1.64476	1.35261
H	-2.47629	0.32683	2.01488
H	-1.78531	-0.08226	3.60524
H	0.20815	1.32807	3.10464
H	-1.28924	2.25564	3.08737
H	-2.39341	2.09674	0.65343
H	-1.64217	3.61642	1.20657
H	-2.07088	3.88509	-1.07594
H	-0.34526	3.65761	-1.01306
H	-1.49977	2.49156	-2.92428
H	-2.47857	1.58037	-1.74547
H	-1.05874	0.07257	-3.77984
H	-2.04611	-0.38621	-2.36964
H	0.83980	-1.28023	-2.90179
H	-0.59903	-2.26391	-3.18319
H	0.01568	-1.67376	3.71429
H	0.80104	-2.24117	2.21554
H	1.08352	-0.59908	2.74696
H	0.70569	3.64388	1.87119
H	1.65943	2.13139	1.67859
H	1.17408	3.04279	0.25911
H	0.69237	1.69460	-3.50080
H	1.11606	2.28709	-1.87636
H	1.57214	0.65591	-2.32665
H	2.00436	-2.11452	-1.30514
H	1.30863	-2.93709	0.08766
H	1.09763	-3.64760	-1.53424
Cl	-3.55986	-0.03743	-0.28059

^{5}FeTMCFOPr
Charge: 0
Energy: -1508408.3246836

Fe	-0.36942	0.00771	0.02575
O	1.53095	0.02579	-0.70009
C	2.74105	-0.01599	-0.24743
O	3.07589	0.03330	0.94591
C	3.80977	-0.13040	-1.34269
H	3.63104	-1.07504	-1.87638
H	3.61397	0.66146	-2.07807
C	5.24292	-0.06300	-0.81977
H	5.96810	-0.16137	-1.63631
H	5.42473	-0.85853	-0.09099
H	5.42311	0.88749	-0.30738
N	-0.01712	1.76961	1.39531
N	-1.18097	1.23362	-1.70656
N	-0.71683	-1.76153	-1.36533
N	-0.37288	-1.22405	1.92733
C	-1.24498	2.59557	1.29145
C	-1.50683	3.21031	-0.09970
C	-2.08826	2.28549	-1.18312
C	-1.96979	0.18519	-2.39661
C	-1.18802	-1.11555	-2.61655
C	-1.78077	-2.57841	-0.73199
C	-1.42996	-3.17698	0.64545
C	-1.46328	-2.22922	1.85702
C	-0.73580	-0.15091	2.88723
C	0.11345	1.11610	2.72456
C	-0.13546	1.79173	-2.57327
C	0.48130	-2.56551	-1.65544
C	0.91282	-1.84979	2.27685
C	1.18631	2.58324	1.13906
H	-2.09085	1.95656	1.54567
H	-1.18304	3.41691	2.02851
H	-0.62161	3.74051	-0.46525
H	-2.26336	3.99182	0.05319
H	-2.44764	2.90858	-2.02180
H	-2.93836	1.76355	-0.74679
H	-2.83220	-0.01868	-1.76343
H	-2.33056	0.54413	-3.37701
H	-0.30348	-0.90828	-3.22383
H	-1.81777	-1.80919	-3.19965
H	-2.64869	-1.93015	-0.60807
H	-2.04818	-3.40601	-1.41449
H	-2.19719	-3.93749	0.84401
H	-0.48672	-3.73121	0.60289
H	-1.45523	-2.83841	2.77841
H	-2.39638	-1.67022	1.81342
H	-0.63380	-0.50680	3.92733
H	-1.78330	0.08765	2.70599
H	1.16821	0.86058	2.84255
H	-0.14855	1.82142	3.53193
H	-0.55524	2.19553	-3.51099
H	0.38440	2.59367	-2.04668
H	0.61112	1.02726	-2.78860
H	0.25446	-3.40161	-2.33897
H	1.23942	-1.91563	-2.09047
H	0.89744	-2.96546	-0.73066
H	0.88825	-2.27262	3.29631
H	1.12611	-2.65724	1.57303
H	1.72281	-1.12685	2.17807
H	2.06967	1.96563	1.29141
H	1.19538	2.92294	0.10301
H	1.22111	3.46274	1.80462
F	-2.28436	0.02602	0.45266

^{5}FeTMCN$_3$OPr
Charge: 0
Energy: -1548786.3069702

Fe	-0.18312	0.03541	0.05532
O	1.74493	-0.10698	-0.52498
C	2.97663	-0.22700	-0.14182
O	3.37656	-0.21149	1.02951
C	3.97224	-0.38970	-1.29746
H	3.71822	-1.32244	-1.82143
H	3.77405	0.41436	-2.01903
C	5.43466	-0.39570	-0.85780
H	6.10471	-0.52870	-1.71523
H	5.61763	-1.20126	-0.14063
H	5.69220	0.54342	-0.35778
N	0.26319	1.77222	1.42672
N	-0.74404	1.28194	-1.74137
N	-0.58672	-1.70714	-1.34521
N	-0.31964	-1.15190	1.94658
C	-0.81803	2.77018	1.21276
C	-0.90354	3.35052	-0.21677
C	-1.51628	2.48853	-1.33844
C	-1.59800	0.33722	-2.50762
C	-0.99394	-1.07098	-2.63110
C	-1.67364	-2.53094	-0.75093
C	-1.38445	-3.10336	0.65405
C	-1.40795	-2.16308	1.87436
C	-0.66805	-0.07961	2.91732
C	0.22431	1.16420	2.78887
C	0.44487	1.66419	-2.52321
C	0.60569	-2.54409	-1.58820
C	0.96427	-1.78884	2.29631
C	1.58481	2.40518	1.23007
H	-1.76521	2.28795	1.45646
H	-0.66151	3.61212	1.91052
H	0.06763	3.74920	-0.52668
H	-1.55872	4.22875	-0.14231
H	-1.66003	3.13300	-2.22314
H	-2.50158	2.15610	-1.01641
H	-2.57327	0.28158	-2.02875
H	-1.76895	0.71477	-3.53086
H	-0.10009	-1.01713	-3.25694
H	-1.71504	-1.70723	-3.16716
H	-2.58650	-1.93651	-0.73073
H	-1.86741	-3.38650	-1.42258
H	-2.17957	-3.83775	0.83903
H	-0.45891	-3.68802	0.63921
H	-1.37699	-2.78710	2.78430
H	-2.35208	-1.62034	1.87433
H	-0.58729	-0.45330	3.95231
H	-1.70503	0.19469	2.72681
H	1.25125	0.89292	3.04109
H	-0.10502	1.90575	3.53417
H	0.15902	2.13903	-3.47668
H	1.05423	2.36022	-1.94613
H	1.06505	0.78819	-2.70579
H	0.37108	-3.38793	-2.25799
H	1.38941	-1.92536	-2.01972
H	0.99102	-2.93227	-0.64604
H	0.93151	-2.20997	3.31519
H	1.17162	-2.59768	1.59337
H	1.78514	-1.07826	2.20018
H	2.36665	1.68041	1.44825
H	1.70370	2.70996	0.19057
H	1.69736	3.29033	1.87808
N	-2.32576	0.29294	0.53615

N	-3.41011	0.06972	0.07606
N	-4.45705	-0.15181	-0.38871

^{5}FeTMCNCSOPr
Charge: 0
Energy: -1753899.1645342

Fe	-0.05298	-0.00199	0.01895
O	-2.02521	0.00771	0.36398
C	-3.20551	-0.01958	-0.17362
O	-3.44801	0.03134	-1.38545
C	-4.34706	-0.11551	0.84514
H	-4.22494	-1.06475	1.38644
H	-4.18657	0.67114	1.59472
C	-5.73939	-0.01901	0.22548
H	-6.51887	-0.10628	0.99122
H	-5.88650	-0.80911	-0.51671
H	-5.86699	0.93654	-0.29300
N	-0.14476	1.75921	-1.38422
N	0.41264	1.19907	1.87847
N	0.06390	-1.76962	1.44208
N	0.26914	-1.19664	-1.84714
C	0.97289	2.67229	-1.02516
C	0.92231	3.24795	0.40733
C	1.32005	2.34297	1.58888
C	1.10377	0.18285	2.71403
C	0.36387	-1.16142	2.77025
C	1.16071	-2.65939	0.97396
C	0.99410	-3.22943	-0.45103
C	1.24446	-2.30451	-1.65689
C	0.82894	-0.15864	-2.75363
C	0.02884	1.15180	-2.73589
C	-0.82247	1.67006	2.52907
C	-1.20211	-2.52285	1.54045
C	-1.01159	-1.71817	-2.36456
C	-1.42942	2.49164	-1.35550
H	1.90715	2.12791	-1.16136
H	0.96920	3.52238	-1.72998
H	-0.04735	3.72079	0.59303
H	1.64740	4.07228	0.42167
H	1.40009	2.97335	2.49116
H	2.30892	1.93403	1.38960
H	2.09521	0.03416	2.29004
H	1.22834	0.54720	3.74822
H	-0.59093	-1.02239	3.28265
H	0.95373	-1.85553	3.38916
H	2.09036	-2.09314	1.02771
H	1.24247	-3.51146	1.67179
H	1.74334	-4.02715	-0.53870
H	0.02885	-3.73671	-0.54859
H	1.25743	-2.92721	-2.56758
H	2.23272	-1.86067	-1.55071
H	0.85837	-0.52758	-3.79277
H	1.85279	0.03174	-2.43484
H	-0.97220	0.96318	-3.12830
H	0.51380	1.86464	-3.42123
H	-0.61130	2.09993	3.52230
H	-1.29516	2.43000	1.90576
H	-1.53490	0.85101	2.61309
H	-1.10620	-3.37835	2.22920
H	-1.98656	-1.85013	1.88121
H	-1.50139	-2.88727	0.55828
H	-0.88731	-2.13261	-3.37880
H	-1.37067	-2.51194	-1.70704
H	-1.77666	-0.94181	-2.35858
H	-2.22907	1.82516	-1.67321
H	-1.65564	2.81093	-0.33837
H	-1.39151	3.37816	-2.00981
N	2.17368	0.03182	-0.08120
C	3.36161	0.03745	-0.10472
S	4.98671	0.04319	-0.12851

^{5}FeTMCOHOPr
Charge: 0
Energy: -1493304.9023239

Fe	-0.46839	0.03254	0.02978
O	1.52220	-0.10079	-0.47381
C	2.73668	-0.19861	-0.05106
O	3.09978	-0.22493	1.13574
C	3.78359	-0.27971	-1.17261
O	-2.46128	0.24157	0.20879
H	3.57586	-1.19168	-1.75082
H	3.59231	0.55359	-1.86228
C	5.22769	-0.26987	-0.67602
H	5.93523	-0.34361	-1.51062
H	5.40424	-1.10423	0.00928
H	5.43927	0.64970	-0.12097
N	-0.01766	1.71090	1.48871
N	-0.91692	1.34818	-1.75090
N	-0.72669	-1.67197	-1.46887
N	-0.59398	-1.25543	1.88312
C	-1.12269	2.67809	1.26922
C	-1.15845	3.33094	-0.13168
C	-1.72991	2.50783	-1.30276
C	-1.74823	0.40619	-2.54079
C	-1.09668	-0.97231	-2.72957
C	-1.84908	-2.47055	-0.91937
C	-1.58469	-3.14154	0.44785
C	-1.65314	-2.27970	1.72457
C	-0.98926	-0.21041	2.85941
C	-0.09575	1.03989	2.81347
C	0.27668	1.77622	-2.49059
C	0.45945	-2.50913	-1.71063
C	0.68498	-1.88475	2.25800
C	1.29236	2.37947	1.36745
H	-2.05956	2.13948	1.41627
H	-1.04217	3.48375	2.02224
H	-0.18116	3.75317	-0.38725
H	-1.82583	4.19857	-0.03826
H	-1.89530	3.18893	-2.15720
H	-2.68826	2.10147	-0.98341
H	-2.68023	0.28836	-1.99009
H	-1.96721	0.81896	-3.54231
H	-0.17973	-0.86029	-3.31339
H	-1.77772	-1.59523	-3.33338
H	-2.69559	-1.78901	-0.82026
H	-2.11022	-3.26670	-1.64114
H	-2.37196	-3.89822	0.56755
H	-0.64977	-3.70976	0.42478
H	-1.64124	-2.95692	2.59714
H	-2.61741	-1.76984	1.73584
H	-0.96871	-0.60701	3.89015
H	-2.01513	0.07771	2.63023
H	0.92233	0.75360	3.08392
H	-0.44914	1.74175	3.58762
H	0.00922	2.24755	-3.45241
H	0.84062	2.49279	-1.89130
H	0.93538	0.92405	-2.65485
H	0.24040	-3.33181	-2.41306
H	1.25749	-1.88133	-2.10296
H	0.82403	-2.92757	-0.77271
H	0.62916	-2.32661	3.26810
H	0.91835	-2.67773	1.54491
H	1.50108	-1.16433	2.19382
H	2.08197	1.66378	1.58963
H	1.44325	2.72170	0.34371
H	1.36183	3.24512	2.04847
H	-3.01745	-0.14908	0.89119

^{5}FeTMCPrBr
Charge: 0
Energy: -3035612.4340540

Fe	-0.34287	0.30721	0.27385
N	-1.22479	-0.34168	-1.69314
C	-0.62663	-1.66747	-2.04260
C	-0.86235	-2.82207	-1.05260
C	-0.18173	-2.76060	0.32464
N	-0.67856	-1.70349	1.24950
C	0.12298	-1.68427	2.50488
C	1.37236	-0.81587	2.40070
N	1.05750	0.57082	1.96447
C	2.33474	1.29495	1.71020
C	2.20407	2.57179	0.87270
C	1.96086	2.33319	-0.62230
N	0.57216	1.91861	-0.96870
C	0.55982	1.33057	-2.33398
C	-0.78107	0.68489	-2.68173
C	-2.09377	-1.93253	1.61289
C	0.25607	1.28881	2.98245
C	-0.33172	3.08476	-0.87786
C	-2.71358	-0.41976	-1.71073
C	-3.45849	0.74535	-1.03687
C	-3.22448	0.82815	0.48043
O	-1.99594	1.12828	0.83490
O	-4.13642	0.60665	1.26434
H	0.45163	-1.51836	-2.13785
H	-1.01933	-1.97629	-3.02670
H	-1.92954	-3.04673	-0.95010
H	-0.43275	-3.70388	-1.54469
H	-0.31137	-3.74233	0.81239
H	0.88681	-2.59088	0.17384
H	-0.52644	-1.31157	3.30064
H	0.41747	-2.70585	2.78818
H	1.88246	-0.80400	3.37819
H	2.05670	-1.23062	1.65697
H	2.79668	1.53637	2.68179
H	2.99469	0.60315	1.18209
H	1.45966	3.25523	1.29732
H	3.16393	3.09746	0.95486
H	2.20286	3.24878	-1.18706
H	2.62909	1.53811	-0.95997
H	0.78509	2.10223	-3.08920
H	1.35420	0.58107	-2.36069
H	-1.55601	1.45051	-2.74043
H	-0.70807	0.23519	-3.68323
H	-2.20942	-2.88404	2.15542

H	-2.71726	-1.96546	0.72217
H	-2.45878	-1.10540	2.22203
H	0.76619	1.28237	3.95840
H	-0.73521	0.84540	3.07465
H	0.10501	2.32049	2.66304
H	-0.05438	3.85359	-1.61634
H	-0.27823	3.51148	0.12404
H	-1.36481	2.78039	-1.02876
H	-3.00716	-1.34194	-1.20932
H	-3.04928	-0.51329	-2.75680
H	-3.18455	1.70076	-1.49893
H	-4.52854	0.59647	-1.20646
Br	2.82244	-1.18384	-0.94599

^{5}FeTMCPrCl
Charge: 0
Energy: -1709083.0197022

Fe	-0.16547	0.02393	0.02977
N	1.58492	-1.05552	-0.92039
C	1.84683	-0.33355	-2.20190
C	2.21273	1.16701	-2.09924
C	1.18255	2.20896	-1.60687
N	0.75987	2.08740	-0.18533
C	-0.32810	3.04949	0.16526
C	-1.75031	2.47972	0.07108
N	-1.90088	1.18251	0.77919
C	-3.20461	0.55257	0.43871
C	-3.31260	-0.95173	0.74928
C	-2.58863	-1.91192	-0.21451
N	-1.11756	-2.00568	-0.01304
C	-0.44567	-2.60844	-1.19205
C	1.08485	-2.44394	-1.16789
C	1.89987	2.33778	0.72168
C	-1.77156	1.35287	2.24006
C	-0.83316	-2.77281	1.21242
C	2.84128	-1.12873	-0.12183
C	2.68962	-1.49012	1.36303
C	1.89599	-0.45273	2.17728
O	0.66106	-0.27753	1.79807
O	2.43874	0.14933	3.09841
H	0.94960	-0.43431	-2.81127
H	2.67907	-0.83746	-2.72527
H	3.15599	1.29270	-1.55713
H	2.44375	1.46521	-3.13057
H	1.62985	3.20749	-1.76085
H	0.28413	2.13723	-2.21848
H	-0.14319	3.38510	1.18834
H	-0.26920	3.94410	-0.47209
H	-2.44865	3.22971	0.48106
H	-2.00453	2.30301	-0.97313
H	-4.00768	1.08551	0.97598
H	-3.36213	0.69651	-0.63112
H	-3.03147	-1.15554	1.78812
H	-4.38032	-1.19889	0.68388
H	-3.02714	-2.91916	-0.10938
H	-2.75853	-1.57489	-1.23748
H	-0.66783	-3.68771	-1.26192
H	-0.85025	-2.11555	-2.07486
H	1.49947	-3.08464	-0.38787
H	1.48361	-2.82248	-2.12088
H	2.27153	3.36949	0.61115
H	2.71728	1.65369	0.50535
H	1.60452	2.15261	1.75385
H	-2.52761	2.05860	2.62126
H	-0.76982	1.69573	2.49246
H	-1.89188	0.38824	2.73259
H	-1.25046	-3.79100	1.14328
H	-1.25511	-2.26142	2.07702
H	0.23792	-2.82949	1.38262
H	3.32810	-0.15548	-0.17855
H	3.52723	-1.84489	-0.60592
H	2.22228	-2.47518	1.47596
H	3.69385	-1.56213	1.79081
Cl	-1.37516	0.31184	-2.36605

^{5}FeTMCPrF
Charge: 0
Energy: -1482963.3316854

Fe	-0.22248	0.02837	-0.04483
N	1.55167	-1.22611	-0.75708
C	1.88700	-0.63706	-2.08246
C	2.34477	0.83691	-2.10267
C	1.32135	1.94635	-1.78567
N	0.88137	2.03230	-0.37104
C	-0.18144	3.05352	-0.18856
C	-1.59698	2.54180	-0.46382
N	-1.96172	1.37082	0.36822
C	-3.22334	0.77731	-0.13243
C	-3.47751	-0.68293	0.27927
C	-2.70373	-1.74156	-0.52844
N	-1.30496	-1.96099	-0.09380
C	-0.52944	-2.62653	-1.16551
C	0.98475	-2.59183	-0.92322
C	1.99921	2.36156	0.53153
C	-2.04806	1.70550	1.79844
C	-1.25297	-2.70452	1.17080
C	2.73526	-1.28305	0.13627
C	2.42377	-1.47937	1.63071
C	1.63882	-0.30777	2.25605
O	0.41827	-0.16678	1.82590
O	2.18915	0.41719	3.08183
H	0.98290	-0.71065	-2.68673
H	2.68231	-1.24337	-2.55320
H	3.25497	0.97292	-1.50981
H	2.65800	1.01946	-3.13955
H	1.76714	2.91288	-2.08488
H	0.42929	1.76439	-2.38465
H	-0.11749	3.40570	0.84383
H	0.00664	3.93001	-0.83093
H	-2.30648	3.37342	-0.30548
H	-1.66616	2.21128	-1.49999
H	-4.07376	1.40149	0.19388
H	-3.17672	0.81631	-1.22246
H	-3.32195	-0.81769	1.35507
H	-4.54559	-0.87366	0.11108
H	-3.25201	-2.69975	-0.49444
H	-2.65857	-1.41014	-1.56695
H	-0.83765	-3.68094	-1.28343
H	-0.75747	-2.08863	-2.08495
H	1.21994	-3.16316	-0.02396
H	1.48216	-3.11178	-1.75840
H	2.41303	3.35995	0.30877
H	2.79778	1.62844	0.43715
H	1.66198	2.31534	1.56729
H	-2.74345	2.54351	1.97612
H	-1.05710	1.94066	2.18653
H	-2.39128	0.83180	2.35422
H	-1.65044	-3.72780	1.05523
H	-1.83146	-2.17819	1.93081
H	-0.22989	-2.74347	1.53937
H	3.28249	-0.34590	0.03029
H	3.41615	-2.08145	-0.20820
H	1.87062	-2.41264	1.78852
H	3.37753	-1.57244	2.15844
F	-0.87264	0.13013	-1.87788

^{5}FeTMCPrN_3
Charge: 0
Energy: -1523342.5666565

Fe	0.06008	0.00918	-0.10274
N	-1.52704	-0.99816	1.18251
C	-1.50289	-0.25530	2.47632
C	-1.82385	1.25782	2.42395
C	-0.86266	2.25022	1.73073
N	-0.74210	2.11988	0.25499
C	0.30041	3.02750	-0.30577
C	1.69129	2.39851	-0.47271
N	1.65993	1.10588	-1.20036
C	2.97911	0.42411	-1.12298
C	2.96097	-1.09039	-1.40052
C	2.41041	-2.00787	-0.29000
N	0.92799	-2.06814	-0.20608
C	0.47293	-2.60760	1.09817
C	-1.03122	-2.39746	1.35197
C	-2.02546	2.42597	-0.40929
C	1.25517	1.29118	-2.60741
C	0.39550	-2.85807	-1.32837
C	-2.91268	-1.03107	0.63891
C	-3.05154	-1.40268	-0.84550
C	-2.39009	-0.39095	-1.79977
O	-1.09719	-0.28169	-1.68121
O	-3.08212	0.25272	-2.58323
H	-0.50285	-0.38212	2.89008
H	-2.22918	-0.72127	3.16612
H	-2.84607	1.41921	2.06631
H	-1.84617	1.57282	3.47591
H	-1.21305	3.26973	1.97308
H	0.13645	2.11857	2.14510
H	-0.05542	3.36253	-1.28270
H	0.40071	3.93084	0.31493
H	2.33279	3.12697	-0.99844
H	2.13191	2.21448	0.50585
H	3.66761	0.90159	-1.84094
H	3.39806	0.59337	-0.12976
H	2.46411	-1.29979	-2.35377
H	4.00901	-1.38163	-1.54717
H	2.80011	-3.02746	-0.45353
H	2.80003	-1.67314	0.67214
H	0.68082	-3.68935	1.17378
H	1.04169	-2.09408	1.87194
H	-1.59806	-3.03224	0.66904
H	-1.25911	-2.75879	2.36643
H	-2.32116	3.47413	-0.23763
H	-2.81511	1.77998	-0.03163
H	-1.94866	2.22623	-1.47774

H	1.93236	1.99090	-3.12454
H	0.22670	1.64392	-2.66079
H	1.26865	0.32806	-3.11761
H	0.77681	-3.89262	-1.30084
H	0.67207	-2.39140	-2.27334
H	-0.69032	-2.86794	-1.29965
H	-3.34652	-0.04029	0.77420
H	-3.52081	-1.72059	1.24973
H	-2.64333	-2.40237	-1.03378
H	-4.11969	-1.44289	-1.07808
N	1.28069	0.22751	1.67117
N	2.42299	0.26473	2.03793
N	3.53407	0.29890	2.38666

[5]FeTMCPrNCS
Charge: 0
Energy: -1728455.5304328

Fe	-0.18765	0.05295	0.23252
N	-1.24142	0.60224	-1.70269
C	-0.74221	-0.37665	-2.71221
C	-1.00671	-1.87522	-2.43181
C	-0.32272	-2.60008	-1.25041
N	-0.73181	-2.16153	0.10971
C	0.07557	-2.81842	1.17818
C	1.32221	-2.03938	1.61714
N	1.02895	-0.62815	1.97241
C	2.29201	0.13937	2.13491
C	2.15098	1.67064	2.06418
C	1.95351	2.29035	0.66757
N	0.57656	2.17330	0.11888
C	0.55998	2.39522	-1.34809
C	-0.76635	1.98494	-2.01122
C	-2.15579	-2.46808	0.35710
C	0.20328	-0.54124	3.19278
C	-0.32095	3.11260	0.81289
C	-2.73019	0.59302	-1.67359
C	-3.38670	1.24169	-0.44478
C	-3.07164	0.51936	0.87785
O	-1.81444	0.52827	1.22739
O	-3.97187	-0.02400	1.50936
H	0.33233	-0.22049	-2.79884
H	-1.20053	-0.14158	-3.68927
H	-2.08347	-2.07264	-2.41299
H	-0.64590	-2.39334	-3.33027
H	-0.53982	-3.67778	-1.35917
H	0.75533	-2.46398	-1.32445
H	-0.58206	-2.95326	2.03988
H	0.38727	-3.82587	0.86278
H	1.77472	-2.57069	2.47196
H	2.05072	-2.02496	0.80801
H	2.74921	-0.12915	3.10231
H	2.98226	-0.18312	1.35327
H	1.37710	2.01990	2.75606
H	3.09334	2.07978	2.45048
H	2.23040	3.35742	0.71169
H	2.63893	1.80917	-0.03112
H	0.74290	3.45700	-1.58820
H	1.37510	1.81108	-1.77178
H	-1.54828	2.67817	-1.69780
H	-0.65924	2.11396	-3.09910
H	-2.33526	-3.55559	0.34273
H	-2.78428	-2.00611	-0.40140
H	-2.46500	-2.04775	1.31378
H	0.69708	-1.04149	4.04194
H	-0.77931	-0.97491	3.01330
H	0.02971	0.50612	3.44021
H	0.00284	4.15569	0.66121
H	-0.33704	2.88755	1.87913
H	-1.34111	2.98963	0.45953
H	-3.05759	-0.44567	-1.71635
H	-3.10925	1.07515	-2.59103
H	-3.09570	2.29524	-0.36205
H	-4.46969	1.21783	-0.59635
N	1.62808	-0.38407	-0.90496
C	2.76274	-0.46932	-1.24857
S	4.32868	-0.55635	-1.67016

[5]FeTMCPrOH
Charge: 0
Energy: -1467861.5446027

Fe	-0.23864	0.03570	-0.14449
O	-0.99838	0.16317	-1.99160
N	1.59519	-1.20731	-0.74581
C	2.00495	-0.60159	-2.03780
C	2.41104	0.89292	-2.02798
C	1.37899	2.00405	-1.72173
N	0.86747	2.05346	-0.33315
C	-0.21224	3.06486	-0.16607
C	-1.63029	2.54381	-0.43135
N	-1.96970	1.34668	0.37363
C	-3.22984	0.73837	-0.11687
C	-3.45570	-0.73228	0.28352
C	-2.67346	-1.78414	-0.52910
N	-1.26501	-1.98002	-0.10789
C	-0.47890	-2.64373	-1.17121
C	1.04063	-2.57806	-0.94009
C	1.94195	2.35601	0.62915
C	-2.03710	1.64488	1.81226
C	-1.19499	-2.70397	1.16627
C	2.74329	-1.26034	0.19574
C	2.38396	-1.47124	1.67472
C	1.55350	-0.31913	2.27809
O	0.37462	-0.15792	1.76111
O	2.04237	0.37187	3.17116
H	1.16801	-0.73949	-2.72282
H	2.86076	-1.16794	-2.44997
H	3.29857	1.03290	-1.40339
H	2.75860	1.09500	-3.05053
H	1.85920	2.96905	-1.97054
H	0.51069	1.88000	-2.36889
H	-0.14917	3.43163	0.86108
H	-0.03268	3.93490	-0.81891
H	-2.34049	3.36709	-0.23380
H	-1.71309	2.23684	-1.47387
H	-4.08533	1.34205	0.23500
H	-3.19769	0.79066	-1.20621
H	-3.30116	-0.87174	1.35894
H	-4.52109	-0.93676	0.11288
H	-3.20647	-2.75047	-0.47646
H	-2.64403	-1.45603	-1.56878
H	-0.76046	-3.70773	-1.27390
H	-0.72631	-2.12253	-2.09587
H	1.29370	-3.16338	-0.05488
H	1.54003	-3.07405	-1.78826
H	2.36348	3.36115	0.45619
H	2.74625	1.62719	0.54881
H	1.55923	2.27698	1.64656
H	-2.76245	2.44989	2.02137
H	-1.04918	1.91158	2.18565
H	-2.33003	0.74624	2.35617
H	-1.61482	-3.72101	1.07550
H	-1.74194	-2.15420	1.93254
H	-0.16493	-2.76132	1.50990
H	3.28443	-0.31681	0.11666
H	3.44480	-2.04796	-0.13262
H	1.84636	-2.41723	1.80832
H	3.32028	-1.55004	2.23512
H	-0.52768	0.16833	-2.83227

[6]FeTMCdmaBr
Charge: 2+
Energy: -3047853.4302353

Fe	0.36733	0.03029	0.05335
N	-0.93275	-0.81684	-1.53841
C	-0.46624	-2.22075	-1.84240
H	0.53531	-2.12532	-2.25865
H	-1.11663	-2.63718	-2.62352
C	-0.45605	-3.20915	-0.65694
H	-1.47942	-3.43154	-0.33584
H	-0.10203	-4.15362	-1.08826
C	0.44013	-2.96984	0.57664
H	0.34583	-3.85033	1.22685
H	1.48257	-2.88965	0.27609
N	0.11213	-1.74936	1.39912
C	1.10305	-1.53252	2.52661
H	0.52779	-1.42209	3.44721
H	1.72012	-2.42808	2.64895
C	2.03689	-0.32321	2.35731
H	2.44634	-0.05667	3.34057
H	2.87012	-0.57934	1.70724
N	1.35780	0.87306	1.75593
C	2.39128	1.89233	1.35269
H	2.78592	2.34375	2.27212
H	3.20692	1.34935	0.87282
C	1.90302	3.00325	0.41269
H	1.05126	3.54258	0.83913
H	2.71477	3.73911	0.37766
C	1.63649	2.59401	-1.04365
H	1.58849	3.49363	-1.67073
H	2.46155	1.98104	-1.40792
N	0.36534	1.81698	-1.24908
C	0.33160	1.18028	-2.60295
H	0.15725	1.94311	-3.37397
H	1.30808	0.73934	-2.78732
C	-0.77115	0.11356	-2.72940
H	-1.73103	0.60649	-2.89201
H	-0.57115	-0.48300	-3.62479
C	-1.22677	-1.93224	2.02636
H	-1.20307	-2.77731	2.72512
H	-1.98258	-2.14134	1.27389
H	-1.51536	-1.02752	2.55881
C	0.39071	1.47144	2.71424
H	0.91438	1.82334	3.61103
H	-0.35876	0.73480	2.99662
H	-0.12419	2.30713	2.24222

C	-0.79492	2.73381	-1.08831
H	-0.66930	3.61177	-1.73316
H	-0.88302	3.05236	-0.05116
H	-1.72021	2.23147	-1.36383
C	-2.34893	-0.81359	-1.09108
H	-2.61927	-1.80282	-0.71607
H	-3.02031	-0.61573	-1.93147
C	-2.55077	0.18668	0.04433
O	-1.51795	0.60947	0.64843
N	-3.77079	0.56239	0.39711
C	-3.97727	1.54127	1.47863
H	-4.44111	1.04509	2.33658
H	-4.64523	2.32841	1.11821
H	-3.02342	1.97251	1.77385
C	-4.99952	0.06549	-0.24902
H	-5.31798	0.74979	-1.04217
H	-5.78559	0.01579	0.50709
H	-4.86403	-0.93676	-0.65554
Br	2.51081	-0.78298	-0.96107

^{6}FeTMCdmaCl
Charge: 2+
Energy: -1721328.5416073

Fe	0.54819	0.09058	0.12007
N	-1.05489	0.36017	1.63543
C	-0.82508	1.68234	2.32492
H	0.12576	1.58996	2.84801
H	-1.61267	1.81899	3.07835
C	-0.81199	2.93181	1.41943
H	-1.81140	3.11860	1.01173
H	-0.64471	3.76996	2.10702
C	0.24774	3.10228	0.31060
H	0.11546	4.10475	-0.11915
H	1.24904	3.05075	0.73381
N	0.18290	2.10367	-0.81607
C	1.31651	2.28240	-1.80450
H	0.87934	2.27595	-2.80421
H	1.77166	3.26887	-1.66837
C	2.42032	1.22132	-1.72128
H	3.01865	1.26353	-2.64104
H	3.08079	1.42711	-0.88168
N	1.88542	-0.16892	-1.53357
C	3.01811	-1.09871	-1.18902
H	3.60792	-1.25286	-2.10195
H	3.64986	-0.57727	-0.46809
C	2.61414	-2.46059	-0.60883
H	1.93297	-2.99641	-1.27757
H	3.53060	-3.06192	-0.59777
C	2.09302	-2.44973	0.83549
H	2.12673	-3.46851	1.24293
H	2.74043	-1.82450	1.45155
N	0.68840	-1.93671	0.98718
C	0.37629	-1.64190	2.42101
H	0.25400	-2.57920	2.98081
H	1.22588	-1.10950	2.84240
C	-0.90879	-0.81535	2.58462
H	-1.77483	-1.46311	2.43887
H	-0.95967	-0.45310	3.61643
C	-1.08547	2.29021	-1.57241
H	-1.09778	3.27624	-2.05285
H	-1.94530	2.23054	-0.91043
H	-1.18180	1.51460	-2.33105
C	1.17160	-0.64138	-2.74835
H	1.85404	-0.66605	-3.60636
H	0.33261	0.01653	-2.96748
H	0.77353	-1.64016	-2.57253
C	-0.26302	-2.94103	0.44381
H	-0.07881	-3.91966	0.90319
H	-0.15034	-3.01853	-0.63638
H	-1.28996	-2.64694	0.65118
C	-2.38498	0.30925	0.98109
H	-2.74511	1.32303	0.79513
H	-3.12338	-0.15866	1.63853
C	-2.28625	-0.40925	-0.36427
O	-1.13161	-0.55663	-0.87192
N	-3.37888	-0.82903	-0.98330
C	-3.29164	-1.54081	-2.27042
H	-3.69281	-0.90641	-3.06676
H	-3.88924	-2.45431	-2.20771
H	-2.25520	-1.79117	-2.48517
C	-4.74406	-0.64224	-0.45926
H	-5.07610	-1.54298	0.06713
H	-5.41218	-0.46389	-1.30452
H	-4.80749	0.21969	0.20446
Cl	2.22823	0.82635	1.49527

^{6}FeTMCdmaF
Charge: 2+
Energy: -1495214.3358332

Fe	0.56254	0.08575	0.16668
N	-1.11711	-0.06333	1.62050
C	-0.93710	1.06393	2.59834
H	0.03189	0.89284	3.06844
H	-1.71420	0.98556	3.37056
C	-0.97453	2.48596	2.01142
H	-1.97024	2.72181	1.62055
H	-0.86173	3.15103	2.87618
C	0.11364	2.92321	1.01390
H	0.00259	4.00279	0.84302
H	1.09841	2.74324	1.44482
N	0.08623	2.23457	-0.32336
C	1.23523	2.68207	-1.18853
H	0.88289	2.70180	-2.22134
H	1.51749	3.71000	-0.93221
C	2.45911	1.78362	-1.07276
H	3.21231	2.09719	-1.80753
H	2.89422	1.86550	-0.07645
N	2.12381	0.33469	-1.27586
C	3.34226	-0.48275	-0.95398
H	4.04357	-0.37942	-1.79224
H	3.80286	-0.02592	-0.07545
C	3.09466	-1.96518	-0.66203
H	2.56778	-2.45923	-1.48469
H	4.08309	-2.43789	-0.63268
C	2.43306	-2.24869	0.69184
H	2.60485	-3.29411	0.97985
H	2.88717	-1.61009	1.45216
N	0.95556	-1.99288	0.73363
C	0.49151	-1.95566	2.15693
H	0.52439	-2.96299	2.59333
H	1.18803	-1.32143	2.70460
C	-0.92839	-1.40653	2.28076
H	-1.63424	-2.10337	1.82504
H	-1.19568	-1.33483	3.34134
C	-1.16454	2.54999	-1.05910
H	-1.20086	3.61626	-1.31558
H	-2.04032	2.32091	-0.45726
H	-1.20750	1.95521	-1.97231
C	1.63637	0.05244	-2.65015
H	2.36677	0.38409	-3.39830
H	0.68251	0.55224	-2.81980
H	1.47264	-1.02007	-2.76023
C	0.23357	-3.02523	-0.05072
H	0.47226	-4.02792	0.32514
H	0.51681	-2.95664	-1.10068
H	-0.84133	-2.86795	0.00862
C	-2.41054	-0.03418	0.90752
H	-2.81406	0.98009	0.90544
H	-3.15254	-0.65827	1.41556
C	-2.20354	-0.47368	-0.54748
O	-1.01537	-0.48820	-1.00204
N	-3.23883	-0.80113	-1.30363
C	-3.04656	-1.24971	-2.69424
H	-3.41150	-0.47913	-3.38034
H	-3.62257	-2.16602	-2.84901
H	-1.99174	-1.44008	-2.87916
C	-4.63952	-0.75957	-0.84749
H	-4.97548	-1.76260	-0.56533
H	-5.25729	-0.40225	-1.67447
H	-4.77231	-0.07586	-0.00977
F	1.69245	0.57311	1.48317

^{6}FeTMCdmaN_3
Charge: 2+
Energy: -1535592.2610602

Fe	-0.47385	-0.01770	0.05396
N	0.81143	0.93150	-1.49685
C	0.31122	2.33743	-1.68004
H	-0.70045	2.25236	-2.07714
H	0.91908	2.82939	-2.45199
C	0.31837	3.24195	-0.42903
H	1.34858	3.46749	-0.13426
H	-0.07495	4.20473	-0.77780
C	-0.51419	2.88787	0.82199
H	-0.43109	3.73337	1.51939
H	-1.56702	2.78219	0.56182
N	-0.10722	1.63595	1.54542
C	-1.03636	1.31967	2.69371
H	-0.41825	1.00963	3.53776
H	-1.56228	2.22745	3.01037
C	-2.06883	0.23143	2.39115
H	-2.54296	-0.07820	3.33227
H	-2.84634	0.62172	1.73536
N	-1.47341	-0.95944	1.70226
C	-2.57809	-1.85933	1.22732
H	-3.00083	-2.36683	2.10443
H	-3.35601	-1.21432	0.81263
C	-2.18709	-2.90314	0.17291
H	-1.36387	-3.53551	0.51968
H	-3.04625	-3.57839	0.08634
C	-1.92193	-2.36043	-1.23905
H	-1.97299	-3.18369	-1.96384
H	-2.70331	-1.64385	-1.50050
N	-0.60204	-1.66764	-1.40576
C	-0.56953	-0.88595	-2.67866

H	-0.50220	-1.56150	-3.54278
H	-1.51162	-0.34615	-2.76291
C	0.61460	0.08899	-2.73777
H	1.53393	-0.47530	-2.90250
H	0.49075	0.74205	-3.60868
C	1.25303	1.80239	2.12159
H	1.25017	2.58233	2.89348
H	1.96798	2.09239	1.35586
H	1.58327	0.85996	2.55764
C	-0.54039	-1.69576	2.59172
H	-1.05657	-2.03865	3.49696
H	0.29686	-1.05562	2.86553
H	-0.13508	-2.55620	2.05955
C	0.49206	-2.67143	-1.37781
H	0.30749	-3.45740	-2.12071
H	0.56318	-3.11644	-0.38641
H	1.44881	-2.20088	-1.59500
C	2.23366	0.89155	-1.08616
H	2.51442	1.84112	-0.62642
H	2.88734	0.77001	-1.95515
C	2.44935	-0.21871	-0.05371
O	1.42905	-0.69883	0.52399
N	3.67611	-0.63163	0.23509
C	3.89479	-1.71598	1.20744
H	4.35060	-1.30860	2.11529
H	4.57423	-2.45118	0.76757
H	2.94644	-2.18940	1.45182
C	4.89836	-0.07515	-0.37025
H	5.23712	-0.70815	-1.19698
H	5.67804	-0.05130	0.39435
H	4.74688	0.94441	-0.72377
N	-2.09059	0.71498	-0.58541
N	-2.93925	1.27373	-1.24724
N	-3.74071	1.80476	-1.87587

^{6}FeTMCdmaNCS2
Energy: -1740702.1054242

Fe	0.25550	0.12222	0.11502
N	-0.74134	-1.15029	-1.41008
C	-0.04167	-2.48140	-1.38372
H	0.98797	-2.28416	-1.68240
H	-0.49158	-3.13004	-2.14794
C	-0.06297	-3.24397	-0.04248
H	-1.08076	-3.57406	0.19100
H	0.47968	-4.17596	-0.24280
C	0.59803	-2.65030	1.21945
H	0.56025	-3.41950	2.00363
H	1.64640	-2.42745	1.02567
N	-0.03164	-1.39658	1.75829
C	0.73909	-0.83670	2.92997
H	0.01078	-0.51901	3.67782
H	1.33857	-1.62740	3.39517
C	1.65648	0.33707	2.58133
H	2.00075	0.80555	3.51332
H	2.53373	-0.01674	2.04157
N	0.98807	1.35978	1.71270
C	2.01587	2.33915	1.22215
H	2.28925	2.98983	2.06335
H	2.90255	1.76163	0.95182
C	1.60237	3.20204	0.02297
H	0.68039	3.75591	0.22578
H	2.37849	3.96988	-0.07546
C	1.53780	2.47870	-1.33014
H	1.55544	3.21816	-2.14172
H	2.42042	1.84645	-1.44291
N	0.33214	1.60604	-1.51660
C	0.51821	0.68878	-2.68243
H	0.46302	1.25077	-3.62510
H	1.51663	0.26081	-2.60962
C	-0.53540	-0.42530	-2.72135
H	-1.49634	-0.00206	-3.01869
H	-0.25837	-1.14617	-3.49845
C	-1.40731	-1.68567	2.24205
H	-1.37641	-2.37041	3.09898
H	-2.00447	-2.15248	1.46280
H	-1.89471	-0.75636	2.53622
C	-0.10452	2.06002	2.43377
H	0.28121	2.56093	3.33040
H	-0.88128	1.35019	2.71458
H	-0.55835	2.79975	1.77434
C	-0.87224	2.45515	-1.69857
H	-0.71607	3.16778	-2.51803
H	-1.08613	2.99848	-0.77919
H	-1.74195	1.84242	-1.92664
C	-2.18876	-1.26207	-1.12239
H	-2.38936	-2.18555	-0.57582
H	-2.76783	-1.32590	-2.04870
C	-2.64077	-0.08585	-0.25122
O	-1.75004	0.58891	0.34706
N	-3.93204	0.18462	-0.11699
C	-4.38112	1.32904	0.69389
H	-4.88102	0.96503	1.59687
H	-5.09085	1.91917	0.10758
H	-3.52702	1.94429	0.96801
C	-5.00544	-0.59662	-0.75594
H	-5.30566	-0.13375	-1.70181
H	-5.86576	-0.60770	-0.08348
H	-4.70449	-1.62986	-0.92859
N	2.01704	-0.46228	-0.32186
C	3.13594	-0.79742	-0.62961
S	4.60144	-1.23427	-1.03144

^{6}FeTMCdmaOH2
Energy: -1480123.3707349

Fe	0.60954	0.12248	0.23458
O	1.82686	0.64403	1.48060
N	-1.12811	0.02848	1.63471
C	-0.99759	1.21319	2.54656
H	-0.06237	1.06832	3.08842
H	-1.81169	1.18571	3.28409
C	-1.00538	2.60262	1.87709
H	-1.99249	2.81331	1.45250
H	-0.91518	3.31529	2.70610
C	0.09652	2.99753	0.87214
H	-0.03621	4.06340	0.63870
H	1.08048	2.87180	1.32344
N	0.10956	2.22829	-0.41712
C	1.27147	2.62811	-1.29310
H	0.91073	2.65209	-2.32272
H	1.58959	3.64846	-1.04969
C	2.47655	1.69541	-1.19172
H	3.19460	1.95206	-1.98217
H	2.96625	1.81673	-0.22646
N	2.09498	0.24900	-1.29997
C	3.29166	-0.59496	-0.96788
H	3.98404	-0.54554	-1.81865
H	3.77681	-0.12384	-0.11097
C	3.00208	-2.06096	-0.62450
H	2.44689	-2.56196	-1.42382
H	3.97641	-2.56244	-0.59798
C	2.35589	-2.29696	0.74759
H	2.49397	-3.34459	1.04634
H	2.85177	-1.66533	1.48672
N	0.89110	-1.98052	0.81263
C	0.44001	-1.90143	2.23472
H	0.42175	-2.90182	2.68904
H	1.17433	-1.30258	2.77170
C	-0.95337	-1.27902	2.37054
H	-1.69972	-1.97680	1.98721
H	-1.17783	-1.13591	3.43368
C	-1.12977	2.49254	-1.19188
H	-1.17007	3.54301	-1.50697
H	-2.01539	2.28887	-0.59517
H	-1.15368	1.84842	-2.07097
C	1.56224	-0.08693	-2.64351
H	2.29774	0.14823	-3.42277
H	0.64072	0.46362	-2.82828
H	1.32357	-1.14987	-2.68277
C	0.12029	-3.00156	0.06134
H	0.35370	-4.00726	0.43292
H	0.36187	-2.94134	-0.99911
H	-0.94875	-2.82652	0.16343
C	-2.40436	0.01627	0.88774
H	-2.81526	1.02616	0.83403
H	-3.15459	-0.59051	1.40421
C	-2.16118	-0.47794	-0.54220
O	-0.96884	-0.49321	-0.97001
N	-3.18334	-0.84829	-1.30160
C	-2.96177	-1.35144	-2.66788
H	-3.33791	-0.62267	-3.39262
H	-3.50907	-2.29013	-2.79055
H	-1.89953	-1.51926	-2.83122
C	-4.58980	-0.80828	-0.86560
H	-4.90668	-1.79237	-0.50482
H	-5.20618	-0.53573	-1.72504
H	-4.75127	-0.06052	-0.08938
H	2.03605	0.90446	2.38860

^{1}FeTMCpyBr
Charge: 2+
Energy: -2964629.3174569

Fe	-0.01077	0.19907	-0.07500
N	0.84258	0.37640	1.78168
C	1.93987	-0.57575	2.16248
H	1.45276	-1.52994	2.35669
H	2.37966	-0.21215	3.10101
C	3.06242	-0.76176	1.13739
H	3.71413	-1.53583	1.56047
H	3.70070	0.12751	1.08795
C	2.68986	-1.24633	-0.26732
H	3.61701	-1.45886	-0.81586
H	2.11033	-2.16429	-0.20815
N	1.89471	-0.25843	-1.08889
C	1.53941	-0.85980	-2.43329
H	1.75816	-0.11397	-3.19984

H	2.19066	-1.71411	-2.64241
C	0.09222	-1.30980	-2.56664
H	-0.07260	-2.28448	-2.11487
H	-0.18700	-1.35444	-3.62602
N	-0.85462	-0.37245	-1.88821
C	-2.27177	-0.87703	-1.92138
H	-2.22755	-1.91515	-1.59243
H	-2.55890	-0.85323	-2.97891
C	-3.27361	-0.09920	-1.07652
H	-3.38218	0.94004	-1.40625
H	-4.24734	-0.55867	-1.28327
C	-3.03923	-0.21480	0.42605
H	-2.89249	-1.26459	0.67580
H	-3.92571	0.13906	0.96652
N	-1.84741	0.54393	0.95317
C	-1.59725	0.04665	2.34961
H	-2.36756	0.43839	3.02572
H	-1.68104	-1.03549	2.32860
C	-0.21459	0.43278	2.85972
H	0.06096	-0.25299	3.66385
H	-0.21447	1.43699	3.29105
C	2.80756	0.88552	-1.41425
H	3.65191	0.53133	-2.01679
H	3.21353	1.33763	-0.51398
H	2.27448	1.65132	-1.97795
C	-0.62233	0.95732	-1.89379
H	0.21966	1.34638	-2.44988
H	-0.89512	3.53715	-1.70798
H	-1.48762	1.59524	-1.79847
C	-2.20998	1.98821	1.02364
H	-2.34511	2.39895	0.02405
H	-1.42279	2.55191	1.52487
H	-3.14132	2.12490	1.58547
C	1.31609	1.73965	1.44240
H	2.40278	1.76856	1.29995
H	1.11318	2.48262	2.22856
C	0.61125	2.00113	0.16560
C	0.77062	3.32794	-0.35479
H	1.57643	3.91569	0.09331
C	-0.01858	3.97546	-1.24743
H	0.17601	5.01534	-1.49682
Br	-0.34349	-2.25011	0.46608

^{1}FeTMCpyCl
Charge: 2+
Energy: -1638104.2614973

Fe	-0.04319	0.02701	0.01588
N	0.79575	-1.70521	-0.68143
C	1.94172	-1.59311	-1.64426
H	1.50581	-1.26683	-2.58752
H	2.35506	-2.60134	-1.78184
C	3.07965	-0.65175	-1.24046
H	3.77160	-0.65313	-2.09132
H	3.66590	-1.07627	-0.41779
C	2.74375	0.81812	-0.97151
H	3.68460	1.36779	-0.83525
H	2.21679	1.24622	-1.82095
N	1.89857	1.05726	0.25692
C	1.58819	2.53057	0.39795
H	1.70572	2.79840	1.45000
H	2.32638	3.12261	-0.15270
C	0.19978	2.92265	-0.07212
H	0.13802	2.97942	-1.15620
H	-0.07905	3.89356	0.35394
N	-0.83387	1.92810	0.34981
C	-2.19065	2.26316	-0.20482
H	-2.03606	2.47424	-1.26299
H	-2.48382	3.19045	0.30066
C	-3.26257	1.19484	-0.03446
H	-3.47372	0.97562	1.01810
H	-4.18685	1.64496	-0.41526
C	-3.00840	-0.06343	-0.85718
H	-2.75183	0.23082	-1.87400
H	-3.92272	-0.66785	-0.90184
N	-1.89821	-0.94888	-0.35293
C	-1.58722	-1.92185	-1.45575
H	-2.39859	-2.65540	-1.54393
H	-1.53269	-1.35719	-2.38164
C	-0.26568	-2.63470	-1.22030
H	0.07716	-3.06189	-2.16557
H	-0.38194	-3.46861	-0.52402
C	2.73887	0.73450	1.45527
H	3.59709	1.41459	1.50449
H	3.12646	-0.27882	1.40870
H	2.15456	0.84303	2.36955
C	-0.72823	1.26910	1.52124
H	0.07582	1.51625	2.20097
H	-1.24042	-0.19524	3.62156
H	-1.64945	0.90946	1.95369
C	-2.40320	-1.70605	0.82737
H	-2.59969	-1.03045	1.65908
H	-1.66658	-2.44211	1.14976
H	-3.33239	-2.23233	0.57937
C	1.17578	-2.08998	0.69845
H	2.25531	-1.99951	0.86422
H	0.93673	-3.13580	0.94379
C	0.43208	-1.09042	1.50372
C	0.47516	-1.29542	2.92186
H	1.24172	-1.98927	3.27735
C	-0.39060	-0.82510	3.85364
H	-0.29284	-1.12367	4.89416
Cl	-0.15585	0.73179	-2.23106

^{1}FeTMCpyF
Charge: 2+
Energy: -1411988.6350103

Fe	-0.06233	0.04000	-0.03494
N	0.77131	-1.75281	-0.54356
C	1.79583	-1.70044	-1.63147
H	1.24255	-1.41449	-2.52710
H	2.19219	-2.71469	-1.76919
C	2.96138	-0.73758	-1.42311
H	3.57098	-0.81139	-2.33153
H	3.62408	-1.08394	-0.62255
C	2.60647	0.73940	-1.25990
H	3.52735	1.33566	-1.30693
H	1.94383	1.04252	-2.06874
N	1.90838	1.07234	0.03146
C	1.58650	2.53900	0.05577
H	1.62391	2.88562	1.09133
H	2.35308	3.10500	-0.48583
C	0.23627	2.82694	-0.54519
H	0.21498	2.59866	-1.61034
H	-0.04337	3.87504	-0.39103
N	-0.82324	1.96629	0.05459
C	-2.14845	2.27271	-0.57392
H	-1.94679	2.37903	-1.64080
H	-2.43927	3.25159	-0.17606
C	-3.24736	1.24599	-0.36695
H	-3.51149	1.11551	0.68783
H	-4.14504	1.66804	-0.83302
C	-2.93567	-0.06766	-1.06835
H	-2.55349	0.15158	-2.06577
H	-3.84733	-0.66864	-1.17463
N	-1.90145	-0.91589	-0.38843
C	-1.52968	-1.97810	-1.38162
H	-2.37446	-2.65920	-1.54351
H	-1.29813	-1.46713	-2.31405
C	-0.31118	-2.73061	-0.90559
H	0.04538	-3.40485	-1.68945
H	-0.53773	-3.34979	-0.03569
C	2.85293	0.87134	1.17224
H	3.68014	1.58793	1.10561
H	3.28461	-0.12512	1.16759
H	2.33011	1.02325	2.11842
C	-0.74125	1.45291	1.30316
H	0.06029	1.76396	1.95992
H	-1.27332	0.11369	3.50631
H	-1.67941	1.18257	1.76697
C	-2.50406	-1.53470	0.82364
H	-2.77625	-0.76319	1.54346
H	-1.79297	-2.20527	1.30427
H	-3.40565	-2.10173	0.56228
C	1.23665	-1.96570	0.84516
H	2.31259	-1.79346	0.94857
H	1.07163	-2.99071	1.20969
C	0.45614	-0.91774	1.56249
C	0.51116	-0.96684	2.99169
H	1.30419	-1.57614	3.43303
C	-0.40343	-0.43785	3.84247
H	-0.32919	-0.60763	4.91348
F	-0.11400	0.39576	-1.83842

^{1}FeTMCpyN_3
Charge: 29
Energy: -1452362.9244476

Fe	-0.05486	-0.13638	0.01887
N	0.81723	0.96975	-1.46774
C	2.00601	1.82549	-1.13969
H	1.62653	2.71765	-0.64509
H	2.44791	2.15019	-2.09142
C	3.10291	1.18251	-0.28638
H	3.80139	1.99557	-0.05497
H	3.69673	0.47750	-0.87720
C	2.70573	0.56386	1.05749
H	3.62485	0.31171	1.60322
H	2.13794	1.27251	1.65811
N	1.87752	-0.68975	0.95051
C	1.55060	-1.21565	2.32747
H	1.61646	-2.30547	2.29772
H	2.30664	-0.88331	3.04695
C	0.18430	-0.79747	2.82591
H	0.15996	0.25987	3.08548
H	-0.10275	-1.39457	3.69897
N	-0.86608	-0.97226	1.78233

C	-2.19653	-0.46554	2.24810
H	-1.99498	0.49846	2.71700
H	-2.52056	-1.17078	3.02203
C	-3.26660	-0.30483	1.17723
H	-3.51189	-1.24901	0.67900
H	-4.18107	-0.02685	1.71394
C	-2.96690	0.81988	0.19257
H	-2.65264	1.69783	0.75692
H	-3.87712	1.08499	-0.35954
N	-1.88781	0.52562	-0.81342
C	-1.54765	1.83018	-1.47298
H	-2.34789	2.11587	-2.16743
H	-1.50749	2.59856	-0.70717
C	-0.22306	1.76677	-2.21860
H	0.14241	2.78471	-2.37300
H	-0.35008	1.32601	-3.20991
C	2.71622	-1.76080	0.32606
H	3.57272	-1.99102	0.97079
H	3.10465	-1.45385	-0.64015
H	2.12672	-2.66813	0.18896
C	-0.77919	-1.91318	0.82405
H	0.01177	-2.64916	0.86861
H	-1.33587	-3.54331	-1.14640
H	-1.70881	-2.21509	0.36583
C	-2.43753	-0.39991	-1.84506
H	-2.64225	-1.37798	-1.41215
H	-1.72022	-0.52836	-2.65577
H	-3.36887	-0.00053	-2.26366
C	1.15356	-0.27541	-2.20230
H	2.22845	-0.48710	-2.16296
H	0.91151	-0.22364	-3.27437
C	0.38448	-1.29760	-1.44813
C	0.40006	-2.61146	-2.02037
H	1.16392	-2.78864	-2.78263
C	-0.48591	-3.61758	-1.81359
H	-0.40554	-4.54439	-2.37542
N	-0.12993	1.44429	1.22695
N	-0.01244	2.63249	1.00922
N	0.08304	3.77273	0.86131

[1]FeTMCpyNCS
Charge: 2+
Energy: -1657474.1461007

Fe	-0.32733	0.07015	0.03995
N	0.13834	-0.81115	-1.74279
C	1.01517	-2.02678	-1.71087
H	2.02221	-1.67269	-1.49060
H	1.02553	-2.45063	-2.72397
C	0.61764	-3.13239	-0.72970
H	1.42292	-3.87444	-0.78782
H	-0.26891	-3.66808	-1.08596
C	0.47592	-2.77302	0.75189
H	0.33467	-3.70254	1.31951
H	1.37969	-2.28782	1.11372
N	-0.68307	-1.86336	1.07071
C	-0.70162	-1.55102	2.54556
H	-1.74322	-1.51914	2.87293
H	-0.22892	-2.36279	3.10931
C	-0.01534	-0.24892	2.89300
H	1.06522	-0.32186	2.78328
H	-0.25457	0.04470	3.92154
N	-0.43740	0.86051	1.98805
C	0.31907	2.12219	2.27807
H	1.36168	1.82133	2.38891
H	-0.05114	2.46218	3.25210
C	0.20853	3.22910	1.23957
H	-0.82160	3.57424	1.09974
H	0.73539	4.08908	1.66914
C	0.90004	2.89028	-0.07559
H	1.88909	2.48798	0.14280
H	1.03600	3.80214	-0.67015
N	0.18504	1.88406	-0.93493
C	1.15796	1.46070	-1.99831
H	1.29669	2.27415	-2.72170
H	2.11766	1.27520	-1.52376
C	0.68377	0.20927	-2.71172
H	1.51870	-0.22593	-3.26666
H	-0.09219	0.44328	-3.44355
C	-1.95504	-2.61475	0.82867
H	-2.02907	-3.45954	1.52352
H	-1.99775	-3.01562	-0.17950
H	-2.81368	-1.95896	0.97968
C	-1.65382	0.89509	1.41315
H	-2.39773	0.16097	1.69097
H	-3.78663	1.64589	0.10299
H	-2.00772	1.86582	1.09969
C	-0.97798	2.55538	-1.58263
H	-1.71959	2.83695	-0.83604
H	-1.45330	1.88465	-2.29780
H	-0.65497	3.45925	-2.11246
C	-1.29811	-1.06872	-2.00961
H	-1.54926	-2.12674	-1.87789
H	-1.59998	-0.82807	-3.03992
C	-1.94483	-0.23484	-0.96232
C	-3.36712	-0.11441	-1.06716
H	-3.85739	-0.82315	-1.74019
C	-4.15989	0.84015	-0.51707
H	-5.22429	0.86448	-0.73511
N	1.54167	-0.04643	0.53216
C	2.71667	-0.14525	0.32420
S	4.28244	-0.27726	0.03610

[1]FeTMCpyOH
Charge: 2+
Energy: -1396893.6677006

Fe	-0.06153	0.05465	-0.06552
N	0.79281	-1.76236	-0.51671
C	1.87751	-1.74266	-1.54598
H	1.37766	-1.48455	-2.47960
H	2.28124	-2.76067	-1.62550
C	3.03094	-0.77110	-1.29817
H	3.68945	-0.87121	-2.16925
H	3.64902	-1.09593	-0.45363
C	2.67959	0.71392	-1.19627
H	3.60857	1.29959	-1.19788
H	2.06946	1.00138	-2.05044
N	1.90464	1.08994	0.03835
C	1.57794	2.55744	0.00118
H	1.61988	2.94582	1.02138
H	2.34178	3.10141	-0.56558
C	0.22186	2.83785	-0.60183
H	0.22153	2.63524	-1.67154
H	-0.06804	3.88019	-0.42661
N	-0.82922	1.95170	-0.02025
C	-2.17507	2.25756	-0.60181
H	-2.02032	2.39747	-1.67483
H	-2.46787	3.22830	-0.18587
C	-3.26434	1.22086	-0.36593
H	-3.50283	1.10759	0.69648
H	-4.17466	1.63222	-0.81701
C	-2.98163	-0.11770	-1.03772
H	-2.68892	0.05643	-2.07571
H	-3.89730	-0.72121	-1.06786
N	-1.90335	-0.93611	-0.39003
C	-1.52559	-2.01236	-1.36674
H	-2.35901	-2.71480	-1.49577
H	-1.31592	-1.52458	-2.31540
C	-0.28054	-2.73986	-0.90610
H	0.08273	-3.38337	-1.71205
H	-0.49196	-3.39247	-0.05637
C	2.78425	0.92251	1.23498
H	3.61974	1.63125	1.19038
H	3.20701	-0.07670	1.28394
H	2.21499	1.10633	2.14784
C	-0.73138	1.45324	1.24466
H	0.05337	1.81187	1.89738
H	-1.30591	0.24280	3.49342
H	-1.66776	1.19547	1.71847
C	-2.46829	-1.55258	0.84335
H	-2.73107	-0.77928	1.56440
H	-1.73737	-2.21166	1.30882
H	-3.36778	-2.13454	0.60869
C	1.20273	-1.95238	0.89107
H	2.27716	-1.78887	1.02556
H	1.01676	-2.96841	1.27226
C	0.41564	-0.88527	1.56638
C	0.43616	-0.91772	2.99809
H	1.20180	-1.54843	3.45778
C	-0.46052	-0.34089	3.83661
H	-0.39407	-0.49749	4.91007
O	0.02846	0.32000	-1.93372
H	-0.75907	0.71257	-2.33685

[6]FeTPOBzOH
Charge: 0
Energy: -2415732.0616617

C	-5.45255	-1.53852	0.76222
C	-4.95990	-0.31826	0.28342
C	-5.80502	0.79409	0.17723
C	-7.14111	0.68534	0.55559
C	-7.63109	-0.53019	1.04447
C	-6.78811	-1.64122	1.14579
C	-3.53395	-0.19903	-0.07950
O	-2.75904	-1.20510	-0.07345
Fe	-1.23478	0.08528	-0.84535
O	-3.03668	0.94117	-0.41046
N	0.20389	1.69929	-1.03247
N	1.48278	1.41430	-0.65475
C	2.26345	2.52222	-0.78701
C	1.45463	3.54408	-1.27030
C	0.16384	2.99812	-1.39842
C	3.70512	2.56284	-0.47298
C	4.19812	2.17436	0.78321
C	5.56634	2.20014	1.04479
C	6.46063	2.63736	0.06407

C	5.97823	3.05308	-1.17955
C	4.60861	3.01402	-1.44773
B	1.84190	0.04200	-0.04312
N	1.51778	-1.13368	-1.00368
N	0.21915	-1.52763	-1.15731
C	0.22535	-2.78463	-1.64615
C	1.56133	-3.19691	-1.81937
C	2.35543	-2.13258	-1.40819
C	-1.06306	3.71802	-1.78526
C	-2.10311	3.10535	-2.50082
C	-3.24581	3.83245	-2.83428
C	-3.36692	5.17481	-2.46993
C	-2.33257	5.79343	-1.76269
C	-1.19077	5.07086	-1.42230
C	3.82212	-2.03621	-1.37656
C	4.49393	-0.84364	-1.69176
C	5.88248	-0.76906	-1.60611
C	6.62460	-1.89094	-1.22913
C	5.96912	-3.09127	-0.94125
C	4.57793	-3.16273	-1.01036
C	-0.97608	-3.60211	-1.89955
C	-2.18118	-3.06607	-2.37845
C	-3.28034	-3.89584	-2.59742
C	-3.19699	-5.26745	-2.35099
C	-1.99929	-5.81102	-1.87994
C	-0.89934	-4.98539	-1.65652
O	-1.58801	0.02641	-2.66981
N	-0.33555	0.06606	1.21245
N	1.01026	-0.13950	1.24636
C	1.41855	-0.38784	2.52160
C	0.28882	-0.33446	3.33299
C	-0.78646	-0.04313	2.47542
C	-2.18761	0.20094	2.86281
C	-2.81343	1.41088	2.52864
C	-4.11840	1.66542	2.94908
C	-4.81266	0.71748	3.70341
C	-4.19478	-0.48892	4.04019
C	-2.88669	-0.74370	3.62837
C	2.82690	-0.60306	2.89588
C	3.37559	0.12151	3.96631
C	4.72118	-0.02748	4.30613
C	5.53619	-0.89801	3.57745
C	4.99440	-1.63442	2.52053
C	3.64787	-1.49763	2.19096
H	2.99258	0.01849	0.21172
H	-2.01715	2.06363	-2.79047
H	-4.04409	3.34185	-3.38498
H	-4.26000	5.73593	-2.73286
H	-2.41774	6.83636	-1.46873
H	-0.40015	5.54905	-0.85061
H	1.76015	4.55616	-1.48905
H	-2.25585	-2.00398	-2.57816
H	-4.20734	-3.46260	-2.96373
H	-4.05780	-5.90857	-2.52258
H	-1.92304	-6.87639	-1.67872
H	0.02206	-5.40891	-1.26632
H	1.90164	-4.12864	-2.24566
H	-2.27765	2.13697	1.92663
H	-4.59754	2.60082	2.67458
H	-5.83632	0.91043	4.01160
H	-4.73444	-1.23553	4.61646
H	-2.40422	-1.68424	3.87946
H	0.24890	-0.47344	4.40319
H	-5.39594	1.72843	-0.19275
H	-4.77583	-2.38326	0.83433
H	-7.80039	1.54528	0.47481
H	-7.17296	-2.58390	1.52503
H	-8.67276	-0.61216	1.34445
H	4.23132	3.31724	-2.42053
H	6.66718	3.40101	-1.94474
H	7.52786	2.65644	0.26839
H	5.92679	1.86984	2.01462
H	3.51174	1.84277	1.55418
H	2.74625	0.81924	4.51187
H	5.13430	0.54466	5.13263
H	6.58708	-1.00346	3.83371
H	5.61714	-2.30906	1.94049
H	3.23175	-2.07860	1.37603
H	4.06526	-4.08620	-0.75552
H	6.53957	-3.97001	-0.65205
H	7.70750	-1.83132	-1.16100
H	6.37751	0.17208	-1.82476
H	3.92766	0.03009	-1.99490
H	-0.83788	-0.26589	-3.21394

^{6}Fetmg3trenBr
Charge: 2+
Energy: -3272364.0890063

Fe	0.00069	0.00053	0.40705
N	0.00099	0.00072	2.71172
C	1.42040	0.10128	3.12866
C	2.30123	-0.64872	2.13534
N	2.01086	-0.13271	0.78805
C	3.04519	0.07088	-0.05602
N	4.17589	-0.68501	-0.02586
C	4.18434	-2.11045	0.30331
C	5.50158	-0.12392	-0.32042
N	3.00087	1.09164	-0.94295
C	3.54803	0.98749	-2.29922
C	2.29634	2.33376	-0.65581
C	-0.79598	1.17963	3.12863
C	-0.58720	2.31725	2.13501
N	-0.88998	1.80740	0.78817
C	-1.58432	2.60055	-0.05592
N	-1.49586	3.95776	-0.02630
C	-0.26565	4.67860	0.30144
C	-2.64527	4.82449	-0.32072
N	-2.44638	2.05077	-0.94204
C	-2.63251	2.57695	-2.29790
C	-3.16859	0.81902	-0.65422
C	-0.62154	-1.27902	3.12832
C	-1.71190	-1.66611	2.13523
N	-1.11998	-1.67384	0.78797
C	-1.46117	-2.67164	-0.05562
N	-2.68088	-3.27340	-0.02433
C	-3.91989	-2.56853	0.30504
C	-2.85735	-4.70222	-0.31834
N	-0.55565	-3.14366	-0.94321
C	-0.92055	-3.56659	-2.29886
C	0.87258	-3.15360	-0.65751
H	1.55259	-0.27959	4.15034
H	1.70585	1.15576	3.12465
H	3.35278	-0.49637	2.39983
H	2.10708	-1.72679	2.19996
H	3.16967	-2.49612	0.33904
H	4.67746	-2.29479	1.26452
H	4.73367	-2.65071	-0.47528
H	5.46396	0.96497	-0.29150
H	5.87233	-0.44955	-1.29827
H	6.20024	-0.47060	0.44785
H	3.83234	-0.04294	-2.51083
H	4.41493	1.64299	-2.43447
H	2.76427	1.27678	-3.00619
H	2.04647	2.36459	0.40453
H	1.37757	2.40674	-1.24576
H	2.94933	3.17905	-0.90102
H	-0.53236	1.48472	4.15029
H	-1.85187	0.89937	3.12460
H	-1.24420	3.15222	2.39972
H	0.44385	2.68730	2.19860
H	0.57593	3.99302	0.33714
H	-0.35211	5.19857	1.26228
H	-0.07324	5.42390	-0.47790
H	-3.56911	4.24692	-0.29085
H	-2.54957	5.30787	-1.29891
H	-2.69429	5.60334	0.44709
H	-1.88476	3.34068	-2.51007
H	-3.63495	2.99733	-2.43165
H	-2.48984	1.75427	-3.00544
H	-3.06735	0.58625	0.40561
H	-2.77370	-0.01248	-1.24599
H	-4.22786	0.96166	-0.89648
H	-1.01696	-1.20366	4.15026
H	0.14887	-2.05359	3.12347
H	-2.10726	-2.65219	2.40019
H	-2.54721	-0.95744	2.19932
H	-3.74708	-1.49690	0.34123
H	-4.32604	-2.90392	1.26608
H	-4.66235	-2.77412	-0.47364
H	-1.89536	-5.21378	-0.28918
H	-3.32472	-4.86110	-1.29609
H	-3.50676	-5.13378	0.45013
H	-1.95579	-3.29941	-2.50939
H	-0.78487	-4.64496	-2.43368
H	-0.27974	-3.03188	-3.00682
H	1.02481	-2.94985	0.40217
H	1.39441	-2.39561	-1.24963
H	1.27823	-4.14222	-0.90072
Br	0.00027	-0.00001	-2.07295

^{6}Fetmg3trenCl
Charge: 2+
Energy: -1945836.6584505

Fe	0.00012	-0.00024	0.28827
N	0.00055	-0.00012	2.59498
C	1.42072	-0.09208	3.01224
C	2.19074	-0.96398	2.02594
N	1.96431	-0.42928	0.67501
C	2.99524	-0.40143	-0.19452
N	4.00162	-1.31622	-0.17263
C	3.80865	-2.71877	0.19673
C	5.38528	-0.96645	-0.52192
N	3.07851	0.59693	-1.10489
C	3.54473	0.37807	-2.47717
C	2.56913	1.93399	-0.83107
C	-0.62975	1.27577	3.01252

C	-0.26027	2.37862	2.02600
N	-0.61047	1.91536	0.67511
C	-1.15023	2.79452	-0.19409
N	-0.86122	4.12350	-0.17197
C	0.45002	4.65772	0.19697
C	-1.85606	5.14687	-0.52107
N	-2.05646	2.36776	-1.10464
C	-2.09943	2.88090	-2.47695
C	-2.95940	1.25773	-0.83133
C	-0.78904	-1.18399	3.01256
C	-1.92932	-1.41507	2.02647
N	-1.35350	-1.48653	0.67534
C	-1.84538	-2.39314	-0.19404
N	-3.14089	-2.80703	-0.17184
C	-4.25880	-1.93857	0.19808
C	-3.53021	-4.17993	-0.52175
N	-1.02296	-2.96462	-1.10484
C	-1.44622	-3.25796	-2.47711
C	0.38978	-3.19226	-0.83182
H	1.50032	-0.47923	4.03700
H	1.84766	0.91341	2.99980
H	3.25483	-0.94953	2.28456
H	1.85524	-2.00576	2.10424
H	2.74942	-2.95185	0.25888
H	4.28841	-2.94892	1.15475
H	4.25809	-3.35294	-0.57498
H	5.50933	0.11638	-0.52661
H	5.67119	-1.36961	-1.49941
H	6.05010	-1.39250	0.23634
H	3.68106	-0.68720	-2.66201
H	4.48436	0.90615	-2.67124
H	2.77523	0.74820	-3.16215
H	2.37498	2.02829	0.23731
H	1.64353	2.12136	-1.38372
H	3.32330	2.67049	-1.13031
H	-0.33373	1.53836	4.03710
H	-1.71400	1.14275	3.00076
H	-0.80476	3.29286	2.28490
H	0.80970	2.60898	2.10389
H	1.18156	3.85700	0.25904
H	0.40969	5.18845	1.15490
H	0.77425	5.36391	-0.57497
H	-2.85579	4.71279	-0.52598
H	-1.64983	5.59633	-1.49843
H	-1.81964	5.93544	0.23742
H	-1.24496	3.53161	-2.66138
H	-3.02651	3.43052	-2.67152
H	-2.03478	2.02940	-3.16187
H	-2.94413	1.04207	0.23698
H	-2.65843	0.36275	-1.38422
H	-3.97433	1.54239	-1.13073
H	-1.16392	-1.05921	4.03737
H	-0.13162	-2.05639	3.00011
H	-2.44877	-2.34379	2.28535
H	-2.66376	-0.60363	2.10485
H	-3.93076	-0.90485	0.26095
H	-4.69810	-2.23952	1.15588
H	-5.03271	-2.00999	-0.57372
H	-2.65460	-4.82892	-0.52728
H	-4.02278	-4.22525	-1.49905
H	-4.23129	-4.54298	0.23663
H	-2.43674	-2.84266	-2.66136
H	-1.45935	-4.33561	-2.67185
H	-0.74093	-2.77654	-3.16203
H	0.56919	-3.07235	0.23657
H	1.01447	-2.48375	-1.38416
H	0.65040	-4.21333	-1.13222
Cl	-0.00006	0.00006	-1.99676

^{6}Fetmg3trenF
Charge: 2+
Energy: -1719713.7378248

Fe	0.00018	0.00028	0.30556
N	-0.00054	0.00003	2.58663
C	1.31576	-0.54580	3.00156
C	1.73992	-1.66543	2.05343
N	1.63610	-1.16622	0.67518
C	2.48694	-1.62234	-0.26118
N	3.04214	-2.86384	-0.21124
C	2.33183	-4.03311	0.30827
C	4.40877	-3.13180	-0.67822
N	2.84581	-0.81695	-1.29131
C	3.02116	-1.32120	-2.65532
C	2.89125	0.63518	-1.16457
C	-0.18593	1.41281	3.00199
C	0.57191	2.34004	2.05421
N	0.19181	2.00011	0.67606
C	0.16143	2.96423	-0.26108
N	0.95933	4.06564	-0.21235
C	2.32677	4.03539	0.30808
C	0.50869	5.38261	-0.68139
N	-0.71520	2.87099	-1.29131
C	-0.36545	3.27221	-2.65596
C	-1.99608	2.18553	-1.16374
C	-1.13162	-0.86693	3.00113
C	-2.31298	-0.67407	2.05262
N	-1.82828	-0.83322	0.67450
C	-2.64847	-1.34180	-0.26210
N	-4.00134	-1.20305	-0.21169
C	-4.65981	-0.00422	0.30880
C	-4.91582	-2.25302	-0.67949
N	-2.13010	-2.05394	-1.29300
C	-2.65465	-1.95239	-2.65684
C	-0.89495	-2.81890	-1.16700
H	1.28352	-0.89816	4.04141
H	2.05025	0.26069	2.94371
H	2.76683	-1.96853	2.28671
H	1.10483	-2.54557	2.20984
H	1.26598	-3.82525	0.38353
H	2.71441	-4.33810	1.28892
H	2.47042	-4.86571	-0.38931
H	4.94578	-2.19434	-0.82308
H	4.41338	-3.70149	-1.61399
H	4.92740	-3.71846	0.08701
H	2.74318	-2.37378	-2.70742
H	4.05427	-1.20228	-2.99880
H	2.35763	-0.75496	-3.31810
H	2.84824	0.90012	-0.10853
H	2.04268	1.09133	-1.68216
H	3.82828	1.00282	-1.59707
H	0.13517	1.56076	4.04194
H	-1.25154	1.64587	2.94410
H	0.32085	3.38094	2.28720
H	1.65163	2.22997	2.21099
H	2.67907	3.00836	0.38555
H	2.39923	4.52100	1.28788
H	2.97926	4.57007	-0.39008
H	-0.57155	5.37881	-0.82723
H	1.00061	5.67015	-1.61712
H	0.75685	6.12610	0.08306
H	0.68524	3.55721	-2.70823
H	-0.98447	4.10707	-3.00128
H	-0.52420	2.41325	-3.31715
H	-2.20473	2.01841	-0.10741
H	-1.96722	1.22126	-1.67890
H	-2.78223	2.81279	-1.59815
H	-1.42099	-0.66293	4.04091
H	-0.80057	-1.90625	2.94333
H	-3.08907	-1.41188	2.28532
H	-2.75775	0.31597	2.20926
H	-3.94765	0.81552	0.38488
H	-5.11517	-0.18429	1.28926
H	-5.45035	0.29200	-0.38858
H	-4.37165	-3.18629	-0.82473
H	-5.41152	-1.97204	-1.61522
H	-5.68326	-2.40988	0.08547
H	-3.42736	-1.18541	-2.70802
H	-3.06823	-2.90621	-3.00124
H	-1.83265	-1.66017	-3.31949
H	-0.64502	-2.91652	-0.11092
H	-0.07544	-2.31032	-1.68253
H	-1.04410	-3.81329	-1.60193
F	0.00078	0.00287	-1.49529

^{6}Fetmg3trenN_3
Charge: 2+
Energy: -1760096.9219138

Fe	-0.02015	-0.08324	0.36454
N	-0.03688	-0.17047	2.65492
C	-0.61202	1.11464	3.12022
C	-0.17567	2.24646	2.19414
N	-0.51782	1.87061	0.81433
C	-0.99691	2.81958	-0.00931
N	-0.66300	4.13494	0.10774
C	0.66746	4.58586	0.51637
C	-1.62891	5.21618	-0.12876
N	-1.87699	2.48089	-0.98676
C	-1.94193	3.17570	-2.27688
C	-2.82524	1.38568	-0.82108
C	-0.88186	-1.33340	3.02486
C	-2.03573	-1.47625	2.03635
N	-1.47137	-1.49823	0.68030
C	-2.01947	-2.29899	-0.24847
N	-3.33574	-2.64482	-0.25016
C	-4.39979	-1.74797	0.20165
C	-3.79903	-3.96594	-0.69536
N	-1.23492	-2.82824	-1.22193
C	-1.69118	-2.98183	-2.60455
C	0.16697	-3.15104	-0.99161
C	1.37249	-0.34697	3.08352
C	2.11515	-1.21971	2.07521
N	1.92883	-0.63010	0.74165
C	2.96808	-0.62133	-0.11085
N	3.92652	-1.58761	-0.11332
C	3.64132	-2.99035	0.18967
C	5.34154	-1.29327	-0.37593

N	3.10047	0.39926	-0.99755
C	3.67702	0.22238	-2.33448
C	2.69532	1.76022	-0.66618
H	-0.32457	1.31793	4.16080
H	-1.70105	1.03409	3.08372
H	-0.68406	3.16928	2.49344
H	0.90175	2.42549	2.30188
H	1.37065	3.75691	0.49006
H	0.65596	5.02004	1.52265
H	1.01072	5.35303	-0.18601
H	-2.64245	4.81609	-0.15975
H	-1.41975	5.75323	-1.06020
H	-1.56259	5.92567	0.70254
H	-1.04321	3.77366	-2.42706
H	-2.82566	3.81888	-2.34828
H	-1.98933	2.42789	-3.07382
H	-2.82717	1.07369	0.22293
H	-2.55352	0.52666	-1.44318
H	-3.82641	1.73106	-1.10244
H	-1.24817	-1.23652	4.05586
H	-0.26428	-2.23303	2.97239
H	-2.58535	-2.39857	2.25403
H	-2.74173	-0.64542	2.16187
H	-4.02219	-0.73310	0.30061
H	-4.82289	-2.07315	1.15886
H	-5.20029	-1.74684	-0.54578
H	-2.95735	-4.65496	-0.76573
H	-4.30743	-3.91233	-1.66426
H	-4.50617	-4.35233	0.04576
H	-2.65875	-2.49763	-2.73778
H	-1.77215	-4.03629	-2.88995
H	-0.96641	-2.49417	-3.26586
H	0.36317	-3.14016	0.08066
H	0.82513	-2.42562	-1.48082
H	0.37381	-4.15099	-1.38938
H	1.42253	-0.77266	4.09493
H	1.84755	0.63649	3.11088
H	3.17500	-1.26231	2.34856
H	1.73274	-2.24771	2.11288
H	2.56852	-3.16769	0.17290
H	4.04274	-3.28264	1.16673
H	4.10861	-3.61819	-0.57642
H	5.52063	-0.21966	-0.31637
H	5.65900	-1.66249	-1.35706
H	5.94503	-1.78761	0.39224
H	3.71409	-0.83775	-2.58682
H	4.68452	0.64693	-2.40462
H	3.03484	0.73040	-3.06021
H	2.40981	1.80018	0.38420
H	1.84985	2.08913	-1.27821
H	3.53576	2.44129	-0.84454
N	-0.00050	-0.00332	-1.53143
N	0.22508	0.59085	-2.55634
N	0.44186	1.15596	-3.53804

^{6}Fetmg3trenNCS
Charge: 2+
Energy: -1965206.9082832

Fe	-0.00031	-0.00025	-0.52638
N	-0.00104	-0.00011	-2.81434
C	-1.41729	0.13690	-3.23640
C	-2.32368	-0.61280	-2.26413
N	-2.01401	-0.14915	-0.90428
C	-3.01893	-0.00031	-0.02230
N	-4.15032	-0.75609	-0.05865
C	-4.15851	-2.16256	-0.46194
C	-5.47013	-0.21132	0.28673
N	-2.93720	0.95938	0.93285
C	-3.47232	0.77816	2.28548
C	-2.23609	2.21646	0.70426
C	0.82539	1.15780	-3.23723
C	0.62982	2.31779	-2.26515
N	0.87740	1.81781	-0.90547
C	1.50918	2.61355	-0.02360
N	1.42040	3.97129	-0.05955
C	0.20643	4.68168	-0.46256
C	2.55221	4.84175	0.28579
N	2.29983	2.06278	0.93115
C	2.41162	2.61703	2.28362
C	3.03780	0.82703	0.70221
C	0.58836	-1.29491	-3.23702
C	1.69149	-1.70496	-2.26547
N	1.13573	-1.66880	-0.90539
C	1.50975	-2.61327	-0.02328
N	2.73020	-3.21478	-0.05974
C	3.95187	-2.51806	-0.46335
C	2.91887	-4.63015	0.28534
N	0.63815	-3.02247	0.93217
C	1.06321	-3.39568	2.28451
C	-0.80112	-3.04436	0.70414
H	-1.55346	-0.21996	-4.26622
H	-1.67930	1.19722	-3.21202
H	-3.36999	-0.41713	-2.52275
H	-2.16634	-1.69442	-2.36206
H	-3.14360	-2.55167	-0.49441
H	-4.63171	-2.29919	-1.44099
H	-4.72543	-2.73776	0.27782
H	-5.43178	0.87770	0.31494
H	-5.82597	-0.58844	1.25164
H	-6.18205	-0.51461	-0.48774
H	-3.73893	-0.26656	2.44628
H	-4.35055	1.40857	2.46212
H	-2.69441	1.04808	3.00660
H	-2.02364	2.31603	-0.36003
H	-1.29337	2.25175	1.25917
H	-2.87385	3.04645	1.02860
H	0.58383	1.45379	-4.26701
H	1.87466	0.85461	-3.21336
H	1.32228	3.12603	-2.52436
H	-0.38560	2.72235	-2.36251
H	-0.63795	3.99723	-0.49485
H	0.32448	5.15982	-1.44162
H	-0.00807	5.46021	0.27729
H	3.47604	4.26384	0.31396
H	2.40368	5.33851	1.25071
H	2.64562	5.60991	-0.48870
H	1.64037	3.37035	2.44496
H	3.39686	3.06240	2.45927
H	2.25707	1.80852	3.00504
H	3.01666	0.59288	-0.36196
H	2.59762	-0.00684	1.25790
H	4.07581	0.96451	1.02542
H	0.96474	-1.23427	-4.26711
H	-0.19879	-2.05202	-3.21210
H	2.04530	-2.70877	-2.52451
H	2.54932	-1.02763	-2.36361
H	3.78059	-1.44471	-0.49600
H	4.30684	-2.85950	-1.44240
H	4.73370	-2.72079	0.27633
H	1.95670	-5.14163	0.31404
H	3.42397	-4.74980	1.24993
H	3.53713	-5.09484	-0.48956
H	2.10137	-3.10437	2.44489
H	0.95639	-4.47152	2.46079
H	0.44088	-2.85717	3.00612
H	-0.99405	-2.90925	-0.35990
H	-1.30317	-2.24633	1.26002
H	-1.20049	-4.01214	1.02778
N	-0.00002	0.00029	1.39091
C	0.00038	0.00019	2.59070
S	0.00156	0.00039	4.18502

^{6}Fetmg3trenOH
Charge: 2+
Energy: -1704622.2733106

Fe	-0.03405	-0.00034	0.23342
N	-0.01569	-0.03406	2.54936
C	-0.20920	1.37125	2.98342
C	0.50125	2.32167	2.02314
N	0.06832	2.00531	0.65594
C	-0.07410	2.99431	-0.24079
N	0.64089	4.15317	-0.19106
C	2.02809	4.21813	0.26781
C	0.07100	5.44325	-0.59998
N	-0.99368	2.87493	-1.23072
C	-0.73142	3.31962	-2.60060
C	-2.21065	2.09107	-1.06366
C	-1.14159	-0.90614	2.96333
C	-2.31582	-0.73108	2.00301
N	-1.81760	-0.93380	0.63638
C	-2.59878	-1.54759	-0.26634
N	-3.95774	-1.48036	-0.24143
C	-4.68939	-0.29686	0.21091
C	-4.80834	-2.60032	-0.66436
N	-2.03131	-2.30987	-1.23634
C	-2.51592	-2.30934	-2.61747
C	-0.78128	-3.02251	-1.01995
C	1.29975	-0.57869	2.95792
C	1.74605	-1.65857	1.97466
N	1.69541	-1.09514	0.61793
C	2.65015	-1.42965	-0.25886
N	3.30972	-2.62029	-0.22515
C	2.66160	-3.87106	0.17223
C	4.74213	-2.73702	-0.52915
N	3.00236	-0.54142	-1.23291
C	3.46207	-0.95707	-2.56080
C	2.98081	0.90069	-1.00073
H	0.14070	1.51485	4.01490
H	-1.27935	1.58941	2.96154
H	0.25318	3.35520	2.28933
H	1.58827	2.21631	2.13182
H	2.45471	3.21917	0.32611
H	2.10916	4.70466	1.24656
H	2.61142	4.79957	-0.45430
H	-1.01111	5.35959	-0.70043
H	0.49697	5.79319	-1.54693

H	0.29584	6.18357	0.17487
H	0.28823	3.69486	-2.68748
H	-1.43152	4.10354	-2.90881
H	-0.84211	2.45814	-3.26845
H	-2.37603	1.91628	-0.00056
H	-2.12971	1.12971	-1.58038
H	-3.05554	2.65530	-1.47411
H	-1.43995	-0.69631	3.99971
H	-0.80442	-1.94432	2.91665
H	-3.09837	-1.45631	2.25221
H	-2.75411	0.26732	2.12524
H	-4.02020	0.55781	0.27874
H	-5.16614	-0.46399	1.18345
H	-5.47090	-0.06532	-0.52053
H	-4.21448	-3.51011	-0.75164
H	-5.30165	-2.39554	-1.62096
H	-5.58017	-2.75613	0.09643
H	-3.32888	-1.59262	-2.73130
H	-2.86319	-3.30239	-2.92223
H	-1.69375	-2.00113	-3.27310
H	-0.56830	-3.05624	0.04860
H	0.04974	-2.52378	-1.52880
H	-0.87845	-4.04324	-1.40662
H	1.26370	-0.96922	3.98430
H	2.02817	0.23557	2.93657
H	2.76010	-1.98212	2.23379
H	1.09614	-2.53819	2.06248
H	1.57980	-3.75124	0.16596
H	2.98553	-4.20028	1.16606
H	2.92771	-4.64861	-0.55157
H	5.20298	-1.74952	-0.55970
H	4.91544	-3.25106	-1.48086
H	5.21953	-3.31552	0.26855
H	3.22274	-2.00752	-2.73042
H	4.54012	-0.80876	-2.68796
H	2.94643	-0.35336	-3.31682
H	2.80694	1.08263	0.05904
H	2.17906	1.38092	-1.57116
H	3.94481	1.33010	-1.29597
O	-0.01569	0.00041	-1.60157
H	0.70844	-0.37316	-2.12449

[6]FeTMG2dienANOH
Charge: 2+
Energy: -1536389.6515305

Fe	-0.05968	0.49223	-0.12501
O	0.08094	-0.29389	-1.76582
N	-1.73525	-0.34025	0.58718
N	-0.55000	2.43002	-1.06088
N	1.73369	0.08908	0.65018
N	-0.22583	1.59920	1.93261
C	1.14367	1.52596	2.50823
C	-0.69474	3.00326	1.92572
C	-1.18618	0.73788	2.67771
C	-2.32942	0.32369	1.75872
C	-2.43607	-1.30612	-0.04908
N	-3.78336	-1.23436	-0.19162
N	-1.78738	-2.38338	-0.54141
C	-0.51169	-2.83580	0.00899
C	-2.18077	-3.03852	-1.79291
C	-4.65326	-2.41818	-0.17151
C	2.77571	-0.42547	-0.04165
N	3.56960	-1.39809	0.47360
N	3.06097	0.05447	-1.27154
C	3.53833	-0.80617	-2.35853
C	5.00746	-1.48606	0.18453
C	3.05381	-2.43033	1.37478
C	2.72316	1.41712	-1.67696
C	-0.78188	3.40228	-1.64657
C	-1.06959	4.63019	-2.37530
H	-1.40553	5.40643	-1.67958
H	-1.85455	4.44906	-3.11718
H	-0.16642	4.97666	-2.88901
H	1.71514	2.36207	2.09522
H	1.11588	1.64032	3.60093
H	1.36322	-0.63044	2.62098
C	1.82914	0.22127	2.11110
H	2.87506	0.25248	2.43498
H	-1.56038	1.25790	3.56955
H	-0.66270	-0.16196	3.00845
H	-2.91649	1.20434	1.47295
H	-3.00594	-0.35498	2.29020
C	-4.47275	0.04634	-0.36089
H	-5.20456	-0.05461	-1.16881
H	-5.00410	0.34406	0.55022
H	-3.75490	0.82080	-0.63639
H	-5.48552	-2.22365	0.51258
H	-5.06283	-2.63746	-1.16334
H	-4.09857	-3.28334	0.19202
H	-0.38813	-2.43459	1.01527
H	0.31623	-2.49879	-0.62310
H	-0.51553	-3.92952	0.05392
H	-2.96811	-2.46962	-2.28696
H	-2.52741	-4.06224	-1.61903
H	-1.30659	-3.06872	-2.45222
H	3.43134	-3.40390	1.04585
H	1.96552	-2.45007	1.33409
H	3.37953	-2.26453	2.40781
H	1.84613	1.41192	-2.33092
H	3.57519	1.84678	-2.21383
H	2.51095	2.02297	-0.79535
H	5.54054	-1.63035	1.12972
H	5.35431	-0.55994	-0.27400
H	5.23749	-2.32877	-0.47607
H	4.55499	-0.53957	-2.66491
H	3.51287	-1.85123	-2.05155
H	2.86437	-0.68171	-3.21238
H	-0.02193	3.60645	1.31390
H	-0.72051	3.41449	2.94358
H	-1.69660	3.05989	1.49585
H	-0.43406	-0.08831	-2.56172

[5]FeTMG2dienBrOH
Charge: 2+
Energy: -3068347.8047351

Fe	-0.05796	0.64965	-0.46684
N	-1.81958	0.56342	0.49264
N	1.66705	0.57693	0.49103
N	-0.03517	2.69766	0.43551
C	1.18529	2.76593	1.28257
C	-0.00868	3.70168	-0.65665
C	-1.29829	2.76927	1.22887
C	-2.36702	1.92712	0.54637
C	-2.68892	-0.48408	0.49713
N	-3.88561	-0.40370	-0.12945
N	-2.35874	-1.60336	1.16718
C	-1.36674	-1.59405	2.23967
C	-2.79932	-2.94068	0.74588
C	-5.10376	-1.05275	0.37493
C	2.75746	-0.18696	0.22145
N	3.45534	-0.78396	1.21985
N	3.17107	-0.31525	-1.05017
C	3.80640	-1.54285	-1.55330
C	4.91650	-0.93704	1.18028
C	2.79526	-1.35424	2.39775
C	2.85991	0.68400	-2.07599
H	1.99533	3.18229	0.68071
H	1.00915	3.43131	2.13628
H	0.79949	0.94252	2.39760
C	1.56577	1.35607	1.73187
H	2.51284	1.37010	2.27886
H	-1.60328	3.81791	1.32584
H	-1.10280	2.36774	2.22540
H	-2.57836	2.33157	-0.44987
H	-3.29764	1.95449	1.12329
C	-4.03887	0.32674	-1.39349
H	-4.55147	-0.32352	-2.10976
H	-4.64055	1.23202	-1.25696
H	-3.05999	0.58901	-1.79682
H	-5.91944	-0.32408	0.33335
H	-5.38233	-1.92011	-0.23247
H	-4.96267	-1.36100	1.41100
H	-1.24486	-0.58223	2.62473
H	-0.40540	-1.96561	1.86623
H	-1.70976	-2.25050	3.04492
H	-3.22540	-2.89823	-0.25568
H	-3.53031	-3.35956	1.44412
H	-1.92251	-3.59411	0.71611
H	3.11746	-2.39470	2.51242
H	1.71440	-1.33678	2.26482
H	3.06805	-0.80652	3.30655
H	1.99731	0.37261	-2.67384
H	3.72851	0.79165	-2.73125
H	2.64005	1.64336	-1.60875
H	5.31779	-0.64209	2.15494
H	5.34008	-0.28912	0.41273
H	5.20659	-1.97490	0.98508
H	4.86616	-1.38090	-1.77193
H	3.69504	-2.34906	-0.82913
H	3.29375	-1.83463	-2.47429
H	0.83225	3.49431	-1.31849
H	0.09364	4.70444	-0.22362
H	-0.92602	3.63953	-1.23919
O	-0.45876	1.34727	-2.07726
H	-0.60613	0.76420	-2.84281
Br	0.05622	-1.67033	-1.19041

[3]FeTMG2dienClOH
Charge: 2+
Energy: -1741815.8414399

Fe	0.08277	0.65602	0.44698
N	1.69433	0.32932	-0.53428
N	-1.61232	0.45253	-0.41500
N	0.07333	2.52484	-0.53174
C	-1.24611	2.66470	-1.22423

C	0.26446	3.65230	0.42505
C	1.21106	2.45254	-1.50063
C	2.31320	1.62395	-0.86535
C	2.51880	-0.76245	-0.35190
N	3.75978	-0.62441	0.16033
N	2.10014	-1.95561	-0.79209
C	1.01843	-2.09336	-1.76649
C	2.50614	-3.21418	-0.14825
C	4.90215	-1.43324	-0.29193
C	-2.66495	-0.34519	-0.05003
N	-3.38744	-1.00342	-0.98260
N	-3.01725	-0.41849	1.24341
C	-3.54572	-1.65055	1.84774
C	-4.82842	-1.26403	-0.83746
C	-2.79375	-1.49872	-2.22790
C	-2.70433	0.64020	2.20786
H	-1.94737	3.10056	-0.50941
H	-1.14976	3.34770	-2.07631
H	-1.12565	0.87084	-2.44260
C	-1.73243	1.28402	-1.62776
H	-2.76719	1.33300	-1.97941
H	1.54711	3.46312	-1.75670
H	0.86255	1.95870	-2.41024
H	2.71364	2.13323	0.01589
H	3.13825	1.46646	-1.56876
C	4.04941	0.30005	1.26571
H	4.53317	-0.26526	2.06914
H	4.73353	1.09005	0.93847
H	3.12678	0.73491	1.64729
H	5.75954	-0.76379	-0.41009
H	5.16468	-2.20758	0.43589
H	4.67718	-1.89395	-1.25408
H	0.90102	-1.16895	-2.33014
H	0.08700	-2.32777	-1.24122
H	1.26602	-2.91098	-2.44922
H	2.98964	-3.00925	0.80578
H	3.17280	-3.79538	-0.79194
H	1.59998	-3.79424	0.04672
H	-3.06842	-2.55076	-2.35532
H	-1.70910	-1.42377	-2.18061
H	-3.16567	-0.93658	-3.09147
H	-1.83432	0.36382	2.81161
H	-3.56730	0.77551	2.86592
H	-2.50290	1.57656	1.68764
H	-5.31564	-1.01336	-1.78469
H	-5.24545	-0.63527	-0.05094
H	-5.02751	-2.31623	-0.61129
H	-4.58766	-1.52751	2.15748
H	-3.46025	-2.48104	1.14856
H	-2.93415	-1.87773	2.72617
H	-0.47681	3.57737	1.22022
H	0.14730	4.60052	-0.11165
H	1.25394	3.59790	0.87381
O	0.82601	1.39918	1.86817
H	0.93563	0.75802	2.59624
Cl	-0.02155	-1.37461	1.44881

^{5}FeTMG2dienFOH
Charge: 2+
Energy: -1515694.1977709

Fe	0.08628	0.60032	0.55756
N	1.71127	0.22452	-0.57093
N	-1.68282	0.55978	-0.28475
N	0.16909	2.51598	-0.44294
C	-1.19709	2.77058	-0.99852
C	0.55831	3.60489	0.49526
C	1.19442	2.34072	-1.52802
C	2.33352	1.47586	-1.01353
C	2.47737	-0.87567	-0.35499
N	3.75933	-0.78090	0.07324
N	1.94482	-2.08866	-0.59580
C	0.79413	-2.26391	-1.47960
C	2.31417	-3.27926	0.18081
C	4.81913	-1.69775	-0.36956
C	-2.65083	-0.34452	0.01563
N	-3.40616	-0.90889	-0.95803
N	-2.89348	-0.64945	1.30314
C	-3.34239	-1.98396	1.72294
C	-4.83504	-1.20683	-0.77436
C	-2.86037	-1.25043	-2.27510
C	-2.59587	0.27271	2.40288
H	-1.79943	3.20479	-0.19778
H	-1.12529	3.49558	-1.81812
H	-1.29641	1.05564	-2.32425
C	-1.81055	1.45354	-1.44225
H	-2.86215	1.59623	-1.71193
H	1.53811	3.32991	-1.85008
H	0.71513	1.84369	-2.37298
H	2.86377	1.99772	-0.21027
H	3.05515	1.28945	-1.81709
C	4.16281	0.21830	1.06997
H	4.72109	-0.28995	1.86322
H	4.81307	0.98236	0.62969
H	3.28053	0.68521	1.51144
H	5.69384	-1.10050	-0.64566
H	5.11090	-2.39463	0.42320
H	4.48758	-2.25776	-1.24437
H	0.72573	-1.41991	-2.16572
H	-0.12451	-2.33097	-0.88701
H	0.92411	-3.18790	-2.05042
H	2.90862	-2.99451	1.04827
H	2.87208	-3.99749	-0.42785
H	1.39410	-3.75447	0.53465
H	-3.16629	-2.27116	-2.52591
H	-1.77201	-1.21096	-2.25088
H	-3.23939	-0.57670	-3.05153
H	-1.69833	-0.05035	2.93850
H	-3.44192	0.27665	3.09636
H	-2.44333	1.27994	2.01588
H	-5.37619	-0.84423	-1.65377
H	-5.21464	-0.69174	0.10829
H	-5.01226	-2.28278	-0.67545
H	-4.37939	-1.96570	2.07211
H	-3.24493	-2.69073	0.89921
H	-2.69945	-2.31445	2.54415
H	-0.11963	3.60750	1.34749
H	0.50228	4.56246	-0.03565
H	1.56943	3.43876	0.86036
O	0.74012	1.38219	2.03798
H	0.87207	0.76786	2.78387
F	-0.06456	-0.99612	1.20696

^{5}FeTMG2dienN_3OH
Charge: 2+
Energy: -1556084.6958216

Fe	-0.00484	0.59141	0.49579
N	1.67182	0.50868	-0.58461
N	-1.78570	0.53787	-0.33815
N	-0.07672	2.62969	-0.26369
C	-1.40705	2.81659	-0.91795
C	0.10859	3.60871	0.84088
C	1.04964	2.71106	-1.24860
C	2.20999	1.86803	-0.74611
C	2.52850	-0.54580	-0.61402
N	3.78457	-0.44998	-0.11953
N	2.11310	-1.70419	-1.16511
C	1.02318	-1.75099	-2.13958
C	2.61632	-3.01590	-0.73581
C	4.94041	-1.12113	-0.73132
C	-2.77382	-0.35439	-0.09424
N	-3.51753	-0.87721	-1.09887
N	-3.04443	-0.71056	1.17848
C	-3.51449	-2.05528	1.53811
C	-4.95047	-1.17472	-0.95297
C	-2.94931	-1.17523	-2.41695
C	-2.74393	0.15944	2.31353
H	-2.10747	3.16399	-0.15542
H	-1.33402	3.58466	-1.69714
H	-1.25979	1.15695	-2.30775
C	-1.88218	1.47886	-1.46450
H	-2.91177	1.56302	-1.82599
H	1.33233	3.76071	-1.38947
H	0.69901	2.31254	-2.20295
H	2.59491	2.28054	0.19252
H	3.02946	1.87721	-1.47323
C	4.07731	0.33580	1.08744
H	4.67812	-0.28315	1.76147
H	4.65189	1.23608	0.84338
H	3.15116	0.60628	1.59685
H	5.75170	-0.39140	-0.81641
H	5.29125	-1.95987	-0.12118
H	4.68454	-1.47528	-1.73016
H	0.84383	-0.75392	-2.54015
H	0.10984	-2.12215	-1.66255
H	1.30324	-2.42719	-2.95308
H	3.14163	-2.92688	0.21483
H	3.28202	-3.45752	-1.48382
H	1.75935	-3.68279	-0.59815
H	-3.24227	-2.19077	-2.70233
H	-1.86177	-1.12668	-2.37412
H	-3.32057	-0.48215	-3.17991
H	-1.84368	-0.18477	2.83663
H	-3.58298	0.13222	3.01526
H	-2.59917	1.18439	1.97029
H	-5.47522	-0.76941	-1.82374
H	-5.34332	-0.69696	-0.05529
H	-5.13578	-2.25280	-0.90574
H	-4.55842	-2.04097	1.86626
H	-3.40503	-2.73053	0.69012
H	-2.89403	-2.42691	2.35945
H	-0.65896	3.44413	1.59750
H	0.02178	4.62734	0.44416
H	1.08445	3.46784	1.30153
O	0.70739	1.10368	2.07402
H	0.21079	1.09237	2.91156
N	-0.09669	-1.23940	0.88907

N	0.70911	-1.67881	1.71402
N	1.44010	-2.16247	2.44647

[5]FeTMG2dienNCSOH
Charge: 2+
Energy: -1761189.6006256

Fe	-0.17832	0.77945	-0.54145
N	-1.91053	0.46990	0.44879
N	1.50711	0.74209	0.45834
N	-0.32036	2.73495	0.41779
C	0.90943	2.89984	1.24940
C	-0.42039	3.81431	-0.60081
C	-1.55996	2.67352	1.26188
C	-2.57908	1.76992	0.58811
C	-2.66722	-0.65211	0.37683
N	-3.88222	-0.65049	-0.22124
N	-2.19978	-1.78998	0.93283
C	-1.24399	-1.77496	2.03909
C	-2.56819	-3.12477	0.44423
C	-5.02534	-1.42973	0.27473
C	2.65548	0.08740	0.15192
N	3.41758	-0.46635	1.12650
N	3.05606	0.01613	-1.13216
C	3.84841	-1.10336	-1.66110
C	4.88747	-0.46536	1.08542
C	2.82578	-1.08788	2.31515
C	2.65299	1.00842	-2.13337
H	1.67542	3.36657	0.62646
H	0.69588	3.56504	2.09441
H	0.68442	1.06350	2.39128
C	1.39332	1.52732	1.69618
H	2.35638	1.61305	2.20750
H	-1.93964	3.69053	1.41008
H	-1.29240	2.25437	2.23384
H	-2.87096	2.19561	-0.37833
H	-3.48006	1.68799	1.20613
C	-4.14133	0.15105	-1.42299
H	-4.61718	-0.49078	-2.17168
H	-4.81642	0.98642	-1.20643
H	-3.20312	0.53007	-1.83031
H	-5.90015	-0.77241	0.30091
H	-5.25036	-2.28097	-0.37614
H	-4.82845	-1.78370	1.28686
H	-1.15358	-0.76407	2.43375
H	-0.26327	-2.12752	1.70168
H	-1.59814	-2.44589	2.82869
H	-2.98593	-3.05373	-0.56002
H	-3.28699	-3.61575	1.10797
H	-1.66273	-3.73620	0.40001
H	3.24998	-2.08995	2.43576
H	1.74732	-1.17769	2.19008
H	3.04549	-0.50802	3.21834
H	1.83351	0.63049	-2.75282
H	3.51159	1.22587	-2.77477
H	2.33292	1.92755	-1.64305
H	5.25808	-0.11929	2.05548
H	5.24191	0.21710	0.31296
H	5.28451	-1.46867	0.89954
H	4.87495	-0.79468	-1.88135
H	3.85444	-1.93005	-0.95269
H	3.37884	-1.44572	-2.58820
H	0.40712	3.72591	-1.30423
H	-0.38192	4.78642	-0.09502
H	-1.35251	3.71616	-1.15321
O	-0.74200	1.54685	-2.07363
H	-0.83903	0.94435	-2.83280
N	0.02052	-0.91976	-1.22490
C	0.51355	-1.99871	-0.99190
S	1.13487	-3.43044	-0.74076

[1]FeTMG2dienOHBr
Charge: 2+
Energy: -3068335.0420020

Fe	0.04650	-0.44234	-0.01066
N	1.47364	0.35439	0.82300
N	-1.70722	-0.43582	0.51860
N	0.26343	-1.88615	1.52463
C	-1.11454	-2.38689	1.79176
C	1.16644	-3.05278	1.30076
C	0.80315	-1.04827	2.63516
C	1.96662	-0.24561	2.07585
C	2.29530	1.29080	0.19352
N	3.54839	0.93981	-0.14072
N	1.83746	2.52408	-0.02106
C	0.69919	3.05598	0.73189
C	2.22312	3.32386	-1.19459
C	4.66393	1.90089	-0.19335
C	-2.65870	0.43915	0.00412
N	-3.21828	1.34838	0.82566
N	-3.04347	0.32328	-1.26639
C	-3.48265	1.47358	-2.07102
C	-4.60332	1.82771	0.67493
C	-2.50282	1.89221	1.98347
C	-2.88146	-0.92392	-2.02460
H	-1.33642	-3.11450	1.00803
H	-1.16980	-2.89188	2.76399
H	-2.08535	-0.61929	2.60760
C	-2.09632	-1.23236	1.69886
H	-3.11609	-1.61538	1.58176
H	1.10113	-1.66730	3.48923
H	0.02032	-0.36032	2.96363
H	2.84672	-0.87581	1.91043
H	2.26076	0.54495	2.77649
C	3.91764	-0.44683	-0.45902
H	4.48384	-0.44708	-1.39529
H	4.55275	-0.86655	0.32863
H	3.02461	-1.05404	-0.59669
H	5.52052	1.44482	0.31147
H	4.94879	2.13009	-1.22451
H	4.39604	2.81828	0.33028
H	0.64345	2.58168	1.71109
H	-0.22381	2.87606	0.17421
H	0.85016	4.12988	0.86939
H	2.78835	2.71501	-1.89873
H	2.80728	4.20230	-0.90690
H	1.30161	3.65115	-1.68476
H	-2.54348	2.98560	1.94340
H	-1.46165	1.57492	1.95602
H	-2.97131	1.56371	2.91743
H	-2.06667	-0.82432	-2.74667
H	-3.81436	-1.12647	-2.55853
H	-2.65506	-1.75038	-1.35470
H	-5.07292	1.81415	1.66285
H	-5.16101	1.16259	0.01625
H	-4.63740	2.84966	0.28562
H	-4.55277	1.42689	-2.29125
H	-3.24555	2.40517	-1.55928
H	-2.92942	1.44580	-3.01435
H	0.75517	-3.69086	0.52203
H	1.26691	-3.62427	2.23091
H	2.14783	-2.71184	0.97408
O	-0.16673	0.88695	-1.20092
H	-0.02300	0.55619	-2.10654
Br	0.54353	-2.01755	-1.73841

[3]FeTMG2dienOHCl
Charge: 2+
Energy: -1741813.2241669

Fe	0.02766	0.55054	0.30967
N	1.67047	0.12375	-0.58791
N	-1.69433	0.41520	-0.44344
N	0.08444	2.36865	-0.81254
C	-1.26525	2.54371	-1.43680
C	0.42079	3.61196	-0.05825
C	1.13821	2.09196	-1.83842
C	2.27212	1.33982	-1.16138
C	2.45831	-0.96045	-0.29608
N	3.76524	-0.82004	0.01734
N	1.93279	-2.18912	-0.42334
C	0.78546	-2.46966	-1.28738
C	2.36120	-3.31417	0.41861
C	4.78695	-1.77569	-0.43825
C	-2.71455	-0.38567	0.01164
N	-3.45373	-1.11291	-0.85346
N	-3.00028	-0.39867	1.32089
C	-3.50457	-1.59824	2.00412
C	-4.88335	-1.39346	-0.64345
C	-2.89160	-1.65803	-2.09332
C	-2.65193	0.70864	2.21862
H	-1.88304	3.09067	-0.72088
H	-1.18783	3.14273	-2.35196
H	-1.39290	0.67081	-2.52715
C	-1.88290	1.17975	-1.68801
H	-2.94287	1.28149	-1.94098
H	1.48227	3.02900	-2.29062
H	0.70682	1.46478	-2.62219
H	2.74641	1.96427	-0.39977
H	3.03977	1.05299	-1.88889
C	4.26584	0.26713	0.87163
H	4.90527	-0.17316	1.64326
H	4.86647	0.97348	0.28851
H	3.43829	0.77942	1.35990
H	5.64824	-1.20189	-0.79326
H	5.11819	-2.43021	0.37456
H	4.39813	-2.37810	-1.25969
H	0.65288	-1.65319	-1.99666
H	-0.11462	-2.57538	-0.67615
H	0.97797	-3.39922	-1.83144
H	2.96607	-2.95422	1.25096
H	2.92801	-4.05358	-0.15550
H	1.46292	-3.79251	0.82031
H	-3.17897	-2.71100	-2.17502
H	-1.80483	-1.59484	-2.06993
H	-3.27593	-1.12489	-2.96966
H	-1.75305	0.46852	2.79305

H	-3.48730	0.87379	2.90473
H	-2.47445	1.61844	1.64595
H	-5.40536	-1.21081	-1.58767
H	-5.28909	-0.72380	0.11482
H	-5.05372	-2.43302	-0.34671
H	-4.54473	-1.47474	2.31976
H	-3.41356	-2.46858	1.35559
H	-2.88441	-1.75999	2.89091
H	-0.25788	3.71460	0.78801
H	0.32417	4.47744	-0.72418
H	1.43732	3.55930	0.32670
O	-0.18500	-0.99820	1.15234
H	0.30678	-0.97540	1.99610
Cl	0.96464	1.45675	2.12720

^{5}FeTMG2dienOHF
Charge: 2+
Energy: -1515695.9926425

Fe	0.06806	-0.03555	0.71475
N	1.70804	0.37025	-0.36027
N	-1.56504	0.27241	-0.41470
N	-0.13133	2.79453	-1.09008
C	-1.26196	2.28790	-1.83314
C	-0.32655	3.58472	0.11274
C	1.22545	2.51643	-1.53403
C	2.09153	1.77408	-0.47700
C	2.70206	-0.55734	-0.23846
N	3.85509	-0.27327	0.41149
N	2.51183	-1.78144	-0.76299
C	1.52159	-2.01605	-1.81298
C	3.01156	-3.00169	-0.11286
C	5.14918	-0.86544	0.04379
C	-2.70124	-0.35916	-0.02010
N	-3.39626	-1.17848	-0.84452
N	-3.12317	-0.17297	1.24820
C	-3.74978	-1.24330	2.03597
C	-4.85348	-1.34584	-0.75260
C	-2.73210	-2.04448	-1.82526
C	-2.89164	1.08574	1.97129
H	-2.17086	2.75298	-1.45044
H	-1.13188	2.56627	-2.88832
H	-0.51856	0.28242	-2.23951
C	-1.40436	0.72851	-1.77842
H	-2.26877	0.49123	-2.40705
H	1.70475	3.48549	-1.73276
H	1.18728	1.94937	-2.46544
H	2.00453	2.30119	0.47876
H	3.13019	1.86316	-0.81261
C	3.87195	0.59357	1.59943
H	4.42576	0.08165	2.39285
H	4.37117	1.54619	1.39189
H	2.85546	0.77831	1.95199
H	5.89280	-0.06332	0.00183
H	5.47974	-1.60614	0.77932
H	5.08077	-1.33272	-0.93889
H	1.39048	-1.11468	-2.41135
H	0.56531	-2.31603	-1.36823
H	1.88013	-2.82283	-2.45800
H	3.44892	-2.76246	0.85536
H	3.75338	-3.50811	-0.73740
H	2.16058	-3.67000	0.05056
H	-3.04104	-3.08024	-1.64840
H	-1.65093	-1.98081	-1.70633
H	-3.00992	-1.77117	-2.84892
H	-2.02242	1.02032	2.63193
H	-3.78307	1.30965	2.56371
H	-2.72651	1.89195	1.25687
H	-5.26508	-1.31960	-1.76630
H	-5.28861	-0.52793	-0.17789
H	-5.12426	-2.30200	-0.29269
H	-4.82195	-1.07102	2.17312
H	-3.58886	-2.20727	1.55338
H	-3.27156	-1.26378	3.02006
H	-0.27913	2.91422	0.98915
H	-1.29794	4.08022	0.08153
H	0.47156	4.32672	0.20351
O	0.06960	-1.75953	1.23406
H	0.18517	-2.04831	2.15500
F	0.22441	1.23159	1.97595

^{3}FeTMG2dienOHN$_3$
Charge: 2+
Energy: -1556079.3062244

Fe	0.03351	0.59020	0.24093
N	1.63502	0.16140	-0.70854
N	-1.74348	0.51716	-0.43065
N	0.09456	2.43401	-0.81747
C	-1.29304	2.70521	-1.30565
C	0.56259	3.61935	-0.04100
C	1.04981	2.14062	-1.92984
C	2.21605	1.35572	-1.34902
C	2.43554	-0.92443	-0.48781
N	3.74226	-0.77715	-0.17658
N	1.91517	-2.15796	-0.63264
C	0.75123	-2.42017	-1.48429
C	2.40251	-3.32125	0.12313
C	4.78825	-1.68794	-0.66826
C	-2.72221	-0.36536	-0.05385
N	-3.46202	-1.01583	-0.98143
N	-2.97726	-0.55084	1.24951
C	-3.43254	-1.84113	1.78415
C	-4.88288	-1.34376	-0.78426
C	-2.90699	-1.42116	-2.27554
C	-2.64276	0.43827	2.27648
H	-1.81699	3.22858	-0.50269
H	-1.26815	3.36006	-2.18506
H	-1.61546	0.93705	-2.51174
C	-1.99872	1.39218	-1.59040
H	-3.07045	1.56232	-1.73590
H	1.37882	3.07132	-2.40650
H	0.53701	1.52952	-2.67702
H	2.77705	1.97601	-0.64448
H	2.90597	1.04735	-2.14225
C	4.21611	0.30685	0.69518
H	4.83657	-0.13071	1.48409
H	4.82643	1.02249	0.13414
H	3.37038	0.81771	1.15639
H	5.61841	-1.07934	-1.03958
H	5.16436	-2.33941	0.12705
H	4.40352	-2.29317	-1.48929
H	0.60475	-1.58336	-2.16632
H	-0.14100	-2.54359	-0.86437
H	0.93691	-3.33280	-2.05814
H	3.03124	-2.99846	0.95347
H	2.96604	-4.00924	-0.51441
H	1.53417	-3.85320	0.52460
H	-3.17995	-2.46464	-2.46273
H	-1.82042	-1.34479	-2.25480
H	-3.30682	-0.80809	-3.09079
H	-1.77312	0.09908	2.84643
H	-3.49582	0.54180	2.95370
H	-2.42860	1.40264	1.81768
H	-5.42592	-1.05779	-1.69042
H	-5.28511	-0.77744	0.05578
H	-5.03310	-2.41414	-0.61150
H	-4.46502	-1.78673	2.14195
H	-3.34418	-2.61676	1.02470
H	-2.78035	-2.10075	2.62344
H	-0.06436	3.74103	0.84159
H	0.49941	4.51365	-0.67154
H	1.58886	3.47636	0.29087
O	-0.19484	-0.98210	1.06168
H	0.63062	-1.35653	1.41552
N	0.81788	1.44757	1.71742
N	0.83399	0.86801	2.80609
N	0.87730	0.39898	3.84808

^{3}FeTMG2dienOHNCS
Charge: 2+
Energy: -1761185.2978873

Fe	-0.05206	-0.45864	0.00830
N	1.41837	0.62386	0.71700
N	-1.88701	-0.33624	0.55193
N	0.14414	-1.55359	1.82848
C	-1.22804	-1.66783	2.42073
C	0.72520	-2.91935	1.69633
C	1.03934	-0.69772	2.67115
C	2.12312	-0.10245	1.78315
C	1.98311	1.70972	0.13183
N	3.32987	1.82036	0.00509
N	1.20215	2.72763	-0.27014
C	-0.11691	2.97667	0.30884
C	1.53067	3.55739	-1.43562
C	4.03855	3.09631	0.17656
C	-2.95045	-0.03548	-0.23801
N	-3.94731	0.77259	0.19706
N	-3.04275	-0.58900	-1.46226
C	-3.61700	0.13119	-2.60494
C	-5.35180	0.57997	-0.19317
C	-3.70467	1.90087	1.09976
C	-2.39322	-1.85477	-1.80118
H	-1.68354	-2.57224	2.01045
H	-1.16297	-1.77886	3.50976
H	-1.71983	0.44322	2.52278
C	-2.05815	-0.46404	2.00664
H	-3.10736	-0.62086	2.27657
H	1.45874	-1.28859	3.49374
H	0.44218	0.11278	3.09517
H	2.77333	-0.89170	1.38871
H	2.75457	0.58417	2.35770
C	4.17547	0.66982	-0.32309
H	4.84810	0.95062	-1.13997
H	4.78409	0.36358	0.53549
H	3.55856	-0.16279	-0.65828
H	4.90456	2.92332	0.82334

H	4.39422	3.49188	-0.78083
H	3.38371	3.82689	0.65203
H	-0.20190	2.45026	1.25971
H	-0.89316	2.62302	-0.37459
H	-0.22871	4.05245	0.47600
H	2.35893	3.11787	-1.99128
H	1.78999	4.57890	-1.13994
H	0.65198	3.58985	-2.08708
H	-4.20336	2.78796	0.69600
H	-2.63715	2.10413	1.16538
H	-4.10505	1.70519	2.10066
H	-1.46317	-1.67697	-2.35042
H	-3.07254	-2.44080	-2.42726
H	-2.17115	-2.41666	-0.89369
H	-5.97000	0.65321	0.70706
H	-5.48660	-0.40957	-0.63025
H	-5.68303	1.34286	-0.90529
H	-4.55258	-0.32741	-2.93987
H	-3.79108	1.17451	-2.34440
H	-2.89272	0.09605	-3.42488
H	0.16908	-3.47838	0.94342
H	0.67023	-3.44005	2.65937
H	1.76774	-2.85855	1.38636
O	-0.34665	0.53529	-1.44372
H	0.24609	0.23642	-2.15763
N	0.98496	-1.78070	-1.02664
C	2.00526	-2.34266	-1.29455
S	3.34854	-3.13897	-1.66813

^{6}FeTPAbpyBr
Charge: 3+
Energy: -3294126.6037048

Fe	-0.99837	-0.27162	0.13684
N	-0.28575	-1.58179	1.68593
N	-0.87578	-1.71253	-1.45174
N	-1.20932	1.35877	-1.27262
N	-0.65761	1.50620	1.32815
N	1.33154	-0.52952	-0.34850
C	-1.05161	-1.92706	2.74792
H	-2.06940	-1.55698	2.74088
C	-0.57130	-2.70672	3.79383
H	-1.22737	-2.96367	4.61871
C	0.75377	-3.14304	3.75127
H	1.16331	-3.75163	4.55192
C	1.54421	-2.79267	2.65336
H	2.57046	-3.14018	2.57953
C	0.99276	-2.02415	1.63192
C	1.75431	-1.77171	0.35022
H	1.55243	-2.61400	-0.31917
H	2.83662	-1.78685	0.52820
C	-1.86779	-2.58240	-1.74196
H	-2.74694	-2.53282	-1.11162
C	-1.77602	-3.48732	-2.79580
H	-2.59826	-4.16668	-2.99396
C	-0.61896	-3.49689	-3.57448
H	-0.51475	-4.19045	-4.40345
C	0.41550	-2.60584	-3.26496
H	1.33355	-2.60027	-3.84423
C	0.25472	-1.72628	-2.20152
C	1.31331	-0.71374	-1.82171
H	2.29039	-1.02942	-2.20825
H	1.07144	0.25765	-2.26726
C	-1.57343	1.18762	-2.55778
H	-1.56065	0.16977	-2.92623
C	-1.97016	2.24118	-3.37430
H	-2.26100	2.05203	-4.40198
C	-2.00071	3.52585	-2.83115
H	-2.31356	4.37512	-3.43073
C	-1.64235	3.70586	-1.49485
H	-1.68738	4.69665	-1.05987
C	-1.25755	2.60301	-0.72756
C	-0.93132	2.68693	0.71432
C	-0.92897	3.88473	1.43567
H	-1.14904	4.82638	0.94806
C	-0.65857	3.86639	2.80362
H	-0.66973	4.79018	3.37388
C	-0.38633	2.64678	3.42519
H	-0.18376	2.58511	4.48904
C	-0.39649	1.49323	2.64875
H	-0.20611	0.52205	3.08782
C	2.07893	0.67431	0.09043
H	1.94933	0.75805	1.17363
H	1.58489	1.54281	-0.35209
C	3.55905	0.73190	-0.26467
N	4.47536	0.42161	0.69670
H	4.13956	0.18001	1.62672
C	4.04862	1.11743	-1.50667
H	3.35101	1.40229	-2.28625
C	5.42915	1.16524	-1.74289
H	5.80193	1.47523	-2.71488
C	5.81785	0.46253	0.51199
H	6.43625	0.20656	1.36551
C	6.32573	0.82999	-0.72351
H	7.39949	0.86569	-0.87381
Br	-3.36349	-0.36059	0.58510

^{6}FeTPAbpyCl
Charge: 3+
Energy: -1967598.5523476

Fe	-1.17803	-0.34949	0.30310
N	-0.25113	-1.48822	1.86459
N	-1.09243	-1.89292	-1.17716
N	-1.61374	1.15074	-1.19535
N	-0.85373	1.53116	1.32763
N	1.12244	-0.50773	-0.36895
C	-0.91682	-1.79666	3.00242
H	-1.95516	-1.49058	3.04318
C	-0.31076	-2.46364	4.06093
H	-0.88635	-2.69721	4.95032
C	1.03424	-2.81971	3.94726
H	1.54009	-3.33886	4.75581
C	1.71922	-2.50828	2.76923
H	2.75794	-2.79854	2.64201
C	1.04561	-1.85514	1.74103
C	1.68733	-1.65779	0.38583
H	1.49674	-2.56384	-0.19835
H	2.77821	-1.58592	0.47509
C	-2.05839	-2.82816	-1.30546
H	-2.88316	-2.76157	-0.60640
C	-2.00388	-3.81564	-2.28530
H	-2.80135	-4.54772	-2.35582
C	-0.91504	-3.83815	-3.15692
H	-0.84159	-4.59600	-3.93111
C	0.09157	-2.87506	-3.01482
H	0.95612	-2.87617	-3.67127
C	-0.02895	-1.91483	-2.01820
C	0.99265	-0.81692	-1.81583
H	1.95189	-1.10782	-2.26172
H	0.65187	0.09808	-2.31332
C	-2.07188	0.85696	-2.42706
H	-2.00516	-0.18115	-2.72670
C	-2.62359	1.81376	-3.27229
H	-2.98438	1.52748	-4.25432
C	-2.71477	3.12868	-2.81529
H	-3.14746	3.90469	-3.43918
C	-2.26008	3.43410	-1.53203
H	-2.35080	4.44772	-1.16152
C	-1.72010	2.42408	-0.73147
C	-1.27877	2.63867	0.66552
C	-1.31406	3.88234	1.30333
H	-1.65414	4.76595	0.77750
C	-0.92470	3.98461	2.63856
H	-0.96323	4.94392	3.14547
C	-0.49829	2.83843	3.31119
H	-0.19936	2.87058	4.35341
C	-0.47947	1.63391	2.61665
H	-0.17069	0.71481	3.09856
C	1.81803	0.77359	-0.09471
H	1.77537	0.93916	0.98595
H	1.22815	1.56909	-0.55678
C	3.25494	0.89445	-0.58579
N	4.26930	0.72704	0.31049
H	4.03183	0.54582	1.28353
C	3.60877	1.20204	-1.89386
H	2.82926	1.37407	-2.62753
C	4.95741	1.31684	-2.25718
H	5.22336	1.56504	-3.28066
C	5.58497	0.83712	0.00230
H	6.29017	0.69550	0.81412
C	5.95880	1.12821	-1.29961
H	7.01069	1.21892	-1.54888
Cl	-3.28935	-0.57506	0.92758

^{6}FeTPAbpyF
Charge: 3+
Energy: -1741474.9561766

Fe	1.21581	0.42362	0.39519
N	0.15041	1.42245	1.93675
N	1.08815	2.00541	-1.00431
N	1.88240	-0.95964	-1.12186
N	1.02443	-1.51228	1.33364
N	-1.08346	0.46592	-0.37182
C	0.79917	1.74092	3.08034
H	1.86046	1.51873	3.09511
C	0.14210	2.32003	4.15997
H	0.69504	2.56867	5.05956
C	-1.22772	2.57253	4.05262
H	-1.77247	3.02004	4.87858
C	-1.88895	2.25803	2.86097
H	-2.94591	2.47699	2.74178
C	-1.16598	1.69633	1.81259
C	-1.77005	1.51070	0.43626
H	-1.66280	2.46331	-0.09317
H	-2.84939	1.32774	0.50210
C	2.02809	2.97386	-1.01947

H	2.82741	2.86467	-0.29479
C	1.96541	4.03554	-1.91807
H	2.73671	4.79831	-1.90758
C	0.89789	4.09224	-2.81568
H	0.81810	4.90982	-3.52587
C	-0.07838	3.08731	-2.78816
H	-0.92144	3.11443	-3.47142
C	0.04996	2.05190	-1.87122
C	-0.91631	0.88857	-1.78795
H	-1.87230	1.15370	-2.25612
H	-0.49893	0.03327	-2.33250
C	2.35609	-0.57793	-2.32349
H	2.19757	0.45893	-2.59191
C	3.03128	-1.44578	-3.17542
H	3.39983	-1.09096	-4.13185
C	3.23180	-2.76180	-2.75835
H	3.76188	-3.46915	-3.38873
C	2.75640	-3.15828	-1.50757
H	2.92690	-4.17287	-1.16913
C	2.08888	-2.23542	-0.69879
C	1.59794	-2.54634	0.66383
C	1.72280	-3.80345	1.26209
H	2.18283	-4.62764	0.73100
C	1.26572	-3.99511	2.56589
H	1.37117	-4.96468	3.04293
C	0.68402	-2.92451	3.24680
H	0.32682	-3.02755	4.26580
C	0.58514	-1.70151	2.59253
H	0.15660	-0.83640	3.08325
C	-1.68084	-0.88357	-0.21738
H	-1.66672	-1.12208	0.85063
H	-1.00929	-1.59546	-0.70461
C	-3.08272	-1.08326	-0.77974
N	-4.14141	-1.06959	0.08003
H	-3.95802	-0.94810	1.07382
C	-3.35903	-1.31298	-2.12209
H	-2.54048	-1.36332	-2.83118
C	-4.67840	-1.50569	-2.55339
H	-4.88300	-1.69195	-3.60376
C	-5.43053	-1.25925	-0.29458
H	-6.17586	-1.23936	0.49316
C	-5.72832	-1.47441	-1.63036
H	-6.75863	-1.62838	-1.93300
F	2.78073	0.91525	1.03810

^{6}FeTPAbpyN$_{3}$
Charge: 3+
Energy: -1781863.7310173

Fe	-1.09488	-0.43386	0.27554
N	-0.16074	-1.44808	1.91162
N	-0.84914	-2.02436	-1.13822
N	-1.54511	1.00136	-1.31553
N	-0.90062	1.53699	1.21613
N	1.26912	-0.49192	-0.30467
C	-0.86472	-1.73838	3.02849
H	-1.92108	-1.49680	2.99409
C	-0.27749	-2.30944	4.15195
H	-0.88141	-2.53328	5.02483
C	1.09128	-2.58432	4.12226
H	1.58508	-3.02721	4.98198
C	1.81670	-2.29349	2.96344
H	2.87614	-2.52471	2.90388
C	1.15842	-1.73831	1.86902
C	1.85244	-1.57198	0.53347
H	1.73347	-2.51475	-0.01046
H	2.93364	-1.44354	0.66905
C	-1.76300	-3.00896	-1.26269
H	-2.61623	-2.94818	-0.59656
C	-1.62205	-4.03791	-2.18959
H	-2.37974	-4.81106	-2.25968
C	-0.49351	-4.04823	-3.01044
H	-0.34979	-4.83727	-3.74241
C	0.46048	-3.03335	-2.87150
H	1.35351	-3.02475	-3.48862
C	0.25024	-2.03383	-1.92830
C	1.21209	-0.87913	-1.73635
H	2.20000	-1.14507	-2.13373
H	0.84899	-0.00709	-2.29263
C	-1.92798	0.63746	-2.55379
H	-1.82105	-0.41321	-2.79511
C	-2.44979	1.53799	-3.47732
H	-2.74964	1.19544	-4.46188
C	-2.58747	2.87270	-3.09529
H	-2.99768	3.60729	-3.78141
C	-2.20599	3.25283	-1.80826
H	-2.32976	4.28331	-1.49873
C	-1.69141	2.29550	-0.92843
C	-1.31216	2.59677	0.47378
C	-1.38737	3.87704	1.03266
H	-1.71605	4.72302	0.44164
C	-1.04898	4.06590	2.37232
H	-1.11647	5.05379	2.81754
C	-0.63481	2.96860	3.12850
H	-0.37429	3.06821	4.17678
C	-0.57557	1.72450	2.50822
H	-0.27151	0.84020	3.05540
C	1.88939	0.83261	-0.06959
H	1.78872	1.05265	0.99779
H	1.28702	1.57498	-0.59951
C	3.34102	0.99743	-0.50196
N	4.31919	0.92107	0.44496
H	4.04417	0.77982	1.41467
C	3.74186	1.25056	-1.80844
H	2.99005	1.34873	-2.58340
C	5.09955	1.40412	-2.11811
H	5.40206	1.60913	-3.14097
C	5.64227	1.07093	0.18906
H	6.31458	1.00187	1.03731
C	6.06308	1.30920	-1.10886
H	7.12067	1.43150	-1.31681
N	-2.87905	-0.71358	0.74666
N	-4.02514	-0.29870	0.75490
N	-5.10645	0.07959	0.76947

^{6}FeTPAbpyNCS
Charge: 3+
Energy: -1986973.1713091

Fe	-0.97716	-0.28718	0.09864
N	-0.29053	-1.57518	1.68254
N	-0.76495	-1.73365	-1.48111
N	-1.12309	1.35345	-1.34131
N	-0.66611	1.53357	1.28061
N	1.41097	-0.56244	-0.29523
C	-1.10973	-1.89258	2.70913
H	-2.12497	-1.52061	2.63248
C	-0.68437	-2.64457	3.79864
H	-1.37826	-2.88212	4.59789
C	0.64190	-3.08020	3.83132
H	1.01076	-3.66743	4.66688
C	1.48690	-2.75977	2.76535
H	2.51485	-3.10990	2.75198
C	0.98592	-2.01671	1.69905
C	1.80098	-1.79087	0.44344
H	1.62045	-2.64552	-0.21661
H	2.87550	-1.81039	0.66564
C	-1.76035	-2.58451	-1.80327
H	-2.66186	-2.50407	-1.20700
C	-1.64213	-3.50663	-2.83949
H	-2.46667	-4.17348	-3.06789
C	-0.44930	-3.55060	-3.56230
H	-0.32111	-4.25931	-4.37486
C	0.58791	-2.67563	-3.21966
H	1.53068	-2.69672	-3.75739
C	0.39539	-1.77686	-2.17642
C	1.44960	-0.77030	-1.76376
H	2.43765	-1.09896	-2.11102
H	1.23200	0.19631	-2.23269
C	-1.42477	1.17358	-2.64039
H	-1.40551	0.15052	-2.99581
C	-1.76216	2.22285	-3.48963
H	-2.00202	2.02632	-4.52904
C	-1.79602	3.51457	-2.96407
H	-2.06109	4.36181	-3.58900
C	-1.49995	3.70530	-1.61426
H	-1.54491	4.70293	-1.19516
C	-1.17173	2.60497	-0.81624
C	-0.89601	2.70688	0.63779
C	-0.88946	3.91970	1.33510
H	-1.07251	4.85619	0.82285
C	-0.65818	3.92373	2.71017
H	-0.66312	4.85917	3.26115
C	-0.43108	2.71149	3.36296
H	-0.25878	2.66718	4.43300
C	-0.44388	1.54331	2.60739
H	-0.28350	0.57680	3.06988
C	2.13684	0.64743	0.15475
H	1.95825	0.75197	1.22945
H	1.66581	1.50923	-0.32491
C	3.63191	0.69638	-0.13277
N	4.50210	0.39606	0.87296
H	4.12217	0.17194	1.79024
C	4.17944	1.05545	-1.35878
H	3.51875	1.33018	-2.17329
C	5.56889	1.08817	-1.53407
H	5.98719	1.37726	-2.49385
C	5.85191	0.42263	0.74752
H	6.42946	0.17622	1.63180
C	6.41684	0.76406	-0.47003
H	7.49636	0.78824	-0.57345
N	-2.82056	-0.44901	0.39883
C	-4.02324	-0.38642	0.52941
S	-5.58979	-0.31224	0.70136

^{2}FeTPAbpyOH
Charge: 3+

Energy: -1726392.1170561

Fe	-1.02097	0.59399	0.01419
N	-1.75882	-0.70878	1.34934
N	-1.80879	-0.69578	-1.30072
N	-0.18249	1.82387	-1.29256
N	-0.13936	1.82461	1.29286
N	0.64129	-0.83210	-0.01977
C	-3.03235	-0.67146	1.78446
H	-3.59228	0.21133	1.49911
C	-3.57942	-1.71070	2.53366
H	-4.60656	-1.64250	2.87582
C	-2.79372	-2.82896	2.81304
H	-3.19781	-3.66229	3.37961
C	-1.47353	-2.86467	2.35107
H	-0.83562	-3.71858	2.55660
C	-0.98720	-1.78078	1.62998
C	0.45824	-1.65579	1.21745
H	0.92619	-2.64147	1.10777
H	0.97920	-1.12668	2.02554
C	-3.09814	-0.66031	-1.68673
H	-3.65346	0.21237	-1.36399
C	-3.66388	-1.68855	-2.43689
H	-4.70349	-1.62255	-2.73950
C	-2.87923	-2.79288	-2.77031
H	-3.29689	-3.61690	-3.34064
C	-1.54259	-2.82653	-2.35865
H	-0.90470	-3.66867	-2.60790
C	-1.03865	-1.75399	-1.63232
C	0.41968	-1.62296	-1.27442
H	0.90377	-2.60418	-1.21175
H	0.90742	-1.06655	-2.08291
C	-0.32177	1.74038	-2.62796
H	-0.88615	0.89206	-2.99511
C	0.20399	2.69940	-3.48979
H	0.06216	2.59980	-4.56061
C	0.88988	3.78620	-2.94444
H	1.30389	4.55792	-3.58612
C	1.02382	3.88143	-1.55800
H	1.53799	4.72936	-1.12063
C	0.47067	2.88795	-0.74808
C	0.49020	2.89119	0.72632
C	1.05407	3.89431	1.51726
H	1.54756	4.74544	1.06260
C	0.95447	3.80595	2.90685
H	1.37498	4.58624	3.53381
C	0.29262	2.71561	3.47522
H	0.17628	2.62229	4.54971
C	-0.24482	1.74696	2.63181
H	-0.79391	0.89609	3.01632
C	1.99420	-0.19426	-0.03181
H	2.05801	0.44695	0.85128
H	2.03570	0.46145	-0.90298
C	3.19160	-1.13384	-0.08555
N	3.79551	-1.49604	1.08308
H	3.43380	-1.11780	1.95565
C	3.74569	-1.62206	-1.26234
H	3.31497	-1.33174	-2.21394
C	4.86908	-2.46032	-1.22620
H	5.29864	-2.82946	-2.15310
C	4.88516	-2.29765	1.16139
H	5.27571	-2.49477	2.15396
C	5.44423	-2.80662	-0.00033
H	6.31879	-3.44575	0.05962
O	-2.53240	1.52737	0.04616
H	-2.40493	2.49310	0.03971

^{4}FeBPMENBr
Charge: 2+
Energy: -2936638.2001069

Fe	0.01960	0.17539	-0.11482
N	-0.40137	-0.99423	1.64753
N	0.44150	-1.66925	-1.06614
N	-1.93957	0.05554	-0.26863
N	1.99581	0.20615	0.00757
C	-0.46726	-2.40027	1.13878
H	-1.46107	-2.56477	0.71692
C	0.60134	-2.63497	0.07415
H	1.59539	-2.49021	0.50183
C	0.58440	-0.85161	2.74859
H	0.25554	-1.40308	3.63753
H	0.69023	0.20546	3.00106
H	1.55294	-1.23527	2.42678
C	-0.56483	-2.15810	-2.04614
H	-0.20733	-3.07239	-2.53394
H	-0.73383	-1.39192	-2.80495
H	-1.50614	-2.36581	-1.53849
C	-1.74309	-0.50891	2.07540
H	-1.60027	0.44259	2.60102
H	-2.21167	-1.20922	2.77792
C	-2.60723	-0.27124	0.86467
C	-3.99666	-0.32716	0.88349
H	-4.51264	-0.60281	1.79752
C	-4.70601	-0.01484	-0.27829
H	-5.79129	-0.04449	-0.27982
C	-4.00559	0.34019	-1.43528
H	-4.52124	0.60132	-2.35290
C	-2.61947	0.36721	-1.39360
H	-2.02506	0.66333	-2.25025
C	1.74784	-1.43081	-1.75160
H	1.54309	-0.87330	-2.67321
H	2.21397	-2.38132	-2.03836
C	2.64280	-0.61616	-0.85738
C	4.03076	-0.66684	-0.90475
H	4.52338	-1.33834	-1.60045
C	4.76938	0.15584	-0.05101
H	5.85459	0.13641	-0.07691
C	4.09555	0.99881	0.83684
H	4.63241	1.65413	1.51401
C	2.70800	1.00110	0.83791
H	2.13727	1.65459	1.48529
H	-0.33781	-3.10949	1.96439
H	0.54618	-3.66276	-0.30206
Br	-0.13259	2.53561	-0.21944

^{4}FeBPMENCl
Charge: 2+
Energy: -1610109.8630760

Fe	-0.01000	-0.33554	-0.30398
N	0.42984	0.02671	1.78135
N	-0.42113	1.73505	-0.42401
N	1.94740	-0.16692	-0.40738
N	-1.98700	-0.39748	-0.19913
C	0.50044	1.51726	1.88484
H	1.49397	1.83640	1.56265
C	-0.56986	2.16323	1.00984
H	-1.56312	1.86261	1.34900
C	-0.55304	-0.54856	2.73392
H	-0.21980	-0.40709	3.76900
H	-0.66281	-1.61654	2.53438
H	-1.52093	-0.06473	2.59948
C	0.58777	2.57046	-1.13046
H	0.23621	3.60592	-1.20558
H	0.74744	2.17434	-2.13489
H	1.53216	2.54910	-0.58798
C	1.77109	-0.59279	1.96751
H	1.62629	-1.67452	2.07096
H	2.25005	-0.23241	2.88639
C	2.62530	-0.33323	0.75376
C	4.01572	-0.31435	0.77495
H	4.54239	-0.43517	1.71607
C	4.71211	-0.15351	-0.42507
H	5.79776	-0.14535	-0.42886
C	3.99921	-0.01105	-1.61964
H	4.50509	0.10055	-2.57239
C	2.61289	-0.02506	-1.57358
H	2.00729	0.05340	-2.46947
C	-1.73375	1.81104	-1.13693
H	-1.53953	1.67970	-2.20791
H	-2.18829	2.80014	-1.00348
C	-2.63289	0.70823	-0.64844
C	-4.02061	0.77503	-0.66727
H	-4.51411	1.67330	-1.02385
C	-4.75809	-0.32722	-0.22752
H	-5.84332	-0.29828	-0.23990
C	-4.08401	-1.46337	0.22792
H	-4.62074	-2.34070	0.57203
C	-2.69604	-1.46658	0.22590
H	-2.12260	-2.32944	0.54023
H	0.37477	1.83337	2.92686
H	-0.51042	3.25545	1.07534
Cl	0.11830	-2.31733	-1.17523

^{4}FeBPMENF
Charge: 2+
Energy: -1383985.7106493

Fe	-0.01368	-0.08461	-0.54743
N	0.49298	-1.19256	1.26863
N	-0.43236	1.51334	0.73301
N	1.94123	0.14195	-0.56486
N	-1.99072	-0.17510	-0.56998
C	0.54007	-0.14798	2.33122
H	1.52139	0.33141	2.30112
C	-0.55967	0.88169	2.09778
H	-1.53957	0.40255	2.14767
C	-0.47041	-2.27531	1.58420
H	-0.13689	-2.86037	2.44981
H	-0.56399	-2.93213	0.71674
H	-1.44865	-1.84288	1.79996
C	0.57350	2.61524	0.74899
H	0.22296	3.43222	1.38930
H	0.71562	2.99150	-0.26554
H	1.52507	2.24279	1.12490
C	1.84193	-1.73681	0.97325
H	1.71074	-2.63389	0.35750
H	2.36312	-2.03838	1.89062

C	2.65132	-0.73548	0.18356
C	4.04224	-0.73399	0.14771
H	4.59833	-1.43284	0.76433
C	4.70130	0.15921	-0.69994
H	5.78600	0.16685	-0.74659
C	3.95354	1.03571	-1.49293
H	4.43035	1.73220	-2.17380
C	2.57016	0.99859	-1.39789
H	1.93689	1.64624	-1.99566
C	-1.76223	2.05434	0.29427
H	-1.58797	2.70871	-0.56761
H	-2.20304	2.66670	1.08934
C	-2.65481	0.91457	-0.11369
C	-4.04282	0.95254	-0.09183
H	-4.55704	1.83036	0.28577
C	-4.75468	-0.15070	-0.57333
H	-5.84032	-0.14177	-0.56962
C	-4.05786	-1.25853	-1.06220
H	-4.57773	-2.12564	-1.45471
C	-2.66851	-1.23911	-1.04856
H	-2.06597	-2.05259	-1.43402
H	0.42619	-0.59763	3.32490
H	-0.52867	1.66623	2.86199
F	0.07472	-1.21969	-1.82382

^{4}FeBPMENN$_{3}$
Charge: 2+
Energy: -1424374.3960887

Fe	0.09623	0.26389	-0.26460
N	-0.33082	-0.35376	1.78561
N	0.67172	-1.72835	-0.56947
N	-1.86421	-0.03154	-0.41715
N	2.08264	0.51504	-0.26254
C	-0.24395	-1.84299	1.75216
H	-1.20137	-2.23583	1.40166
C	0.87985	-2.27824	0.81803
H	1.83767	-1.90111	1.18285
C	0.60115	0.24393	2.77297
H	0.30845	-0.01441	3.79794
H	0.59600	1.32896	2.65199
H	1.61243	-0.12104	2.58720
C	-0.28280	-2.57613	-1.33702
H	0.14410	-3.57153	-1.50467
H	-0.48759	-2.10850	-2.30185
H	-1.21817	-2.67290	-0.78756
C	-1.72210	0.11097	2.00674
H	-1.68066	1.17948	2.24628
H	-2.18384	-0.39880	2.86192
C	-2.54704	-0.07170	0.75316
C	-3.93074	-0.21820	0.76479
H	-4.45956	-0.26403	1.71148
C	-4.62080	-0.28879	-0.44754
H	-5.70153	-0.39193	-0.45522
C	-3.90753	-0.22228	-1.64808
H	-4.40829	-0.26602	-2.60905
C	-2.52651	-0.09758	-1.59310
H	-1.92204	-0.03852	-2.49267
C	1.97901	-1.66023	-1.29716
H	1.76102	-1.48209	-2.35665
H	2.50573	-2.61942	-1.22779
C	2.80362	-0.52233	-0.75743
C	4.19172	-0.48792	-0.78792
H	4.74806	-1.33257	-1.18122
C	4.84937	0.65073	-0.31239
H	5.93374	0.70136	-0.33071
C	4.09815	1.71888	0.18379
H	4.57371	2.62009	0.55497
C	2.71258	1.61806	0.19282
H	2.07012	2.41732	0.54261
H	-0.07438	-2.24499	2.75824
H	0.94610	-3.37131	0.77192
N	-0.14757	2.09032	-0.25281
N	-1.18710	2.69132	-0.54156
N	-2.11115	3.31263	-0.78847

^{6}FeBPMENNCS
Charge: 2+
Energy: -1629482.6180144

Fe	0.10533	0.10701	-0.15851
N	-0.55630	-0.47738	1.78324
N	0.71829	-2.04945	-0.36517
N	-1.92538	-0.36864	-0.59613
N	2.20113	0.23278	-0.34311
C	-0.39372	-1.96491	1.86830
H	-1.29971	-2.42676	1.47135
C	0.82862	-2.42710	1.07926
H	1.73098	-1.95492	1.47850
C	0.23002	0.22435	2.83305
H	-0.15766	-0.00857	3.83183
H	0.17630	1.30104	2.66092
H	1.27426	-0.08931	2.77306
C	-0.20518	-2.96564	-1.08550
H	0.19387	-3.98743	-1.10098
H	-0.33207	-2.61668	-2.11236
H	-1.18209	-2.97138	-0.60433
C	-1.99183	-0.07999	1.82444
H	-2.02485	1.00386	1.97849
H	-2.49801	-0.55194	2.67543
C	-2.69108	-0.40529	0.51975
C	-4.05748	-0.66209	0.45073
H	-4.64953	-0.70126	1.35963
C	-4.64922	-0.85722	-0.79958
H	-5.71416	-1.05430	-0.87501
C	-3.85642	-0.79601	-1.94842
H	-4.28022	-0.93603	-2.93685
C	-2.49580	-0.55412	-1.80290
H	-1.83397	-0.50362	-2.66218
C	2.05535	-2.09626	-1.01423
H	1.89876	-2.09591	-2.09936
H	2.57900	-3.02903	-0.76750
C	2.88918	-0.89252	-0.64937
C	4.27963	-0.90965	-0.68264
H	4.80499	-1.82838	-0.92339
C	4.97967	0.26786	-0.41090
H	6.06506	0.27669	-0.43583
C	4.26691	1.43044	-0.10537
H	4.77401	2.36459	0.10988
C	2.88050	1.37314	-0.07896
H	2.27506	2.24095	0.15267
H	-0.30396	-2.27060	2.91698
H	0.95198	-3.51323	1.18180
N	-0.23254	1.97335	-0.12903
C	-0.55746	3.13313	-0.21464
S	-0.98083	4.65540	-0.31864

^{4}FeBPMENOH
Charge: 2+
Energy: -1368904.7746960

Fe	-0.02228	-0.11552	-0.57185
N	0.48879	-1.15729	1.29183
N	-0.41832	1.52887	0.67863
N	1.95122	0.09557	-0.61178
N	-2.01583	-0.18144	-0.57373
C	0.54132	-0.08675	2.32672
H	1.52569	0.38606	2.28605
C	-0.55102	0.94298	2.06166
H	-1.53368	0.47112	2.12616
C	-0.48149	-2.22564	1.63090
H	-0.15391	-2.79378	2.51017
H	-0.57999	-2.89718	0.77573
H	-1.45651	-1.78077	1.83586
C	0.59789	2.61866	0.66151
H	0.26291	3.45829	1.28089
H	0.73991	2.96572	-0.36360
H	1.54778	2.24622	1.04259
C	1.83085	-1.71654	1.00694
H	1.68986	-2.62486	0.41058
H	2.35385	-2.00282	1.92838
C	2.65011	-0.73687	0.19861
C	4.04141	-0.70235	0.22253
H	4.58488	-1.36455	0.88890
C	4.71844	0.17946	-0.62291
H	5.80367	0.21276	-0.62081
C	3.98640	1.01675	-1.47078
H	4.47660	1.71016	-2.14540
C	2.60084	0.94925	-1.43408
H	1.98066	1.57614	-2.06691
C	-1.74082	2.07054	0.22525
H	-1.56082	2.68891	-0.66179
H	-2.17216	2.71944	0.99648
C	-2.65465	0.93060	-0.13596
C	-4.04122	0.99108	-0.08400
H	-4.53359	1.88791	0.27772
C	-4.78028	-0.11579	-0.51302
H	-5.86529	-0.09004	-0.48515
C	-4.11052	-1.24967	-0.97890
H	-4.65184	-2.12235	-1.32748
C	-2.72082	-1.24944	-0.99753
H	-2.13548	-2.08292	-1.36761
H	0.42393	-0.50827	3.33245
H	-0.51671	1.74930	2.80312
O	0.02476	-1.38280	-1.78514
H	0.79197	-1.43588	-2.38338

^{2}FePy5Me2Br
Charge: 2+
Energy: -3283168.7461461

Fe	0.00002	0.00007	-0.49088
N	-0.00007	-0.00016	1.54934
N	-1.53586	-1.36156	-0.43822
N	-1.53644	1.36122	-0.43819
N	1.53602	1.36155	-0.43799
N	1.53658	-1.36100	-0.43861
C	-3.69546	-0.00063	2.35291

H	-4.62418	-0.00098	1.77959
H	-3.69874	0.88118	2.99602
H	-3.69819	-0.88227	2.99626
C	-2.47300	-0.00038	1.41291
C	-1.17307	-0.00010	2.22688
C	-1.19529	0.00005	3.62141
H	-2.12824	0.00035	4.16383
C	-0.00018	-0.00028	4.32681
H	-0.00023	-0.00033	5.41236
C	1.19498	-0.00057	3.62151
H	2.12789	-0.00093	4.16401
C	1.17287	-0.00031	2.22698
C	2.47284	0.00003	1.41309
C	3.69524	0.00001	2.35318
H	4.62400	0.00030	1.77991
H	3.69835	-0.88186	2.99620
H	3.69804	0.88158	2.99663
C	2.50012	1.24866	0.50746
C	3.50683	2.21071	0.61888
H	4.26776	2.12769	1.38033
C	3.55521	3.28844	-0.26276
H	4.33864	4.03439	-0.17323
C	2.59937	3.36287	-1.26750
H	2.60439	4.15162	-2.01156
C	1.62066	2.38099	-1.31915
H	0.90521	2.38317	-2.12174
C	2.50061	-1.24816	0.50692
C	3.50773	-2.20982	0.61794
H	4.26861	-2.12680	1.37944
C	3.55662	-3.28712	-0.26418
H	4.34037	-4.03278	-0.17497
C	2.60085	-3.36149	-1.26900
H	2.60623	-4.14988	-2.01343
C	1.62172	-2.37999	-1.32025
H	0.90637	-2.38209	-2.12293
C	-2.50075	1.24799	0.50700
C	-3.50802	2.20949	0.61799
H	-4.26917	2.12610	1.37919
C	-3.55668	3.28713	-0.26372
H	-4.34055	4.03267	-0.17453
C	-2.60047	3.36205	-1.26808
H	-2.60556	4.15080	-2.01213
C	-1.62126	2.38064	-1.31937
H	-0.90554	2.38321	-2.12171
C	-2.50012	-1.24885	0.50707
C	-3.50679	-2.21097	0.61822
H	-4.26787	-2.12806	1.37953
C	-3.55492	-3.28864	-0.26350
H	-4.33832	-4.03465	-0.17419
C	-2.59883	-3.36297	-1.26802
H	-2.60360	-4.15171	-2.01209
C	-1.62019	-2.38100	-1.31942
H	-0.90453	-2.38315	-2.12181
Br	-0.00020	0.00039	-2.95124

[2]FePy5Me2Cl
Charge: 2+
Energy: -1956643.0779066

Fe	0.00002	0.00008	-0.67954
N	-0.00009	-0.00003	1.35538
N	-1.53623	-1.35132	-0.63563
N	-1.53706	1.35078	-0.63597
N	1.53639	1.35131	-0.63548
N	1.53712	-1.35059	-0.63612
C	-3.69693	-0.00064	2.15687
H	-4.62391	-0.00118	1.58063
H	-3.70226	0.88140	2.79981
H	-3.70147	-0.88240	2.80018
C	-2.47248	-0.00029	1.22020
C	-1.17318	0.00013	2.03393
C	-1.19537	0.00037	3.42829
H	-2.12864	0.00082	3.97029
C	-0.00025	-0.00008	4.13381
H	-0.00031	-0.00009	5.21936
C	1.19495	-0.00052	3.42842
H	2.12816	-0.00101	3.97053
C	1.17292	-0.00023	2.03406
C	2.47228	0.00015	1.22045
C	3.69667	0.00026	2.15722
H	4.62369	0.00067	1.58105
H	3.70180	-0.88179	2.80013
H	3.70129	0.88200	2.80057
C	2.49877	1.24729	0.31162
C	3.50471	2.21080	0.41311
H	4.26398	2.13850	1.17762
C	3.55456	3.27484	-0.48560
H	4.33671	4.02311	-0.40443
C	2.60539	3.33165	-1.49834
H	2.61720	4.10688	-2.25640
C	1.62506	2.35033	-1.53798
H	0.91172	2.33342	-2.34298
C	2.49944	-1.24652	0.31103
C	3.50598	-2.20946	0.41201
H	4.26518	-2.13712	1.17657
C	3.55651	-3.27298	-0.48728
H	4.33913	-4.02081	-0.40651
C	2.60740	-3.32978	-1.50008
H	2.61970	-4.10457	-2.25859
C	1.62647	-2.34905	-1.53918
H	0.91319	-2.33213	-2.34425
C	-2.49962	1.24645	0.31090
C	-3.50630	2.20926	0.41178
H	-4.26573	2.13668	1.17608
C	-3.55666	3.27298	-0.48729
H	-4.33938	4.02070	-0.40661
C	-2.60719	3.33015	-1.49972
H	-2.61928	4.10515	-2.25802
C	-1.62617	2.34951	-1.53877
H	-0.91260	2.33291	-2.34357
C	-2.49878	-1.24737	0.31130
C	-3.50466	-2.21094	0.41263
H	-4.26407	-2.13868	1.17699
C	-3.55424	-3.27503	-0.48604
H	-4.33635	-4.02336	-0.40501
C	-2.60482	-3.33184	-1.49854
H	-2.61636	-4.10715	-2.25653
C	-1.62457	-2.35044	-1.53804
H	-0.91100	-2.33358	-2.34283
Cl	-0.00007	0.00026	-2.93446

[2]FePy5Me2F
Charge: 2+
Energy: -1730525.2394613

Fe	-0.00002	0.00002	-0.71877
N	0.00006	-0.00017	1.31445
N	-1.53123	-1.30735	-0.71510
N	-1.53108	1.30756	-0.71486
N	1.53112	1.30746	-0.71495
N	1.53107	-1.30752	-0.71509
C	-3.70207	-0.00020	2.08213
H	-4.62036	-0.00012	1.49175
H	-3.71623	0.88211	2.72515
H	-3.71625	-0.88277	2.72479
C	-2.46518	-0.00004	1.16467
C	-1.17363	-0.00033	1.99033
C	-1.19725	-0.00077	3.38440
H	-2.13101	-0.00093	3.92651
C	0.00016	-0.00098	4.08839
H	0.00020	-0.00131	5.17397
C	1.19752	-0.00074	3.38432
H	2.13131	-0.00086	3.92636
C	1.17380	-0.00036	1.99024
C	2.46530	-0.00012	1.16451
C	3.70224	0.00005	2.08189
H	4.62050	0.00095	1.49146
H	3.71697	-0.88274	2.72423
H	3.71594	0.88214	2.72524
C	2.48677	1.23982	0.23909
C	3.49122	2.20700	0.29769
H	4.24434	2.17826	1.07217
C	3.54810	3.21329	-0.66747
H	4.32743	3.96755	-0.62226
C	2.62211	3.20139	-1.70531
H	2.65965	3.92097	-2.51561
C	1.63459	2.22524	-1.69363
H	0.92809	2.13367	-2.50236
C	2.48693	-1.23986	0.23875
C	3.49153	-2.20693	0.29697
H	4.24482	-2.17824	1.07126
C	3.54831	-3.21310	-0.66833
H	4.32775	-3.96726	-0.62340
C	2.62202	-3.20125	-1.70590
H	2.65940	-3.92079	-2.51625
C	1.63439	-2.22522	-1.69385
H	0.92762	-2.13374	-2.50236
C	-2.48667	1.23996	0.23926
C	-3.49100	2.20728	0.29793
H	-4.24405	2.17868	1.07247
C	-3.54786	3.21357	-0.66723
H	-4.32710	3.96792	-0.62195
C	-2.62198	3.20156	-1.70517
H	-2.65952	3.92114	-2.51547
C	-1.63455	2.22532	-1.69354
H	-0.92811	2.13368	-2.50232
C	-2.48693	-1.23972	0.23890
C	-3.49161	-2.20667	0.29720
H	-4.24478	-2.17793	1.07162
C	-3.54865	-3.21272	-0.66820
H	-4.32817	-3.96681	-0.62323
C	-2.62257	-3.20082	-1.70595
H	-2.66019	-3.92023	-2.51640
C	-1.63483	-2.22489	-1.69398
H	-0.92824	-2.13331	-2.50265
F	-0.00004	0.00013	-2.48607

^{2}FePy5Me2N$_{3}$
Charge: 2+
Energy: -1770909.1597884

Fe	-0.01897	-0.00016	-0.61229
N	-0.13073	0.00006	1.42996
N	1.46894	1.37981	-0.43443
N	1.46907	-1.38016	-0.43371
N	-1.58032	-1.30666	-0.70515
N	-1.58017	1.30630	-0.70566
C	3.52774	0.00072	2.41687
H	4.48450	0.00123	1.89140
H	3.49938	-0.88228	3.05811
H	3.49858	0.88346	3.05842
C	2.35459	0.00037	1.41733
C	1.00817	-0.00002	2.16526
C	0.95812	-0.00030	3.55881
H	1.86107	-0.00058	4.15027
C	-0.27350	-0.00017	4.20156
H	-0.32820	-0.00032	5.28573
C	-1.43208	0.00019	3.43743
H	-2.39245	0.00043	3.93065
C	-1.33437	0.00020	2.04563
C	-2.57844	0.00023	1.15270
C	-3.85996	0.00039	2.00882
H	-4.74891	0.00034	1.37522
H	-3.90471	0.88187	2.65131
H	-3.90480	-0.88094	2.65151
C	-2.56006	-1.24154	0.22673
C	-3.56661	-2.20906	0.26005
H	-4.33403	-2.18414	1.02011
C	-3.61149	-3.20861	-0.71191
H	-4.39334	-3.96112	-0.68463
C	-2.67236	-3.18522	-1.73704
H	-2.70142	-3.89154	-2.55934
C	-1.68130	-2.21380	-1.69588
H	-0.96792	-2.10994	-2.49942
C	-2.55995	1.24162	0.22626
C	-3.56645	2.20921	0.25917
H	-4.33382	2.18463	1.01927
C	-3.61133	3.20835	-0.71320
H	-4.39316	3.96090	-0.68621
C	-2.67222	3.18449	-1.73832
H	-2.70125	3.89045	-2.56094
C	-1.68118	2.21311	-1.69678
H	-0.96777	2.10900	-2.50024
C	2.42327	-1.24874	0.51669
C	3.43330	-2.20485	0.64809
H	4.19327	-2.10493	1.40899
C	3.48044	-3.30159	-0.21033
H	4.26800	-4.04163	-0.10893
C	2.51037	-3.41490	-1.19960
H	2.50520	-4.23430	-1.90969
C	1.53264	-2.43417	-1.27310
H	0.77949	-2.47972	-2.04061
C	2.42256	1.24955	0.51676
C	3.43149	2.20670	0.64876
H	4.19087	2.10780	1.41038
C	3.47837	3.30318	-0.21004
H	4.26506	4.04407	-0.10809
C	2.50927	3.41504	-1.20040
H	2.50411	4.23402	-1.91097
C	1.53247	2.43341	-1.27436
H	0.78009	2.47788	-2.04268
N	0.09817	-0.00080	-2.48767
N	1.20652	-0.00089	-3.02617
N	2.20372	-0.00099	-3.58803

^{6}FePy5Me2NCS
Charge: 2+
Energy: -1976013.5262206

Fe	0.00005	0.57493	0.00011
N	-0.00037	-1.62871	-0.00043
N	1.64233	0.36236	1.40683
N	1.64225	0.36275	-1.40685
N	-1.64234	0.36366	-1.40667
N	-1.64213	0.36271	1.40705
C	3.70361	-2.47182	-0.00062
H	4.64523	-1.91961	-0.00044
H	3.69373	-3.11420	-0.88287
H	3.69372	-3.11485	0.88115
C	2.50272	-1.50191	-0.00029
C	1.17513	-2.30378	-0.00066
C	1.19587	-3.70034	-0.00126
H	2.12384	-4.25072	-0.00149
C	-0.00093	-4.40273	-0.00157
H	-0.00115	-5.48831	-0.00203
C	-1.19745	-3.69986	-0.00127
H	-2.12564	-4.24987	-0.00148
C	-1.17614	-2.30331	-0.00071
C	-2.50342	-1.50091	-0.00038
C	-3.70468	-2.47038	-0.00044
H	-4.64609	-1.91781	-0.00018
H	-3.69492	-3.11326	0.88144
H	-3.69514	-3.11290	-0.88258
C	-2.57765	-0.60062	-1.26442
C	-3.59394	-0.73048	-2.21619
H	-4.34637	-1.50047	-2.13004
C	-3.66007	0.15057	-3.29636
H	-4.45069	0.04610	-4.03293
C	-2.71946	1.17092	-3.39837
H	-2.74808	1.90052	-4.20008
C	-1.73194	1.23862	-2.42567
H	-0.99543	2.03030	-2.43538
C	-2.57747	-0.60143	1.26423
C	-3.59368	-0.73197	2.21598
H	-4.34611	-1.50191	2.12932
C	-3.65968	0.14830	3.29678
H	-4.45028	0.04338	4.03332
C	-2.71896	1.16849	3.39949
H	-2.74743	1.89746	4.20179
C	-1.73151	1.23685	2.42676
H	-0.99487	2.02840	2.43710
C	2.57731	-0.60171	-1.26436
C	3.59370	-0.73197	-2.21595
H	4.34594	-1.50213	-2.12951
C	3.66015	0.14885	-3.29627
H	4.45090	0.04414	-4.03268
C	2.71968	1.16929	-3.39866
H	2.74848	1.89866	-4.20058
C	1.73204	1.23739	-2.42610
H	0.99559	2.02912	-2.43619
C	2.57713	-0.60238	1.26429
C	3.59310	-0.73334	2.21624
H	4.34509	-1.50374	2.12987
C	3.65950	0.14711	3.29688
H	4.44988	0.04179	4.03360
C	2.71949	1.16799	3.39917
H	2.74837	1.89718	4.20124
C	1.73222	1.23676	2.42629
H	0.99619	2.02888	2.43622
N	0.00042	2.46968	0.00056
C	0.00071	3.67684	0.00084
S	0.00190	5.25963	0.00079

^{2}FePy5Me2OH
Charge: 2+
Energy: -1715439.7733917

Fe	0.00669	-0.00009	-0.76077
O	0.07291	-0.00007	-2.55408
N	-0.06068	-0.00020	1.29491
N	-1.50638	-1.35242	-0.74283
N	-1.50669	1.35194	-0.74322
N	1.56006	1.29926	-0.70921
N	1.56056	-1.29890	-0.70962
C	-3.78893	0.00001	1.94590
H	-4.69222	0.00040	1.33257
H	-3.81960	0.88174	2.58876
H	-3.82002	-0.88206	2.58828
C	-2.52739	-0.00004	1.06110
C	-1.25700	-0.00042	1.92944
C	-1.32982	-0.00105	3.32188
H	-2.28084	-0.00123	3.83284
C	-0.15753	-0.00148	4.06792
H	-0.19625	-0.00201	5.15279
C	1.06317	-0.00118	3.40669
H	1.97753	-0.00147	3.98098
C	1.08569	-0.00050	2.01158
C	2.40106	-0.00002	1.22658
C	3.60690	0.00009	2.18542
H	4.54503	0.00052	1.62713
H	3.59879	-0.88181	2.82902
H	3.59824	0.88164	2.82949
C	2.45889	1.24057	0.30020
C	3.45740	2.21034	0.40930
H	4.16112	2.19195	1.22913
C	3.57723	3.20312	-0.56388
H	4.35247	3.95819	-0.47889
C	2.72517	3.17027	-1.66261
H	2.82157	3.87128	-2.48431
C	1.73581	2.19627	-1.69711
H	1.09061	2.07348	-2.55355
C	2.45948	-1.24018	0.29969
C	3.45858	-2.20941	0.40821
H	4.16240	-2.19098	1.22795
C	3.57885	-3.20168	-0.56543
H	4.35454	-3.95634	-0.48090
C	2.72663	-3.16880	-1.66404
H	2.82333	-3.86938	-2.48607
C	1.73672	-2.19535	-1.69798
H	1.09139	-2.07245	-2.55432
C	-2.51547	1.24834	0.15218
C	-3.51703	2.22093	0.20493
H	-4.31868	2.15181	0.92577
C	-3.50218	3.29304	-0.68629
H	-4.28024	4.04876	-0.64346
C	-2.49010	3.35797	-1.63810

H	-2.44627	4.15053	-2.37690
C	-1.51943	2.36624	-1.63073
H	-0.73306	2.35958	-2.36703
C	-2.51575	-1.24820	0.15185
C	-3.51795	-2.22018	0.20387
H	-4.32019	-2.15045	0.92399
C	-3.50291	-3.29250	-0.68709
H	-4.28148	-4.04772	-0.64482
C	-2.48989	-3.35837	-1.63782
H	-2.44568	-4.15129	-2.37621
C	-1.51875	-2.36710	-1.62991
H	-0.73161	-2.36123	-2.36539
H	-0.82512	-0.00045	-2.92881

^{6}FeLBr2
Charge: 3+
Energy: -3294126.6037048

Fe	-0.99837	-0.27162	0.13684
N	-0.28575	-1.58179	1.68593
N	-0.87578	-1.71253	-1.45174
N	-1.20932	1.35877	-1.27262
N	-0.65761	1.50620	1.32815
N	1.33154	-0.52952	-0.34850
C	-1.05161	-1.92706	2.74792
H	-2.06940	-1.55698	2.74088
C	-0.57130	-2.70672	3.79383
H	-1.22737	-2.96367	4.61871
C	0.75377	-3.14304	3.75127
H	1.16331	-3.75163	4.55192
C	1.54421	-2.79267	2.65336
H	2.57046	-3.14018	2.57953
C	0.99276	-2.02415	1.63192
C	1.75431	-1.77171	0.35022
H	1.55243	-2.61400	-0.31917
H	2.83662	-1.78685	0.52820
C	-1.86779	-2.58240	-1.74196
H	-2.74694	-2.53282	-1.11162
C	-1.77602	-3.48732	-2.79580
H	-2.59826	-4.16668	-2.99396
C	-0.61896	-3.49689	-3.57448
H	-0.51475	-4.19045	-4.40345
C	0.41550	-2.60584	-3.26496
H	1.33355	-2.60027	-3.84423
C	0.25472	-1.72628	-2.20152
C	1.31331	-0.71374	-1.82171
H	2.29039	-1.02942	-2.20825
H	1.07144	0.25765	-2.26726
C	-1.57343	1.18762	-2.55778
H	-1.56065	0.16977	-2.92623
C	-1.97016	2.24118	-3.37430
H	-2.26100	2.05203	-4.40198
C	-2.00071	3.52585	-2.83115
H	-2.31356	4.37512	-3.43073
C	-1.64235	3.70586	-1.49485
H	-1.68738	4.69665	-1.05987
C	-1.25755	2.60301	-0.72756
C	-0.93132	2.68693	0.71432
C	-0.92897	3.88473	1.43567
H	-1.14904	4.82638	0.94806
C	-0.65857	3.86639	2.80362
H	-0.66973	4.79018	3.37388
C	-0.38633	2.64678	3.42519
H	-0.18376	2.58511	4.48904
C	-0.39649	1.49323	2.64875
H	-0.20611	0.52205	3.08782
C	2.07893	0.67431	0.09043
H	1.94933	0.75805	1.17363
H	1.58489	1.54281	-0.35209
C	3.55905	0.73190	-0.26467
N	4.47536	0.42161	0.69670
H	4.13956	0.18001	1.62672
C	4.04862	1.11743	-1.50667
H	3.35101	1.40229	-2.28625
C	5.42915	1.16524	-1.74289
H	5.80193	1.47523	-2.71488
C	5.81785	0.46253	0.51199
H	6.43625	0.20656	1.36551
C	6.32573	0.82999	-0.72351
H	7.39949	0.86569	-0.87381
Br	-3.36349	-0.36059	0.58510

^{6}FeLCl2
Charge: 3+
Energy: -1967598.5523476

Fe	-1.17803	-0.34949	0.30310
N	-0.25113	-1.48822	1.86459
N	-1.09243	-1.89292	-1.17716
N	-1.61374	1.15074	-1.19535
N	-0.85373	1.53116	1.32763
N	1.12244	-0.50773	-0.36895
C	-0.91682	-1.79666	3.00242
H	-1.95516	-1.49058	3.04318
C	-0.31076	-2.46364	4.06093
H	-0.88635	-2.69721	4.95032
C	1.03424	-2.81971	3.94726
H	1.54009	-3.33886	4.75581
C	1.71922	-2.50828	2.76923
H	2.75794	-2.79854	2.64201
C	1.04561	-1.85514	1.74103
C	1.68733	-1.65779	0.38583
H	1.49674	-2.56384	-0.19835
H	2.77821	-1.58592	0.47509
C	-2.05839	-2.82816	-1.30546
H	-2.88316	-2.76157	-0.60640
C	-2.00388	-3.81564	-2.28530
H	-2.80135	-4.54772	-2.35582
C	-0.91504	-3.83815	-3.15692
H	-0.84159	-4.59600	-3.93111
C	0.09157	-2.87506	-3.01482
H	0.95612	-2.87617	-3.67127
C	-0.02895	-1.91483	-2.01820
C	0.99265	-0.81692	-1.81583
H	1.95189	-1.10782	-2.26172
H	0.65187	0.09808	-2.31332
C	-2.07188	0.85696	-2.42706
H	-2.00516	-0.18115	-2.72670
C	-2.62359	1.81376	-3.27229
H	-2.98438	1.52748	-4.25432
C	-2.71477	3.12868	-2.81529
H	-3.14746	3.90469	-3.43918
C	-2.26008	3.43410	-1.53203
H	-2.35080	4.44772	-1.16152
C	-1.72010	2.42408	-0.73147
C	-1.27877	2.63867	0.66552
C	-1.31406	3.88234	1.30333
H	-1.65414	4.76595	0.77750
C	-0.92470	3.98461	2.63856
H	-0.96323	4.94392	3.14547
C	-0.49829	2.83843	3.31119
H	-0.19936	2.87058	4.35341
C	-0.47947	1.63391	2.61665
H	-0.17069	0.71481	3.09856
C	1.81803	0.77359	-0.09471
H	1.77537	0.93916	0.98595
H	1.22815	1.56909	-0.55678
C	3.25494	0.89445	-0.58579
N	4.26930	0.72704	0.31049
H	4.03183	0.54582	1.28353
C	3.60877	1.20204	-1.89386
H	2.82926	1.37407	-2.62753
C	4.95741	1.31684	-2.25718
H	5.22336	1.56504	-3.28066
C	5.58497	0.83712	0.00230
H	6.29017	0.69550	0.81412
C	5.95880	1.12821	-1.29961
H	7.01069	1.21892	-1.54888
Cl	-3.28935	-0.57506	0.92758

^{6}FeLF2
Charge: 3+
Energy: -1741474.9561766

Fe	1.21581	0.42362	0.39519
N	0.15041	1.42245	1.93675
N	1.08815	2.00541	-1.00431
N	1.88240	-0.95964	-1.12186
N	1.02443	-1.51228	1.33364
N	-1.08346	0.46592	-0.37182
C	0.79917	1.74092	3.08034
H	1.86046	1.51873	3.09511
C	0.14210	2.32003	4.15997
H	0.69504	2.56867	5.05956
C	-1.22772	2.57253	4.05262
H	-1.77247	3.02004	4.87858
C	-1.88895	2.25803	2.86097
H	-2.94591	2.47699	2.74178
C	-1.16598	1.69633	1.81259
C	-1.77005	1.51070	0.43626
H	-1.66280	2.46331	-0.09317
H	-2.84939	1.32774	0.50210
C	2.02809	2.97386	-1.01947
H	2.82741	2.86467	-0.29479
C	1.96541	4.03554	-1.91807
H	2.73671	4.79831	-1.90758
C	0.89789	4.09224	-2.81568
H	0.81810	4.90982	-3.52587
C	-0.07838	3.08731	-2.78816
H	-0.92144	3.11443	-3.47142
C	0.04996	2.05190	-1.87122
C	-0.91631	0.88857	-1.78795
H	-1.87230	1.15370	-2.25612
H	-0.49893	0.03327	-2.33250
C	2.35609	-0.57793	-2.32349
H	2.19757	0.45893	-2.59191
C	3.03128	-1.44578	-3.17542
H	3.39983	-1.09096	-4.13185

C	3.23180	-2.76180	-2.75835
H	3.76188	-3.46915	-3.38873
C	2.75640	-3.15828	-1.50757
H	2.92690	-4.17287	-1.16913
C	2.08888	-2.23542	-0.69879
C	1.59794	-2.54634	0.66383
C	1.72280	-3.80345	1.26209
H	2.18283	-4.62764	0.73100
C	1.26572	-3.99511	2.56589
H	1.37117	-4.96468	3.04293
C	0.68402	-2.92451	3.24680
H	0.32682	-3.02755	4.26580
C	0.58514	-1.70151	2.59253
H	0.15660	-0.83640	3.08325
C	-1.68084	-0.88357	-0.21738
H	-1.66672	-1.12208	0.85063
H	-1.00929	-1.59546	-0.70461
C	-3.08272	-1.08326	-0.77974
N	-4.14141	-1.06959	0.08003
H	-3.95802	-0.94810	1.07382
C	-3.35903	-1.31298	-2.12209
H	-2.54048	-1.36332	-2.83118
C	-4.67840	-1.50569	-2.55339
H	-4.88300	-1.69195	-3.60376
C	-5.43053	-1.25925	-0.29458
H	-6.17586	-1.23936	0.49316
C	-5.72832	-1.47441	-1.63036
H	-6.75863	-1.62838	-1.93300
F	2.78073	0.91525	1.03810

$^{6}FeLN_{3}2$
Charge: 3+
Energy: -1781863.7310048

Fe	-1.09488	-0.43386	0.27554
N	-0.16074	-1.44808	1.91162
N	-0.84914	-2.02436	-1.13822
N	-1.54511	1.00136	-1.31553
N	-0.90062	1.53699	1.21613
N	1.26912	-0.49192	-0.30467
C	-0.86472	-1.73838	3.02849
H	-1.92108	-1.49680	2.99409
C	-0.27749	-2.30944	4.15195
H	-0.88141	-2.53327	5.02483
C	1.09128	-2.58432	4.12226
H	1.58508	-3.02721	4.98198
C	1.81670	-2.29349	2.96344
H	2.87614	-2.52471	2.90388
C	1.15842	-1.73831	1.86902
C	1.85244	-1.57198	0.53347
H	1.73348	-2.51475	-0.01046
H	2.93364	-1.44354	0.66905
C	-1.76300	-3.00896	-1.26269
H	-2.61623	-2.94818	-0.59656
C	-1.62205	-4.03791	-2.18959
H	-2.37974	-4.81106	-2.25968
C	-0.49351	-4.04823	-3.01044
H	-0.34979	-4.83727	-3.74241
C	0.46048	-3.03335	-2.87150
H	1.35351	-3.02475	-3.48862
C	0.25024	-2.03383	-1.92830
C	1.21209	-0.87913	-1.73635
H	2.20000	-1.14507	-2.13373
H	0.84899	-0.00709	-2.29263
C	-1.92798	0.63746	-2.55379
H	-1.82105	-0.41321	-2.79511
C	-2.44979	1.53799	-3.47732
H	-2.74964	1.19544	-4.46188
C	-2.58747	2.87270	-3.09529
H	-2.99769	3.60729	-3.78141
C	-2.20599	3.25283	-1.80826
H	-2.32976	4.28331	-1.49873
C	-1.69141	2.29550	-0.92843
C	-1.31216	2.59677	0.47378
C	-1.38737	3.87704	1.03266
H	-1.71605	4.72302	0.44163
C	-1.04898	4.06590	2.37232
H	-1.11647	5.05379	2.81754
C	-0.63481	2.96860	3.12850
H	-0.37429	3.06821	4.17678
C	-0.57557	1.72450	2.50822
H	-0.27151	0.84020	3.05540
C	1.88939	0.83261	-0.06960
H	1.78872	1.05265	0.99779
H	1.28702	1.57498	-0.59951
C	3.34102	0.99743	-0.50196
N	4.31919	0.92107	0.44496
H	4.04417	0.77982	1.41467
C	3.74186	1.25056	-1.80844
H	2.99005	1.34873	-2.58340
C	5.09955	1.40412	-2.11811
H	5.40206	1.60913	-3.14097
C	5.64227	1.07093	0.18906
H	6.31458	1.00187	1.03731
C	6.06308	1.30920	-1.10886
H	7.12067	1.43150	-1.31682
N	-2.87905	-0.71358	0.74666
N	-4.02514	-0.29871	0.75490
N	-5.10645	0.07959	0.76947

$^{6}FeLNCS2$
Charge: 3+
Energy: -1986973.1713091

Fe	-0.97716	-0.28718	0.09864
N	-0.29053	-1.57518	1.68254
N	-0.76495	-1.73365	-1.48111
N	-1.12309	1.35345	-1.34131
N	-0.66611	1.53357	1.28061
N	1.41097	-0.56244	-0.29523
C	-1.10973	-1.89258	2.70913
H	-2.12497	-1.52061	2.63248
C	-0.68437	-2.64457	3.79864
H	-1.37826	-2.88212	4.59789
C	0.64190	-3.08020	3.83132
H	1.01076	-3.66743	4.66688
C	1.48690	-2.75977	2.76535
H	2.51485	-3.10990	2.75198
C	0.98592	-2.01671	1.69905
C	1.80098	-1.79087	0.44344
H	1.62045	-2.64552	-0.21661
H	2.87550	-1.81039	0.66564
C	-1.76035	-2.58451	-1.80327
H	-2.66186	-2.50407	-1.20700
C	-1.64213	-3.50663	-2.83949
H	-2.46667	-4.17348	-3.06789
C	-0.44930	-3.55060	-3.56230
H	-0.32111	-4.25931	-4.37486
C	0.58791	-2.67563	-3.21966
H	1.53068	-2.69672	-3.75739
C	0.39539	-1.77686	-2.17642
C	1.44960	-0.77030	-1.76376
H	2.43765	-1.09896	-2.11102
H	1.23200	0.19631	-2.23269
C	-1.42477	1.17358	-2.64039
H	-1.40551	0.15052	-2.99581
C	-1.76216	2.22285	-3.48963
H	-2.00202	2.02632	-4.52904
C	-1.79602	3.51457	-2.96407
H	-2.06109	4.36181	-3.58900
C	-1.49995	3.70530	-1.61426
H	-1.54491	4.70293	-1.19516
C	-1.17173	2.60497	-0.81624
C	-0.89601	2.70688	0.63779
C	-0.88946	3.91970	1.33510
H	-1.07251	4.85619	0.82285
C	-0.65818	3.92373	2.71017
H	-0.66312	4.85917	3.26115
C	-0.43108	2.71149	3.36296
H	-0.25878	2.66718	4.43300
C	-0.44388	1.54331	2.60739
H	-0.28350	0.57680	3.06988
C	2.13684	0.64743	0.15475
H	1.95825	0.75197	1.22945
H	1.66581	1.50923	-0.32491
C	3.63191	0.69638	-0.13277
N	4.50210	0.39606	0.87296
H	4.12217	0.17194	1.79024
C	4.17944	1.05545	-1.35878
H	3.51875	1.33018	-2.17329
C	5.56889	1.08817	-1.53407
H	5.98719	1.37726	-2.49385
C	5.85191	0.42263	0.74752
H	6.42946	0.17622	1.63180
C	6.41684	0.76406	-0.47003
H	7.49636	0.78824	-0.57345
N	-2.82056	-0.44901	0.39883
C	-4.02324	-0.38642	0.52941
S	-5.58979	-0.31224	0.70136

$^{2}FeLOH2$
Charge: 3+
Energy: -1726392.1177401

Fe	-1.02090	0.59415	0.01404
O	-2.53214	1.52787	0.04588
N	-1.75941	-0.70835	1.34897
N	-1.80872	-0.69542	-1.30110
N	-0.18207	1.82404	-1.29254
N	-0.13911	1.82446	1.29286
N	0.64100	-0.83209	-0.01957
C	-3.03296	-0.67070	1.78397
H	-3.59269	0.21217	1.49844
C	-3.58031	-1.70972	2.53328
H	-4.60745	-1.64128	2.87536
C	-2.79485	-2.82809	2.81292
H	-3.19919	-3.66127	3.37953
C	-1.47459	-2.86411	2.35115

H	-0.83684	-3.71806	2.55696
C	-0.98799	-1.78041	1.62996
C	0.45756	-1.65565	1.21773
H	0.92541	-2.64139	1.10824
H	0.97842	-1.12650	2.02587
C	-3.09790	-0.65961	-1.68754
H	-3.65311	0.21321	-1.36497
C	-3.66369	-1.68774	-2.43784
H	-4.70318	-1.62143	-2.74080
C	-2.87926	-2.79231	-2.77089
H	-3.29696	-3.61628	-3.34128
C	-1.54275	-2.82631	-2.35879
H	-0.90503	-3.66866	-2.60778
C	-1.03874	-1.75387	-1.63240
C	0.41953	-1.62317	-1.27412
H	0.90335	-2.60450	-1.21110
H	0.90768	-1.06709	-2.08259
C	-0.32083	1.74046	-2.62797
H	-0.88537	0.89231	-2.99527
C	0.20559	2.69923	-3.48969
H	0.06417	2.59958	-4.56056
C	0.89159	3.78588	-2.94417
H	1.30608	4.55741	-3.58575
C	1.02504	3.88117	-1.55769
H	1.53935	4.72896	-1.12018
C	0.47130	2.88791	-0.74790
C	0.49057	2.89106	0.72651
C	1.05446	3.89404	1.51760
H	1.54794	4.74524	1.06307
C	0.95488	3.80545	2.90718
H	1.37542	4.58562	3.53427
C	0.29301	2.71502	3.47537
H	0.17673	2.62149	4.54985
C	-0.24454	1.74658	2.63180
H	-0.79377	0.89574	3.01617
C	1.99406	-0.19459	-0.03145
H	2.05796	0.44652	0.85170
H	2.03575	0.46119	-0.90256
C	3.19128	-1.13440	-0.08521
N	3.79454	-1.49748	1.08349
H	3.43246	-1.11975	1.95612
C	3.74583	-1.62200	-1.26203
H	3.31560	-1.33104	-2.21366
C	4.86906	-2.46047	-1.22587
H	5.29900	-2.82911	-2.15279
C	4.88403	-2.29929	1.16183
H	5.27405	-2.49711	2.15447
C	5.44358	-2.80762	0.00005
H	6.31800	-3.44692	0.06000
H	-2.40448	2.49355	0.03756

^{5}FeTQABrOH
Charge: 2+
Energy: -3319903.8997327

Fe	-0.27110	-0.82084	-0.40872
N	-2.22229	-0.76336	0.21178
N	0.41500	0.15163	1.34635
N	1.70070	-1.22170	-0.66052
N	-0.32397	-2.44781	0.71564
C	-1.64967	-3.08702	0.46205
C	-2.69431	-2.00477	0.39046
C	-4.07016	-2.28965	0.43806
C	-4.97076	-1.26228	0.24052
C	-4.49564	0.06110	0.07694
C	-5.35743	1.17410	-0.14330
C	-4.84968	2.46247	-0.28455
C	-3.47521	2.69007	-0.15573
C	-2.58782	1.62230	0.06394
C	-3.09166	0.28032	0.12581
C	-0.21091	-2.05296	2.15155
C	0.48496	-0.73274	2.34469
C	1.10083	-0.47181	3.58303
C	1.65935	0.76598	3.80182
C	1.60787	1.74300	2.78344
C	2.16695	3.03594	2.96083
C	2.10611	3.97006	1.95199
C	1.48456	3.63477	0.72732
C	0.93724	2.38394	0.52253
C	0.97696	1.40406	1.53850
C	0.81821	-3.28239	0.24780
C	1.99048	-2.40733	-0.10684
C	3.30330	-2.87560	0.06380
C	4.35251	-2.09374	-0.36823
C	4.09146	-0.86279	-1.00669
C	5.13539	-0.04550	-1.51634
C	4.84682	1.12319	-2.18191
C	3.49828	1.50965	-2.36791
C	2.46249	0.74959	-1.86643
C	2.72534	-0.44527	-1.16320
H	-1.88088	-3.82780	1.23697
H	-1.60850	-3.58979	-0.50546
H	-4.40425	-3.31082	0.58869
H	-6.03893	-1.45880	0.21792
H	-6.42804	1.00015	-0.20682
H	-5.52470	3.29419	-0.45651
H	-3.08242	3.70080	-0.19726
H	-1.58639	1.81909	0.42440
H	0.28267	-2.84904	2.71841
H	-1.22397	-1.95595	2.55521
H	1.12422	-1.24357	4.34523
H	2.14246	0.99865	4.74674
H	2.64089	3.27199	3.90918
H	2.53211	4.95824	2.09153
H	1.44033	4.37060	-0.07011
H	0.47894	2.14588	-0.42374
H	0.49619	-3.78549	-0.66744
H	1.07828	-4.04133	0.99279
H	3.47219	-3.84078	0.52895
H	5.37949	-2.42264	-0.23624
H	6.16279	-0.37246	-1.38543
H	5.64586	1.73959	-2.58068
H	3.27318	2.41538	-2.92281
H	1.43939	1.04580	-2.03672
O	-0.69519	-1.90278	-1.75787
H	-0.70442	-1.43147	-2.60894
Br	-1.12165	1.19206	-2.18699

^{5}FeTQAClOH
Charge: 2+
Energy: -1993379.4576342

Fe	-0.43508	-0.69236	-0.76382
N	-2.58452	-0.53939	0.01432
N	0.30768	0.49321	0.92702
N	1.80274	-1.34014	-0.59091
N	-0.55672	-2.17865	0.69505
C	-1.89410	-2.81120	0.52895
C	-2.97643	-1.76012	0.38351
C	-4.32769	-2.09956	0.59118
C	-5.29551	-1.13155	0.39802
C	-4.91009	0.17814	0.03133
C	-5.84487	1.22953	-0.17178
C	-5.41164	2.50650	-0.50990
C	-4.03730	2.77198	-0.64733
C	-3.09742	1.76503	-0.46037
C	-3.51671	0.44538	-0.13878
C	-0.44852	-1.54405	2.03797
C	0.33568	-0.25916	2.03588
C	0.99896	0.12040	3.21748
C	1.66065	1.32693	3.25967
C	1.65161	2.16024	2.12114
C	2.31352	3.41697	2.11291
C	2.28626	4.22313	0.99115
C	1.58832	3.79289	-0.15463
C	0.93527	2.57012	-0.18088
C	0.95239	1.71593	0.94962
C	0.54546	-3.14141	0.42272
C	1.86217	-2.43675	0.16859
C	3.07331	-2.95751	0.66166
C	4.25629	-2.30579	0.35778
C	4.22509	-1.14602	-0.44777
C	5.39340	-0.42556	-0.81574
C	5.30493	0.70024	-1.62686
C	4.05380	1.13160	-2.10447
C	2.88959	0.45455	-1.75931
C	2.95318	-0.69238	-0.91959
H	-2.10552	-3.48006	1.37321
H	-1.86607	-3.40852	-0.38504
H	-4.59556	-3.10883	0.88707
H	-6.34712	-1.36575	0.53831
H	-6.90545	1.01982	-0.06529
H	-6.13550	3.30009	-0.66360
H	-3.70571	3.77372	-0.90127
H	-2.03852	1.96615	-0.54735
H	-0.02502	-2.25841	2.75279
H	-1.45934	-1.30801	2.38375
H	0.98166	-0.54026	4.07774
H	2.18680	1.64227	4.15647
H	2.83676	3.73513	3.01017
H	2.78966	5.18442	0.99489
H	1.55100	4.42991	-1.03321
H	0.39188	2.26285	-1.06114
H	0.27501	-3.67967	-0.48985
H	0.63075	-3.86539	1.24153
H	3.07176	-3.85593	1.27017
H	5.20531	-2.67923	0.73260
H	6.36087	-0.77478	-0.46587
H	6.20602	1.23687	-1.90561
H	3.99567	1.99498	-2.75972
H	1.92508	0.75606	-2.14722
O	-0.80283	-2.01701	-1.88575
H	-0.91488	-1.71279	-2.80491
Cl	-0.61626	0.76686	-2.50321

^{3}FeTQAFOH
Charge: 2+

Energy: -1767266.3403380

Fe	-0.31831	-0.84276	-0.57191
N	-2.29104	-0.66022	-0.22790
N	0.15125	0.46823	0.99652
N	1.67216	-1.27427	-0.45605
N	-0.53092	-2.19608	0.88886
C	-1.81638	-2.88779	0.57289
C	-2.81300	-1.82435	0.19748
C	-4.19141	-2.04872	0.28541
C	-5.05354	-1.03966	-0.09577
C	-4.54449	0.21024	-0.50494
C	-5.40294	1.28854	-0.84696
C	-4.88084	2.51368	-1.19267
C	-3.47927	2.70088	-1.19806
C	-2.61133	1.67278	-0.88492
C	-3.11809	0.40048	-0.54654
C	-0.62845	-1.48715	2.20400
C	0.03100	-0.13718	2.18173
C	0.41634	0.45037	3.39778
C	0.93927	1.72375	3.38289
C	1.08831	2.40588	2.15684
C	1.62998	3.71719	2.10186
C	1.77827	4.36322	0.89630
C	1.38923	3.71067	-0.29544
C	0.86145	2.43422	-0.28066
C	0.69088	1.74655	0.94137
C	0.66620	-3.08022	0.79449
C	1.87798	-2.27043	0.41891
C	3.15231	-2.61642	0.88869
C	4.24607	-1.91648	0.42147
C	4.07725	-0.91870	-0.56011
C	5.18536	-0.23426	-1.12734
C	4.99926	0.67312	-2.14365
C	3.69482	0.91712	-2.63545
C	2.58973	0.29482	-2.09091
C	2.74762	-0.62035	-1.02629
H	-2.15409	-3.48413	1.42806
H	-1.64857	-3.55495	-0.27492
H	-4.55815	-3.00566	0.64106
H	-6.12860	-1.19240	-0.05994
H	-6.47660	1.12762	-0.81865
H	-5.53801	3.33756	-1.45063
H	-3.07339	3.67515	-1.45276
H	-1.54851	1.83973	-0.89844
H	-0.21299	-2.12094	2.99354
H	-1.68924	-1.34312	2.43094
H	0.29248	-0.10020	4.32434
H	1.24499	2.20738	4.30648
H	1.92185	4.19772	3.03112
H	2.18981	5.36646	0.85698
H	1.50725	4.22137	-1.24646
H	0.57288	1.95314	-1.19985
H	0.47929	-3.79595	-0.01130
H	0.80908	-3.63797	1.72496
H	3.25999	-3.42358	1.60508
H	5.24382	-2.14621	0.78487
H	6.18118	-0.46338	-0.75937
H	5.84857	1.18304	-2.58645
H	3.55929	1.60099	-3.46793
H	1.60273	0.47348	-2.48805
O	-0.55292	-2.15530	-1.71843
H	-0.38715	-1.80896	-2.61760
F	-0.30422	0.31483	-1.89582

^{5}FeTQAN$_{3}$OH

Charge: 2+

Energy: -1807649.6229586

Fe	-0.52439	-0.58282	-0.88425
N	-2.57139	-0.52898	0.06455
N	0.42075	0.31777	1.17590
N	1.66509	-1.25700	-0.75870
N	-0.58283	-2.28110	0.55726
C	-1.93472	-2.85463	0.35490
C	-2.97557	-1.75852	0.39727
C	-4.30590	-2.05888	0.74854
C	-5.24473	-1.04818	0.74262
C	-4.84810	0.27090	0.42582
C	-5.75711	1.36230	0.43328
C	-5.32160	2.64483	0.14418
C	-3.96296	2.87547	-0.15286
C	-3.05227	1.83161	-0.17500
C	-3.47421	0.50458	0.09885
C	-0.39424	-1.84371	1.95986
C	0.50563	-0.63525	2.10963
C	1.34132	-0.53197	3.24031
C	2.13194	0.58864	3.39576
C	2.07525	1.61339	2.42455
C	2.85505	2.79586	2.51492
C	2.76504	3.78417	1.54120
C	1.88715	3.61999	0.45700
C	1.10329	2.47532	0.34030
C	1.18506	1.44168	1.31720
C	0.48605	-3.19590	0.09217
C	1.77681	-2.45008	-0.16389
C	3.02066	-3.01518	0.17594
C	4.17805	-2.30833	-0.09037
C	4.09119	-1.04244	-0.71123
C	5.23462	-0.25550	-1.01581
C	5.10234	0.97757	-1.64180
C	3.82700	1.45253	-1.99518
C	2.68591	0.71002	-1.71026
C	2.79357	-0.54731	-1.05199
H	-2.15651	-3.63270	1.09736
H	-1.95441	-3.30696	-0.64031
H	-4.57680	-3.07645	1.01040
H	-6.28151	-1.25314	0.99465
H	-6.80030	1.17445	0.67073
H	-6.02357	3.47220	0.15044
H	-3.62618	3.88476	-0.36831
H	-2.00988	2.00537	-0.40620
H	-0.02415	-2.67455	2.57384
H	-1.37346	-1.56454	2.36185
H	1.35986	-1.33291	3.97208
H	2.79419	0.68813	4.25145
H	3.51829	2.92413	3.36595
H	3.36246	4.68603	1.62711
H	1.80555	4.40035	-0.29347
H	0.40928	2.35575	-0.48293
H	0.15534	-3.61477	-0.86305
H	0.64244	-4.02030	0.79969
H	3.05808	-3.99184	0.64686
H	5.14991	-2.71571	0.17445
H	6.21902	-0.63942	-0.76287
H	5.98504	1.56384	-1.87563
H	3.72991	2.40309	-2.51037
H	1.70335	1.04758	-2.01527
O	-0.95855	-1.82359	-2.15609
H	-1.08326	-1.60468	-3.09463
N	-0.53702	1.03495	-1.91943
N	-1.05408	1.24903	-3.00839
N	-1.53013	1.48627	-4.02262

^{5}FeTQANCSOH

Charge: 2+

Energy: -2012759.2650010

Fe	-0.42175	-0.50257	-0.88643
N	-2.42341	-0.82237	0.05675
N	0.47287	-0.12451	1.28123
N	1.77541	-1.03829	-1.02755
N	-0.36487	-2.51877	-0.02257
C	-1.69015	-3.09197	-0.36889
C	-2.78251	-2.10564	-0.02583
C	-4.10672	-2.54386	0.16667
C	-5.08443	-1.61082	0.43900
C	-4.73432	-0.24763	0.57993
C	-5.68450	0.75482	0.90911
C	-5.28807	2.06683	1.08702
C	-3.92581	2.41587	0.95784
C	-2.97822	1.46581	0.62393
C	-3.36145	0.11924	0.40494
C	-0.16721	-2.47152	1.44830
C	0.64569	-1.28463	1.91982
C	1.49237	-1.42939	3.03745
C	2.19603	-0.33508	3.49550
C	2.03999	0.91050	2.84678
C	2.72721	2.08031	3.26541
C	2.53769	3.28617	2.60867
C	1.64845	3.35904	1.51933
C	0.95394	2.23618	1.09192
C	1.14449	0.98117	1.73206
C	0.74217	-3.20803	-0.73028
C	1.97717	-2.33887	-0.79912
C	3.26288	-2.89895	-0.67636
C	4.36714	-2.07637	-0.78126
C	4.18810	-0.69636	-1.02384
C	5.27778	0.20762	-1.14896
C	5.05542	1.55044	-1.40403
C	3.73853	2.02926	-1.55526
C	2.65205	1.17603	-1.43345
C	2.85145	-0.20243	-1.15722
H	-1.85326	-4.05111	0.13979
H	-1.70365	-3.26535	-1.44806
H	-4.34151	-3.60026	0.08718
H	-6.11920	-1.91541	0.56906
H	-6.72650	0.47136	1.02605
H	-6.01947	2.82757	1.33938
H	-3.61893	3.44336	1.12684
H	-1.93339	1.72889	0.54127
H	0.28138	-3.40870	1.79903
H	-1.15249	-2.39376	1.91821
H	1.58659	-2.39603	3.52116
H	2.86531	-0.42137	4.34710
H	3.39924	2.01741	4.11672
H	3.06276	4.17547	2.94183
H	1.48989	4.30873	1.01754
H	0.24667	2.29961	0.27591

H	0.40669	-3.38584	-1.75616
H	0.96472	-4.17634	-0.26527
H	3.37204	-3.96348	-0.49798
H	5.37050	-2.48035	-0.67824
H	6.29003	-0.17508	-1.05403
H	5.89468	2.23088	-1.50467
H	3.57135	3.07793	-1.78080
H	1.64224	1.53516	-1.57865
O	-0.82734	-1.32823	-2.46211
H	-0.95919	-0.81238	-3.27568
N	-0.63478	1.34490	-1.51578
C	-1.20558	2.16228	-2.18737
S	-1.94666	3.28593	-3.03992

^{6}FeTQAOH
Charge: 2+
Energy: -1704606.9208396

Fe	-0.00366	-0.09216	-0.06710
N	0.22072	1.88898	0.52480
N	1.82221	-1.19331	0.33454
N	-1.98254	-0.82967	0.33253
N	0.05645	-0.32196	2.08950
O	0.17399	-0.19368	-1.85413
C	0.95408	0.76024	2.55874
C	0.69597	2.03000	1.77334
C	0.97451	3.28426	2.33535
C	0.75588	4.42001	1.57974
C	0.24507	4.31521	0.26767
C	-0.01673	5.45447	-0.53785
C	-0.52869	5.30431	-1.80685
C	-0.79422	4.00971	-2.31381
C	-0.55136	2.87792	-1.55926
C	-0.02508	3.00615	-0.25470
C	0.57608	-1.68120	2.35245
C	1.71734	-1.98611	1.40701
C	2.60584	-3.04329	1.66536
C	3.63191	-3.27902	0.77384
C	3.82020	-2.42174	-0.33568
C	4.90494	-2.57463	-1.23837
C	5.09079	-1.67296	-2.26314
C	4.20859	-0.57645	-2.40835
C	3.13268	-0.40529	-1.55689
C	2.89846	-1.33925	-0.52114
C	-1.32777	-0.14106	2.57475
C	-2.31257	-0.79352	1.63472
C	-3.52993	-1.27534	2.13680
C	-4.45234	-1.80540	1.25872
C	-4.16450	-1.85127	-0.12084
C	-5.09178	-2.38017	-1.05701
C	-4.79122	-2.40215	-2.39919
C	-3.55062	-1.89101	-2.84628
C	-2.62165	-1.37623	-1.96263
C	-2.89844	-1.34485	-0.57832
H	1.98815	0.44283	2.39325
H	0.83022	0.93489	3.63483
H	1.35241	3.34785	3.35028
H	0.96353	5.40278	1.99421
H	0.19213	6.44072	-0.13395
H	-0.73035	6.17501	-2.42216
H	-1.19653	3.90371	-3.31666
H	-0.74186	1.89413	-1.97146
H	-0.24390	-2.38958	2.18782
H	0.89809	-1.79193	3.39661
H	2.47258	-3.65744	2.54994
H	4.32150	-4.10332	0.93400
H	5.59143	-3.40427	-1.09681
H	5.92414	-1.78786	-2.94847
H	4.38752	0.15060	-3.19472
H	2.48118	0.45517	-1.65786
H	-1.53404	0.93471	2.60478
H	-1.44052	-0.52322	3.59686
H	-3.72992	-1.22489	3.20181
H	-5.40170	-2.19029	1.62098
H	-6.04117	-2.76068	-0.69175
H	-5.50105	-2.80373	-3.11490
H	-3.32329	-1.90064	-3.90807
H	-1.68235	-0.97662	-2.31979
H	0.71678	-0.75883	-2.42975

^{3}FeTQAOHBr
Charge: 2+
Energy: -3319910.8336810

Fe	-0.42917	-0.48420	-0.36897
N	-2.56605	-0.11392	0.27238
N	0.50373	1.02254	0.91229
N	1.68491	-1.29330	-0.08208
N	-0.60972	-1.51880	1.45069
C	-1.98023	-2.09891	1.53217
C	-3.00586	-1.09159	1.06931
C	-4.35401	-1.22720	1.44825
C	-5.27745	-0.32137	0.96308
C	-4.84822	0.73009	0.12335
C	-5.74235	1.70720	-0.39282
C	-5.27709	2.73137	-1.20447
C	-3.90772	2.80902	-1.52236
C	-3.00635	1.87168	-1.03536
C	-3.45795	0.81219	-0.20482
C	-0.43203	-0.51602	2.54388
C	0.50754	0.60572	2.18528
C	1.28472	1.20434	3.19372
C	2.09566	2.27213	2.87082
C	2.11829	2.74677	1.54177
C	2.92974	3.84490	1.14914
C	2.92608	4.29613	-0.16116
C	2.10312	3.66588	-1.11222
C	1.29611	2.58850	-0.76518
C	1.29057	2.09668	0.56944
C	0.42470	-2.59194	1.50776
C	1.75205	-2.12220	0.96264
C	2.97129	-2.59576	1.48033
C	4.15347	-2.17999	0.89312
C	4.11176	-1.30750	-0.21755
C	5.27972	-0.84734	-0.88359
C	5.18233	-0.00473	-1.98585
C	3.92032	0.39126	-2.46240
C	2.75452	-0.03795	-1.83506
C	2.83169	-0.88556	-0.69398
H	-2.19230	-2.43920	2.55399
H	-2.02002	-2.96619	0.86815
H	-4.65316	-2.03743	2.10517
H	-6.32763	-0.40628	1.22818
H	-6.79661	1.64033	-0.13974
H	-5.96843	3.47077	-1.59529
H	-3.55111	3.61055	-2.16176
H	-1.95794	1.90455	-1.30351
H	-0.11403	-1.01735	3.46502
H	-1.40923	-0.06642	2.74405
H	1.24070	0.82103	4.20761
H	2.71441	2.74852	3.62635
H	3.54836	4.33177	1.89784
H	3.54548	5.13956	-0.44852
H	2.08582	4.03226	-2.13424
H	0.64619	2.11786	-1.49017
H	0.07886	-3.40679	0.86364
H	0.52161	-2.97935	2.52881
H	2.97546	-3.27635	2.32532
H	5.11092	-2.52205	1.27627
H	6.25278	-1.17454	-0.52800
H	6.08284	0.33136	-2.48958
H	3.85143	1.02530	-3.34075
H	1.77242	0.22252	-2.21187
O	-0.38463	0.49465	-1.87715
H	-0.74037	-0.00637	-2.63587
Br	-1.01193	-2.46904	-1.70906

^{5}FeTQAOHCl
Charge: 2+
Energy: -1993390.4640687

Fe	-0.55202	-0.55673	-0.75469
N	-2.63584	-0.34608	0.00918
N	0.43513	0.67896	1.04922
N	1.58073	-1.32123	-0.49548
N	-0.68841	-1.93736	1.00647
C	-2.04935	-2.52177	0.92663
C	-3.06602	-1.43776	0.65070
C	-4.40547	-1.62012	1.04088
C	-5.32887	-0.63802	0.74691
C	-4.90998	0.53806	0.08751
C	-5.80984	1.59509	-0.21835
C	-5.36174	2.74038	-0.85244
C	-4.00102	2.86176	-1.19927
C	-3.09634	1.84928	-0.91827
C	-3.52941	0.66290	-0.27276
C	-0.53190	-1.18364	2.27604
C	0.44032	-0.03039	2.18236
C	1.25527	0.28748	3.28638
C	2.10431	1.37336	3.20619
C	2.12915	2.14384	2.02289
C	2.97890	3.27123	1.86604
C	2.97466	4.00795	0.68699
C	2.11569	3.64193	-0.36168
C	1.26573	2.54380	-0.24333
C	1.25985	1.76506	0.95075
C	0.36807	-2.95952	0.81886
C	1.67088	-2.34395	0.36224
C	2.90461	-2.87478	0.78255
C	4.07589	-2.31469	0.30873
C	4.01101	-1.23136	-0.59532
C	5.17098	-0.60531	-1.12639
C	5.06249	0.44943	-2.02625
C	3.79447	0.89842	-2.42997
C	2.63491	0.30948	-1.93087
C	2.72124	-0.76022	-0.99376
H	-2.30295	-3.06790	1.84468
H	-2.06578	-3.23109	0.09439

H	-4.69529	-2.52734	1.56071
H	-6.37158	-0.75597	1.02843
H	-6.85569	1.48728	0.05444
H	-6.05535	3.54200	-1.08408
H	-3.65494	3.76118	-1.69922
H	-2.05645	1.93109	-1.20896
H	-0.25063	-1.86200	3.09128
H	-1.50767	-0.76007	2.53495
H	1.21137	-0.32189	4.18302
H	2.75068	1.63674	4.03895
H	3.62988	3.55606	2.68806
H	3.62476	4.87079	0.58447
H	2.09927	4.22924	-1.27470
H	0.58088	2.27459	-1.03864
H	0.03403	-3.63306	0.02263
H	0.51289	-3.55516	1.72910
H	2.92418	-3.71233	1.47190
H	5.04171	-2.69970	0.62415
H	6.14903	-0.97211	-0.82750
H	5.95794	0.91083	-2.42975
H	3.71265	1.70267	-3.15444
H	1.65211	0.61712	-2.26835
O	-0.42395	0.81941	-1.97513
H	-0.74918	0.58899	-2.86449
Cl	-1.02965	-2.24221	-2.20398

^{3}FeTQAOHF
Charge: 2+
Energy: -1767264.5932889

Fe	-0.31677	-0.80788	-0.54266
N	-2.29421	-0.65412	-0.19515
N	0.15975	0.50201	0.97923
N	1.65425	-1.28826	-0.43625
N	-0.54270	-2.16386	0.93540
C	-1.81566	-2.87074	0.60834
C	-2.81610	-1.82518	0.20453
C	-4.19482	-2.06629	0.24329
C	-5.05457	-1.06627	-0.16407
C	-4.54610	0.19640	-0.53685
C	-5.40298	1.26859	-0.90132
C	-4.88333	2.50693	-1.20418
C	-3.48726	2.71588	-1.13430
C	-2.62003	1.69363	-0.79585
C	-3.12333	0.40515	-0.51640
C	-0.64810	-1.43065	2.22865
C	0.02070	-0.08336	2.17592
C	0.41070	0.51783	3.38351
C	0.96185	1.77846	3.35373
C	1.13089	2.43880	2.11881
C	1.69863	3.73835	2.05186
C	1.85955	4.37067	0.84078
C	1.45362	3.71521	-0.34292
C	0.90241	2.44817	-0.31627
C	0.72304	1.77171	0.91093
C	0.64491	-3.05786	0.85936
C	1.85994	-2.27445	0.45117
C	3.13477	-2.63872	0.90456
C	4.23368	-1.96719	0.41097
C	4.06672	-0.97796	-0.57916
C	5.18122	-0.32225	-1.16713
C	5.00255	0.58237	-2.18710
C	3.69702	0.85099	-2.66038
C	2.58836	0.25484	-2.09407
C	2.73566	-0.65808	-1.02830
H	-2.16350	-3.46239	1.46314
H	-1.62907	-3.54116	-0.23179
H	-4.56175	-3.03037	0.57883
H	-6.12799	-1.23370	-0.17392
H	-6.47453	1.09328	-0.92437
H	-5.54027	3.32553	-1.47898
H	-3.08501	3.70289	-1.34130
H	-1.56207	1.88317	-0.72708
H	-0.24158	-2.04042	3.04194
H	-1.70924	-1.27334	2.44625
H	0.27163	-0.01662	4.31730
H	1.27440	2.26833	4.27172
H	1.99840	4.22171	2.97711
H	2.29079	5.36515	0.79171
H	1.57639	4.21577	-1.29873
H	0.59772	1.97541	-1.23467
H	0.45062	-3.79468	0.07450
H	0.79166	-3.59384	1.80234
H	3.23739	-3.43780	1.63058
H	5.23281	-2.21064	0.76143
H	6.17642	-0.57129	-0.81055
H	5.85642	1.07080	-2.64502
H	3.56247	1.53277	-3.49471
H	1.59913	0.45483	-2.47735
O	-0.34636	0.31859	-1.89898
H	-0.75346	-0.16479	-2.64868
F	-0.57603	-2.12697	-1.67334

^{6}FeTQAOHMeCN
Charge: 2+
Energy: -1787970.5792176

Fe	-0.33131	-0.56913	-0.30087
N	-2.45410	-0.28362	0.22766
N	0.36100	1.11689	0.81830
N	1.68720	-1.32944	0.06792
N	-0.56245	-1.42677	1.71243
O	-0.45723	-0.07560	-2.03912
N	-0.80053	-2.71773	-1.01865
C	-1.89973	-2.06084	1.78096
C	-2.92230	-1.17917	1.09928
C	-4.29226	-1.32678	1.38557
C	-5.19755	-0.51608	0.73573
C	-4.74066	0.47864	-0.16001
C	-5.62519	1.37729	-0.81170
C	-5.13229	2.36552	-1.63410
C	-3.73579	2.49607	-1.82291
C	-2.84709	1.63221	-1.21372
C	-3.32841	0.59221	-0.38444
C	-0.48238	-0.26840	2.64795
C	0.33174	0.89963	2.13530
C	0.94323	1.76375	3.06202
C	1.59053	2.88985	2.60138
C	1.63147	3.16397	1.21634
C	2.27800	4.31354	0.69114
C	2.29395	4.54387	-0.66557
C	1.66377	3.62955	-1.54292
C	1.03051	2.49848	-1.06798
C	0.99754	2.23882	0.32182
C	0.54102	-2.39618	1.91494
C	1.81828	-1.93768	1.24852
C	3.06829	-2.21779	1.82878
C	4.21390	-1.85078	1.15378
C	4.11941	-1.22730	-0.11017
C	5.26445	-0.84631	-0.85860
C	5.12249	-0.26181	-2.09627
C	3.82977	-0.04523	-2.63298
C	2.69443	-0.39389	-1.93073
C	2.81195	-0.98250	-0.64970
H	-2.19422	-2.26272	2.81941
H	-1.84762	-3.02136	1.26215
H	-4.61547	-2.07009	2.10713
H	-6.26292	-0.61537	0.92508
H	-6.69314	1.27725	-0.64071
H	-5.80953	3.05499	-2.12758
H	-3.35632	3.29593	-2.45170
H	-1.78082	1.75251	-1.34939
H	-0.10563	-0.59857	3.62297
H	-1.50058	0.10052	2.80829
H	0.89434	1.53836	4.12216
H	2.07273	3.57216	3.29610
H	2.75324	5.00632	1.37956
H	2.78485	5.42508	-1.06572
H	1.67803	3.82198	-2.61160
H	0.55453	1.80508	-1.74927
H	0.24090	-3.33853	1.44615
H	0.69992	-2.59605	2.98155
H	3.11719	-2.71068	2.79399
H	5.19325	-2.04090	1.58446
H	6.24929	-1.03347	-0.44044
H	5.99846	0.02407	-2.66960
H	3.73151	0.39826	-3.61934
H	1.70879	-0.24202	-2.35335
C	-0.87155	-3.66559	-1.68109
C	-0.95914	-4.85642	-2.51661
H	-1.98940	-4.99682	-2.85984
H	-0.30390	-4.74505	-3.38701
H	-0.64843	-5.73831	-1.94689
H	-1.17747	-0.27966	-2.65853

^{5}FeTQAOHN$_{3}$
Charge: 2+
Energy: -1807652.4672519

Fe	0.56184	-0.70124	0.61155
N	2.62389	-0.29945	-0.16643
N	-0.43554	0.86392	-0.95954
N	-1.60155	-1.38291	0.20781
N	0.66901	-1.73055	-1.38073
C	2.03725	-2.30241	-1.40559
C	3.04475	-1.24413	-1.01295
C	4.35804	-1.29244	-1.51692
C	5.26308	-0.32890	-1.12059
C	4.85243	0.69374	-0.23728
C	5.73049	1.72525	0.19230
C	5.28671	2.71312	1.05228
C	3.95218	2.69962	1.51015
C	3.06911	1.70923	1.11256
C	3.49853	0.68379	0.23097
C	0.48129	-0.77938	-2.50346
C	-0.47483	0.35177	-2.19354
C	-1.31158	0.85572	-3.20938
C	-2.14956	1.91676	-2.92825

C	-2.14247	2.47620	-1.63109
C	-2.97717	3.56423	-1.26288
C	-2.93962	4.08719	0.02611
C	-2.06333	3.54136	0.97690
C	-1.22463	2.47615	0.65065
C	-1.25121	1.91730	-0.66128
C	-0.37615	-2.77993	-1.34496
C	-1.68640	-2.23602	-0.81872
C	-2.91688	-2.64698	-1.36474
C	-4.09027	-2.13784	-0.83997
C	-4.03124	-1.22848	0.23938
C	-5.19176	-0.65960	0.83069
C	-5.08559	0.22165	1.90023
C	-3.82074	0.54887	2.41804
C	-2.66074	0.01198	1.86530
C	-2.74469	-0.87903	0.75650
H	2.27820	-2.72623	-2.38924
H	2.07297	-3.10958	-0.66777
H	4.64227	-2.08140	-2.20543
H	6.28487	-0.34365	-1.48966
H	6.75609	1.72318	-0.16550
H	5.96369	3.49620	1.37782
H	3.61330	3.47585	2.18948
H	2.05087	1.67983	1.48194
H	0.16518	-1.31298	-3.40879
H	1.45268	-0.32548	-2.72481
H	-1.29342	0.40607	-4.19673
H	-2.81187	2.31952	-3.68971
H	-3.64254	3.99186	-2.00794
H	-3.57923	4.92329	0.28987
H	-2.02440	3.96073	1.97760
H	-0.53111	2.06004	1.37329
H	-0.03653	-3.55312	-0.64820
H	-0.51094	-3.24455	-2.33023
H	-2.93287	-3.35067	-2.19040
H	-5.05323	-2.42925	-1.25032
H	-6.16827	-0.93405	0.44131
H	-5.98142	0.64096	2.34665
H	-3.74421	1.21598	3.27102
H	-1.68046	0.22448	2.27843
O	0.40788	0.42040	2.07842
H	0.78801	0.14469	2.93003
N	1.00786	-2.37210	1.45063
N	1.07812	-2.67396	2.63125
N	1.14986	-2.98430	3.73372

[1]FeTQAOHNCS
Charge: 2+
Energy: -2012757.1414462

Fe	-0.35130	-0.55777	-0.03220
N	-2.33067	-0.13104	0.25879
N	0.35292	1.20503	0.77330
N	1.60643	-1.19293	0.24872
N	-0.58075	-1.14383	1.90325
C	-1.93102	-1.76832	1.98650
C	-2.88720	-0.92180	1.18634
C	-4.26829	-0.96703	1.43332
C	-5.10205	-0.16644	0.68324
C	-4.55382	0.72935	-0.26067
C	-5.37073	1.62496	-1.00010
C	-4.80525	2.53488	-1.86400
C	-3.39905	2.58510	-2.00684
C	-2.57334	1.71865	-1.31806
C	-3.12773	0.75552	-0.44322
C	-0.52501	0.08340	2.74573
C	0.28970	1.17692	2.11098
C	0.87567	2.14386	2.94637
C	1.55899	3.19281	2.37657
C	1.65248	3.27485	0.97190
C	2.34845	4.34329	0.34578
C	2.43312	4.42002	-1.02795
C	1.81644	3.42493	-1.81395
C	1.13284	2.36760	-1.23842
C	1.03105	2.25552	0.17063
C	0.51410	-2.10111	2.20712
C	1.77092	-1.72841	1.46647
C	3.02851	-2.01537	2.02166
C	4.16083	-1.75263	1.28049
C	4.03333	-1.23520	-0.02520
C	5.16912	-0.98515	-0.84176
C	5.01883	-0.51900	-2.13101
C	3.72339	-0.29575	-2.64546
C	2.59482	-0.51159	-1.87446
C	2.71814	-0.97062	-0.54038
H	-2.25763	-1.86046	3.02972
H	-1.87345	-2.77383	1.56515
H	-4.65538	-1.62692	2.20261
H	-6.17770	-0.19335	0.83358
H	-6.44682	1.58600	-0.85835
H	-5.43122	3.22203	-2.42384
H	-2.95744	3.32392	-2.66881
H	-1.50350	1.76813	-1.43714
H	-0.15399	-0.15886	3.74742
H	-1.54676	0.45743	2.86500
H	0.78043	2.05052	4.02299
H	2.02724	3.95410	2.99421
H	2.80778	5.10128	0.97370
H	2.96259	5.24052	-1.50115
H	1.87286	3.48776	-2.89663
H	0.65821	1.62379	-1.85738
H	0.19878	-3.08825	1.85516
H	0.68377	-2.17555	3.28682
H	3.09186	-2.43615	3.01942
H	5.14850	-1.95223	1.68672
H	6.15655	-1.17951	-0.43313
H	5.88954	-0.33886	-2.75305
H	3.60698	0.04413	-3.67013
H	1.60319	-0.36112	-2.27595
O	-0.30319	-0.04984	-1.74267
H	-0.91461	-0.60068	-2.26384
N	-0.81759	-2.36233	-0.63894
C	-0.94100	-3.38224	-1.22656
S	-1.12128	-4.79398	-2.00818

[5]FeTQAOHOTF
Charge: 2+
Energy: -2308101.3404695

Fe	-0.48562	-0.10655	-0.05273
N	1.55599	0.83429	0.57481
N	0.90209	-1.85201	0.54717
N	-2.37521	-1.05294	0.40314
N	-0.56894	-0.06072	2.16928
O	-0.31748	-0.17669	-1.87070
O	-0.02543	2.65380	-1.87066
O	-1.24161	1.70036	0.08165
O	0.33361	3.58842	0.45477
S	-0.55049	2.96301	-0.52977
F	-2.89453	3.44976	-1.58698
F	-1.68045	5.22221	-1.20956
F	-2.64343	4.18386	0.45106
C	0.29618	1.04504	2.63917
C	1.59909	1.13065	1.88018
C	2.76589	1.59431	2.51230
C	3.91899	1.75819	1.76560
C	3.89550	1.46189	0.38533
C	5.03135	1.61838	-0.45325
C	4.96070	1.33667	-1.82072
C	3.75402	0.90659	-2.38270
C	2.61366	0.74638	-1.58925
C	2.66945	1.00457	-0.18573
C	-0.15491	-1.38608	2.68930
C	0.94671	-2.02506	1.87427
C	1.93176	-2.80343	2.51124
C	2.91329	-3.40410	1.74904
C	2.90727	-3.22844	0.34731
C	3.89353	-3.80554	-0.49632
C	3.85775	-3.60847	-1.87035
C	2.82923	-2.83805	-2.43935
C	1.84071	-2.26208	-1.64542
C	1.86337	-2.43880	-0.23147
C	-2.00236	0.19603	2.45725
C	-2.87367	-0.68476	1.58984
C	-4.15750	-1.05565	2.02562
C	-4.94647	-1.82841	1.19928
C	-4.45365	-2.24637	-0.05664
C	-5.21762	-3.05675	-0.93776
C	-4.69872	-3.44724	-2.15459
C	-3.39983	-3.03633	-2.53069
C	-2.62701	-2.24942	-1.69718
C	-3.13474	-1.83592	-0.44178
C	-2.05948	4.04469	-0.73897
H	0.47414	0.97883	3.71994
H	-0.22406	1.98705	2.43676
H	2.74918	1.82913	3.57130
H	4.83381	2.11683	2.22915
H	5.96136	1.97434	-0.01831
H	5.83731	1.47469	-2.44523
H	3.68783	0.72072	-3.44991
H	1.65617	0.49129	-2.02233
H	-1.02398	-2.05099	2.63711
H	0.13460	-1.31741	3.74538
H	1.91308	-2.91820	3.58995
H	3.69009	-4.00333	2.21612
H	4.67599	-4.41228	-0.04899
H	4.61435	-4.06043	-2.50352
H	2.78967	-2.70286	-3.51593
H	1.02549	-1.70105	-2.08688
H	-2.20734	1.24009	2.20613
H	-2.23050	0.04530	3.52016
H	-4.50957	-0.73153	2.99928
H	-5.94344	-2.12836	1.51023
H	-6.21619	-3.35980	-0.63661
H	-5.28637	-4.06426	-2.82646
H	-3.00391	-3.33902	-3.49529
H	-1.64721	-1.90936	-2.00708
H	-0.51609	0.67810	-2.31099

^{6}FeTPPh2OBzBr
Charge: 2+
Energy: -3983089.8899685

Fe	-1.24634	-0.36638	0.07336
B	1.87855	0.26017	-0.01600
H	3.03352	0.46423	-0.05643
O	-2.67645	0.48416	-1.18882
C	-3.47510	0.58145	-0.19112
O	-2.97645	0.21959	0.94523
N	-0.25070	1.55397	0.04699
N	1.08468	1.53656	-0.22904
C	-2.00058	3.33297	0.23630
C	-2.67220	4.19147	-0.65578
H	-2.22489	4.41589	-1.61962
C	-3.91099	4.72294	-0.31321
H	-4.43611	5.36686	-1.01156
C	-4.47680	4.43228	0.93481
H	-5.44020	4.85413	1.20373
C	-3.80228	3.60075	1.83661
H	-4.23577	3.38976	2.80917
C	-2.57536	3.04610	1.48981
H	-2.04550	2.40194	2.18253
C	-0.66197	2.84148	-0.09312
C	0.42843	3.63659	-0.48735
H	0.41785	4.70134	-0.66614
C	1.53029	2.79181	-0.55319
C	2.93478	3.11479	-0.83095
C	3.50997	4.23387	-0.20167
H	2.90686	4.84358	0.46499
C	4.85362	4.54255	-0.41002
H	5.29020	5.40682	0.08137
C	5.63447	3.74193	-1.24956
H	6.68072	3.98411	-1.41077
C	5.06423	2.63887	-1.89319
H	5.66201	2.01883	-2.55387
C	3.72197	2.33071	-1.69230
H	3.28145	1.48769	-2.21346
N	0.26354	-0.98349	-1.51504
N	1.52435	-0.76700	-1.14400
C	-0.84401	-2.34744	-3.29352
C	-0.69903	-3.50131	-4.12184
H	0.25843	-4.00542	-4.18526
C	-1.78376	-4.01023	-4.80325
H	-1.67501	-4.89977	-5.41501
C	-3.04342	-3.37705	-4.70112
H	-3.89142	-3.78060	-5.24652
C	-3.20187	-2.23415	-3.90392
H	-4.16905	-1.74726	-3.83473
C	-2.12513	-1.72452	-3.20022
H	-2.24886	-0.83172	-2.60499
C	0.30610	-1.83879	-2.60400
C	1.66104	-2.12405	-2.89828
H	2.04241	-2.74095	-3.69679
C	2.42085	-1.44109	-1.97783
C	3.87941	-1.34426	-1.88758
C	4.56550	-1.49654	-0.67044
H	4.01712	-1.71293	0.23872
C	5.95222	-1.39557	-0.63084
H	6.46879	-1.51049	0.31644
C	6.67206	-1.14981	-1.80508
H	7.75439	-1.06933	-1.77148
C	6.00008	-1.01713	-3.02447
H	6.55720	-0.83483	-3.93832
C	4.61117	-1.11707	-3.06919
H	4.08546	-0.99336	-4.01169
N	0.27212	-0.79645	1.62071
N	1.50145	-0.32865	1.37700
C	-0.79321	-2.12955	3.44460
C	-0.54319	-3.23881	4.30121
H	0.47153	-3.60072	4.42791
C	-1.59011	-3.88534	4.92746
H	-1.39925	-4.74495	5.56156
C	-2.91307	-3.43201	4.73722
H	-3.73166	-3.94140	5.23684
C	-3.17434	-2.32955	3.91162
H	-4.19235	-1.98011	3.77540
C	-2.13328	-1.68392	3.26576
C	0.32800	-1.47532	2.82001
C	1.64541	-1.40225	3.31986
H	1.99371	-1.75989	4.27661
C	2.36737	-0.63717	2.42367
C	3.75325	-0.18562	2.50834
C	4.72444	-1.06438	3.03201
H	4.43583	-2.06838	3.32954
C	6.05202	-0.66020	3.13495
H	6.79543	-1.34380	3.53323
C	6.42708	0.62415	2.72106
H	7.46439	0.93583	2.79821
C	5.46637	1.50942	2.21734
H	5.75006	2.50872	1.90282
C	4.13780	1.11385	2.11877
H	3.39768	1.81770	1.75540
H	-2.34220	-0.81819	2.65447
C	-4.84258	1.06722	-0.32034
C	-5.70768	1.03280	0.78660
C	-5.27995	1.59126	-1.54883
C	-7.00517	1.51795	0.66159
H	-5.34984	0.62903	1.72745
C	-6.57656	2.08164	-1.66478
H	-4.59347	1.62039	-2.38831
C	-7.43759	2.04381	-0.56171
H	-7.68127	1.48935	1.51041
H	-6.92012	2.49343	-2.60863
H	-8.45058	2.42419	-0.65610
Br	-1.95835	-2.75704	0.04865

^{4}FeTPPh2OBzCl
Charge: 2+
Energy: -2656545.8593775

Fe	1.31515	0.57251	0.25139
B	-1.76980	-0.20575	-0.07151
H	-2.90773	-0.46781	-0.19521
O	2.66152	0.11231	-1.31032
C	3.51709	-0.24736	-0.43000
O	3.10197	-0.20123	0.79366
N	0.42232	-1.38470	-0.26070
N	-0.89136	-1.32915	-0.61305
C	2.21453	-3.10557	-0.40289
C	2.94669	-3.79359	-1.39615
H	2.54853	-3.85552	-2.40446
C	4.17985	-4.35344	-1.09094
H	4.75312	-4.85885	-1.86129
C	4.68282	-4.26721	0.21597
H	5.64183	-4.71577	0.45571
C	3.94837	-3.61209	1.21602
H	4.33340	-3.56722	2.22990
C	2.72930	-3.02528	0.91029
H	2.15037	-2.51867	1.67378
C	0.89271	-2.57388	-0.70828
C	-0.14013	-3.26331	-1.38296
H	-0.07664	-4.24227	-1.83413
C	-1.26943	-2.46397	-1.28616
C	-2.64844	-2.73034	-1.71870
C	-3.22072	-3.98217	-1.43573
H	-2.63414	-4.73649	-0.91885
C	-4.54296	-4.24631	-1.79348
H	-4.97731	-5.21641	-1.57120
C	-5.30463	-3.26546	-2.43487
H	-6.33440	-3.47227	-2.71060
C	-4.73640	-2.02363	-2.73282
H	-5.32015	-1.26005	-3.23745
C	-3.41431	-1.75914	-2.38457
H	-2.97267	-0.80074	-2.63757
N	-0.24943	1.49650	-1.15509
N	-1.48626	1.12186	-0.86339
C	0.77104	3.40258	-2.41705
C	0.55506	4.74187	-2.86556
H	-0.43196	5.18423	-2.79449
C	1.60606	5.49587	-3.34205
H	1.44220	6.51966	-3.66191
C	2.90170	4.93702	-3.40772
H	3.72459	5.53456	-3.78882
C	3.12962	3.61752	-2.98600
H	4.12548	3.19117	-3.04810
C	2.08703	2.85723	-2.48896
H	2.26360	1.83566	-2.18485
C	-0.34693	2.64665	-1.93371
C	-1.71504	2.93401	-2.13452
H	-2.13687	3.74392	-2.70863
C	-2.42945	1.97138	-1.45972
C	-3.87586	1.77426	-1.41087
C	-4.55564	1.48102	-0.21364
H	-4.01035	1.41740	0.71977
C	-5.93421	1.30442	-0.21667
H	-6.44455	1.07607	0.71319
C	-6.65439	1.42200	-1.41126
H	-7.73058	1.27766	-1.41233
C	-5.99143	1.73467	-2.60397
H	-6.55038	1.83337	-3.52938
C	-4.61170	1.91578	-2.60605
H	-4.09169	2.13523	-3.53399
N	-0.21218	0.44653	1.79472
N	-1.42280	-0.00943	1.42474
C	0.82874	1.22578	3.92578
C	0.54375	2.04034	5.05379
H	-0.48440	2.30560	5.27727
C	1.57163	2.53553	5.83636
H	1.35035	3.17441	6.68514
C	2.90660	2.21603	5.52591
H	3.71095	2.60402	6.14358
C	3.20120	1.39644	4.42599
H	4.23125	1.14371	4.19674
C	2.17828	0.90525	3.63119
C	-0.27613	0.72444	3.13764
C	-1.57241	0.42005	3.60050

H	-1.91740	0.45331	4.62259
C	-2.27326	-0.08121	2.51671
C	-3.63452	-0.61289	2.46952
C	-4.64097	0.02578	3.22219
H	-4.39777	0.91264	3.80030
C	-5.94636	-0.45773	3.20040
H	-6.71678	0.04173	3.77981
C	-6.26353	-1.58329	2.43027
H	-7.28295	-1.95690	2.41196
C	-5.26670	-2.23353	1.69327
H	-5.50505	-3.11118	1.10073
C	-3.95974	-1.76034	1.71857
H	-3.19027	-2.28942	1.16768
H	2.41670	0.25083	2.80448
C	4.86119	-0.70044	-0.77375
C	5.78961	-0.98239	0.24163
C	5.20833	-0.87937	-2.12394
C	7.06049	-1.44103	-0.09505
H	5.50350	-0.83904	1.27766
C	6.47811	-1.34405	-2.45304
H	4.47526	-0.66340	-2.89413
C	7.40256	-1.62386	-1.43991
H	7.78554	-1.65397	0.68437
H	6.75149	-1.48830	-3.49368
H	8.39441	-1.98243	-1.69944
Cl	1.89024	2.68511	0.80552

^{6}FeTPPh2OBzF
Charge: 2+
Energy: -2430439.7106367

Fe	1.32398	-0.94076	0.06354
B	-1.67139	0.30771	-0.20275
H	-2.77896	0.69639	-0.31587
O	2.35622	0.42328	1.30281
C	3.34325	0.37841	0.48518
O	3.16546	-0.33928	-0.56848
N	0.51337	1.39745	-0.61306
N	-0.69842	1.52921	-0.11321
C	2.38799	2.86894	-1.22465
C	3.17514	3.98979	-0.85530
H	2.83264	4.64722	-0.06260
C	4.39104	4.21896	-1.47456
H	5.00495	5.06177	-1.17504
C	4.83299	3.35401	-2.49180
H	5.78338	3.54312	-2.98156
C	4.05608	2.25183	-2.87972
H	4.40081	1.59715	-3.67355
C	2.85288	1.99562	-2.24411
H	2.24629	1.14422	-2.52660
C	1.09688	2.65584	-0.62519
C	0.19802	3.58017	-0.07842
H	0.34750	4.64206	0.04211
C	-0.95524	2.87276	0.23189
C	-2.21912	3.37198	0.73649
C	-2.60696	4.69231	0.40067
H	-1.97826	5.28723	-0.25423
C	-3.80856	5.21076	0.86251
H	-4.10475	6.21763	0.58601
C	-4.64287	4.43029	1.67486
H	-5.58433	4.83676	2.03180
C	-4.26225	3.12978	2.03042
H	-4.89966	2.52458	2.66647
C	-3.06340	2.60464	1.56892
H	-2.76225	1.61613	1.88552
N	-0.33281	-0.95007	1.51274
N	-1.54273	-0.55886	1.08659
C	0.52735	-2.41112	3.33890
C	0.22365	-3.57820	4.09650
H	-0.77823	-3.99265	4.07043
C	1.21120	-4.21583	4.82131
H	0.98228	-5.11845	5.37832
C	2.52158	-3.69474	4.83413
H	3.29290	-4.19486	5.41223
C	2.83127	-2.53100	4.11135
H	3.83790	-2.12673	4.14090
C	1.85424	-1.89556	3.36672
H	2.08319	-0.98242	2.83314
C	-0.52860	-1.76957	2.59694
C	-1.91870	-1.86459	2.84450
H	-2.40653	-2.41061	3.63710
C	-2.54669	-1.09694	1.88739
C	-3.97944	-0.80435	1.76244
C	-4.66075	-0.89361	0.53784
H	-4.13619	-1.20360	-0.35628
C	-6.02285	-0.61403	0.46991
H	-6.53240	-0.68488	-0.48591
C	-6.72404	-0.25404	1.62472
H	-7.78668	-0.03742	1.57040
C	-6.05957	-0.18617	2.85393
H	-6.60418	0.07932	3.75508
C	-4.69524	-0.46105	2.92584
H	-4.17435	-0.39149	3.87673
N	-0.10276	-1.28534	-1.39166
N	-1.27441	-0.57735	-1.40563
C	0.89933	-3.15966	-2.67517
C	0.57535	-4.45498	-3.13561
H	-0.46619	-4.74568	-3.23259
C	1.58159	-5.36763	-3.42154
H	1.32630	-6.36698	-3.75943
C	2.92676	-5.00006	-3.26921
H	3.71169	-5.71450	-3.49797
C	3.25864	-3.71083	-2.83503
H	4.29981	-3.42079	-2.73523
C	2.25607	-2.79413	-2.54487
C	-0.17967	-2.23134	-2.36516
C	-1.42597	-2.11949	-3.00773
H	-1.76033	-2.67491	-3.87067
C	-2.08943	-1.06024	-2.40349
C	-3.39628	-0.49598	-2.75493
C	-4.44351	-1.36915	-3.10081
H	-4.27841	-2.44252	-3.07543
C	-5.69516	-0.86287	-3.44726
H	-6.49839	-1.54464	-3.70970
C	-5.91195	0.51824	-3.46083
H	-6.88573	0.91227	-3.73572
C	-4.87047	1.39270	-3.13509
H	-5.03204	2.46590	-3.16538
C	-3.61881	0.89177	-2.78676
H	-2.80535	1.57442	-2.56179
H	2.52654	-1.78492	-2.25734
C	4.57788	1.13055	0.71040
C	5.66907	0.96364	-0.15604
C	4.65012	2.04427	1.77791
C	6.82476	1.71463	0.04075
H	5.59543	0.25282	-0.97148
C	5.80704	2.79487	1.96660
H	3.79676	2.15633	2.43865
C	6.89203	2.63114	1.09860
H	7.67569	1.58592	-0.62108
H	5.86873	3.50217	2.78782
H	7.79649	3.21328	1.24970
F	1.78760	-2.56658	0.54598

^{6}FeTPPh2OBzN$_3$
Charge: 2+
Energy: -2470830.9126213

Fe	1.24144	-0.71371	0.02418
B	-1.82246	0.29078	-0.19666
H	-2.95387	0.60858	-0.28966
O	2.25318	0.67648	1.29950
C	3.23785	0.66619	0.48376
O	3.10030	-0.06568	-0.56816
N	0.30086	1.52222	-0.58339
N	-0.92627	1.57227	-0.10392
C	2.08647	3.11649	-1.15832
C	2.80173	4.27305	-0.75524
H	2.41091	4.89205	0.04607
C	4.01037	4.58610	-1.35258
H	4.57005	5.45629	-1.02638
C	4.51524	3.77071	-2.38054
H	5.45916	4.02493	-2.85287
C	3.80836	2.63406	-2.80230
H	4.20052	2.01827	-3.60520
C	2.61450	2.29449	-2.18875
H	2.06024	1.41784	-2.50053
C	0.80216	2.81580	-0.58110
C	-0.16297	3.67672	-0.04544
H	-0.08393	4.74524	0.08310
C	-1.27262	2.89431	0.24407
C	-2.57096	3.30804	0.73825
C	-3.04506	4.59828	0.39580
H	-2.45413	5.23206	-0.25790
C	-4.28162	5.03525	0.84935
H	-4.64436	6.01854	0.56734
C	-5.06502	4.20269	1.66104
H	-6.03371	4.54568	2.01175
C	-4.59861	2.93252	2.02458
H	-5.19573	2.28808	2.66117
C	-3.36490	2.48808	1.57058
H	-2.99857	1.52380	1.89335
N	-0.36818	-0.90390	1.47001
N	-1.61450	-0.57729	1.07848
C	0.63296	-2.33946	3.23501
C	0.44577	-3.57613	3.90901
H	-0.52316	-4.06320	3.88193
C	1.50725	-4.18805	4.54980
H	1.36729	-5.14527	5.04154
C	2.77598	-3.57229	4.56046
H	3.60336	-4.05535	5.07158
C	2.96910	-2.33627	3.92666
H	3.94132	-1.85490	3.95947
C	1.91554	-1.72162	3.26879
H	2.05122	-0.75133	2.80766
C	-0.48723	-1.73971	2.54704
C	-1.85979	-1.92053	2.83145
H	-2.29117	-2.50300	3.63109

C	-2.55811	-1.17969	1.89863
C	-4.01011	-0.97563	1.81306
C	-4.71612	-1.10676	0.60672
H	-4.19653	-1.38367	-0.30129
C	-6.09433	-0.91055	0.57451
H	-6.62338	-1.01261	-0.36780
C	-6.78591	-0.59396	1.74746
H	-7.86099	-0.44348	1.72128
C	-6.09481	-0.48488	2.95877
H	-6.63079	-0.25342	3.87440
C	-4.71444	-0.67557	2.99459
H	-4.17408	-0.57469	3.93173
N	-0.16089	-1.14484	-1.44671
N	-1.38787	-0.54856	-1.42289
C	0.98937	-2.88846	-2.76392
C	0.80870	-4.22829	-3.17227
H	-0.19448	-4.63871	-3.23507
C	1.90983	-5.02898	-3.44458
H	1.76755	-6.06421	-3.73798
C	3.20703	-4.50363	-3.33351
H	4.06517	-5.13331	-3.54758
C	3.39624	-3.16604	-2.96156
H	4.39842	-2.75440	-2.89959
C	2.29826	-2.36108	-2.68501
C	-0.17462	-2.07984	-2.43126
C	-1.44221	-2.08039	-3.04202
H	-1.74570	-2.65479	-3.90415
C	-2.18332	-1.09203	-2.40790
C	-3.54489	-0.64478	-2.71757
C	-4.51997	-1.60590	-3.04066
H	-4.25957	-2.66045	-3.02727
C	-5.82083	-1.21134	-3.34889
H	-6.56758	-1.96056	-3.59356
C	-6.15968	0.14508	-3.34618
H	-7.17195	0.45234	-3.59108
C	-5.19119	1.10708	-3.04196
H	-5.44832	2.16177	-3.05908
C	-3.89071	0.71781	-2.73238
H	-3.13538	1.46900	-2.52390
H	2.44941	-1.31676	-2.43726
C	4.44234	1.47110	0.70615
C	5.53629	1.35585	-0.16471
C	4.47969	2.38351	1.77633
C	6.65902	2.15617	0.02991
H	5.49043	0.64604	-0.98311
C	5.60376	3.18334	1.96393
H	3.62470	2.45543	2.44049
C	6.69106	3.07099	1.09116
H	7.51176	2.06742	-0.63621
H	5.63755	3.88942	2.78786
H	7.56986	3.69157	1.24061
N	1.90204	-2.45773	0.40176
N	3.02173	-2.93235	0.37455
N	4.06258	-3.41486	0.35778

^{6}FeTPPh2OBzNCS
Charge: 2+
Energy: -2675941.7469379

Fe	-1.16976	-0.34431	0.07503
B	1.95211	0.29169	0.18593
H	3.10934	0.50350	0.25785
O	-2.15962	0.96553	-1.28104
C	-3.12379	1.04521	-0.44488
O	-2.96408	0.39307	0.65960
N	-0.07602	1.70667	0.49920
N	1.17349	1.65332	0.07677
C	-1.73882	3.46771	1.02719
C	-2.36386	4.63648	0.52803
H	-1.92290	5.16095	-0.31397
C	-3.55236	5.08105	1.08424
H	-4.04501	5.96082	0.68370
C	-4.12103	4.38841	2.16602
H	-5.04746	4.74504	2.60552
C	-3.49930	3.24279	2.68380
H	-3.93694	2.72313	3.53010
C	-2.32807	2.77156	2.11207
H	-1.83780	1.88815	2.50304
C	-0.46674	3.04079	0.49461
C	0.58744	3.81374	0.00670
H	0.60228	4.88605	-0.11372
C	1.63843	2.93829	-0.25041
C	2.97363	3.23882	-0.72042
C	3.54400	4.49392	-0.38670
H	2.99549	5.18180	0.24892
C	4.81808	4.82257	-0.82359
H	5.25625	5.77611	-0.54676
C	5.54381	3.91797	-1.61445
H	6.54216	4.17792	-1.95330
C	4.98165	2.68488	-1.97397
H	5.53167	1.98805	-2.59783
C	3.71111	2.34605	-1.53382
H	3.27258	1.41202	-1.85475
N	0.31300	-0.80994	-1.36413
N	1.61985	-0.55637	-1.06154
C	-0.92749	-2.28822	-2.92029
C	-0.93620	-3.67070	-3.17426
H	-0.02972	-4.25021	-3.03198
C	-2.12026	-4.30396	-3.53330
H	-2.13424	-5.37639	-3.69928
C	-3.31118	-3.55611	-3.68116
H	-4.22868	-4.05846	-3.97132
C	-3.29436	-2.17070	-3.49265
H	-4.20024	-1.58998	-3.63468
C	-2.11743	-1.53757	-3.11105
H	-2.09893	-0.46753	-2.94414
C	0.30073	-1.67419	-2.40871
C	1.62137	-1.95186	-2.79047
H	1.94782	-2.59480	-3.59416
C	2.43981	-1.23508	-1.92129
C	3.90972	-1.15980	-1.92246
C	4.66652	-1.36478	-0.75807
H	4.17418	-1.61026	0.17471
C	6.05664	-1.27852	-0.79843
H	6.62570	-1.43611	0.11261
C	6.70779	-1.00199	-2.00346
H	7.79157	-0.94091	-2.03514
C	5.96334	-0.82108	-3.17351
H	6.46610	-0.62297	-4.11556
C	4.57096	-0.90009	-3.13596
H	3.99093	-0.74732	-4.04185
N	0.17013	-0.90889	1.50576
N	1.45928	-0.45385	1.45841
C	-1.15509	-2.58720	2.72277
C	-1.14738	-3.98714	2.84057
H	-0.20703	-4.52653	2.78091
C	-2.34676	-4.67969	2.97635
H	-2.34132	-5.76298	3.04422
C	-3.56735	-3.98103	3.02161
H	-4.49795	-4.52815	3.13623
C	-3.57771	-2.58519	2.94786
H	-4.51572	-2.04192	3.00094
C	-2.38199	-1.89061	2.79677
C	0.09849	-1.87717	2.45679
C	1.36307	-2.04322	3.02665
H	1.62436	-2.68587	3.85397
C	2.20375	-1.12134	2.39365
C	3.61989	-0.86386	2.66067
C	4.46986	-1.95026	2.93912
H	4.07055	-2.96038	2.93350
C	5.82383	-1.73650	3.18989
H	6.47360	-2.58108	3.39757
C	6.34103	-0.43748	3.17717
H	7.39489	-0.27108	3.37923
C	5.49841	0.64904	2.91986
H	5.89555	1.65945	2.93067
C	4.14611	0.44056	2.66474
H	3.48948	1.28702	2.49063
H	-2.38986	-0.80766	2.73478
C	-4.31878	1.84878	-0.69708
C	-5.38527	1.82840	0.21588
C	-4.37661	2.66710	-1.83986
C	-6.50186	2.62786	-0.01199
H	-5.32195	1.19208	1.09157
C	-5.49449	3.46638	-2.06005
H	-3.54207	2.66941	-2.53327
C	-6.55481	3.44739	-1.14706
H	-7.33275	2.61345	0.68666
H	-5.54476	4.10092	-2.93940
H	-7.42839	4.06863	-1.32212
N	-2.02668	-2.14227	-0.20870
C	-2.67561	-3.13355	-0.29458
S	-3.54555	-4.47693	-0.44736

^{6}FeTPPh2OBzOH
Charge: 2+
Energy: -2415349.3709457

Fe	1.19727	0.65816	0.10635
B	-1.83103	-0.11889	-0.08352
H	-2.97132	-0.37035	-0.19891
O	4.14634	1.08314	-0.13950
C	3.87327	-0.08733	0.15108
O	2.63341	-0.50093	0.37736
N	0.36162	-0.83432	-1.05746
N	-0.96211	-1.06800	-0.92111
C	2.25657	-1.87882	-2.25332
C	2.87826	-0.68331	-2.67597
H	2.31171	0.24241	-2.65839
C	4.18542	-0.69793	-3.13358
H	4.66021	0.22402	-3.45271
C	4.89763	-1.90986	-3.18189
H	5.92488	-1.91844	-3.53168
C	4.28340	-3.10679	-2.78978
H	4.83795	-4.03849	-2.82611
C	2.97081	-3.09736	-2.33757
H	2.49537	-4.01769	-2.01264
C	0.88475	-1.86637	-1.77838

C	-0.14085	-2.79027	-2.05931
H	-0.06337	-3.67718	-2.67019
C	-1.30852	-2.24538	-1.54223
C	-2.68686	-2.74635	-1.61373
C	-2.95581	-4.07538	-1.24067
H	-2.14560	-4.70968	-0.89260
C	-4.25904	-4.56797	-1.29716
H	-4.46133	-5.59323	-1.00308
C	-5.30106	-3.74334	-1.73421
H	-6.31416	-4.13171	-1.78431
C	-5.03718	-2.42399	-2.12092
H	-5.84004	-1.78151	-2.46886
C	-3.73865	-1.92725	-2.06709
H	-3.53990	-0.90909	-2.38538
N	-0.28694	1.77781	-0.66391
N	-1.55205	1.31116	-0.59770
C	0.84388	3.80770	-1.55652
C	0.67330	5.20983	-1.68827
H	-0.31431	5.64379	-1.57323
C	1.76504	6.03266	-1.91048
H	1.62729	7.10604	-1.99117
C	3.05363	5.47985	-2.01969
H	3.90654	6.12877	-2.19393
C	3.23801	4.09318	-1.91180
H	4.22902	3.66055	-2.00076
C	2.14824	3.26784	-1.69179
H	2.31308	2.19938	-1.64814
C	-0.32111	2.98238	-1.30263
C	-1.66349	3.25988	-1.65273
H	-2.03474	4.12589	-2.17905
C	-2.41888	2.18810	-1.21211
C	-3.85636	1.92392	-1.37397
C	-4.67146	1.59825	-0.27753
H	-4.25030	1.56889	0.72158
C	-6.02356	1.32533	-0.46749
H	-6.64329	1.07491	0.38762
C	-6.57677	1.37903	-1.75076
H	-7.63228	1.16932	-1.89691
C	-5.77498	1.71802	-2.84456
H	-6.20352	1.76910	-3.84079
C	-4.42012	1.99407	-2.65907
H	-3.79211	2.24609	-3.50889
N	-0.18509	0.00455	1.80326
N	-1.43101	-0.22409	1.43169
C	1.01283	0.37691	3.94054
C	0.93118	0.95818	5.23752
H	-0.02982	1.28089	5.62415
C	2.07698	1.15179	5.98465
H	2.01760	1.61236	6.96534
C	3.32807	0.75492	5.46958
H	4.22471	0.90683	6.06314
C	3.42169	0.16287	4.19874
H	4.38633	-0.15471	3.81537
C	2.28243	-0.02130	3.43616
C	-0.18721	0.16689	3.18232
C	-1.51186	0.04714	3.64718
H	-1.84312	0.04408	4.67428
C	-2.28957	-0.24620	2.54316
C	-3.70772	-0.56317	2.47942
C	-4.59979	0.14938	3.31202
H	-4.22139	0.94831	3.94277
C	-5.95819	-0.14429	3.29550
H	-6.64081	0.41651	3.92609
C	-6.44355	-1.16364	2.46454
H	-7.50459	-1.39484	2.45698
C	-5.56385	-1.88986	1.65125
H	-5.93404	-2.68755	1.01600
C	-4.20667	-1.59540	1.65391
H	-3.53216	-2.18090	1.03991
O	1.82811	2.02814	0.98488
H	2.34415	-0.49146	2.46419
C	4.90222	-1.15424	0.24908
C	4.57752	-2.44766	0.68163
C	6.21591	-0.85896	-0.14957
C	5.56240	-3.43597	0.72143
H	3.55839	-2.67222	0.97594
C	7.19435	-1.85344	-0.12077
H	6.44970	0.14760	-0.47957
C	6.86836	-3.14109	0.31606
H	5.31286	-4.43582	1.06411
H	8.20928	-1.62363	-0.43070
H	7.63171	-3.91314	0.34434
H	2.80556	2.02420	0.85192

^{6}FeTMCpyBr
Charge: 2+
Energy: -3047694.3568923

Fe	0.23775	0.00541	0.06395
N	-0.64236	-1.59550	-1.20532
N	-0.19598	1.29835	-1.70808
N	1.15101	1.69571	1.26315
N	0.63841	-1.13160	1.88271
C	-0.23813	-1.12825	-2.57450
C	-0.61737	0.33893	-2.80179
C	1.08530	2.01763	-2.05762
C	1.65353	2.93493	-0.95778
C	2.18480	2.33608	0.35768
C	1.80350	1.03868	2.46693
C	1.88624	-0.49326	2.42092
C	0.89054	-2.58696	1.57608
C	-0.13183	-3.26498	0.64924
C	-0.04946	-2.93411	-0.85147
C	-2.12792	-1.68428	-1.11148
C	-1.28137	2.31475	-1.57429
C	0.27887	2.78907	1.78359
C	-0.45897	-1.01479	2.87980
H	-0.73461	-1.73938	-3.33966
H	0.83285	-1.27615	-2.67785
H	-1.70322	0.41814	-2.88818
H	-0.20053	0.66827	-3.76003
H	0.88491	2.63905	-2.94075
H	1.81713	1.26482	-2.34205
H	2.52292	3.42196	-1.41623
H	0.95893	3.75440	-0.74955
H	2.95005	1.59187	0.15591
H	2.65425	3.14856	0.92782
H	2.81556	1.43589	2.59570
H	1.23686	1.34425	3.34748
H	2.07606	-0.85935	3.43847
H	2.71471	-0.81085	1.79459
H	0.91219	-3.12429	2.53269
H	1.88384	-2.66183	1.13387
H	-1.15098	-3.12336	1.02827
H	0.05667	-4.34121	0.73593
H	0.98841	-2.94082	-1.18037
H	-0.58135	-3.70284	-1.42644
H	-2.56258	-1.71751	-2.11664
H	-2.39740	-2.63661	-0.64529
H	-1.37201	2.88817	-2.50495
H	-1.06260	3.00577	-0.76474
H	-2.23187	1.82885	-1.36657
H	0.89332	3.58684	2.21856
H	-0.37163	2.40917	2.56970
H	-0.33182	3.21442	0.99094
H	-0.17086	-1.50290	3.81856
H	-1.36460	-1.47994	2.49462
C	-2.77101	-0.58984	-0.30675
C	-2.58147	1.06912	1.29184
C	-4.15690	-0.41767	-0.35799
C	-3.95032	1.28845	1.31231
H	-1.93179	1.64443	1.93020
C	-4.76006	0.53419	0.45856
H	-4.75023	-1.03489	-1.02598
H	-4.36821	2.03585	1.97800
H	-5.83531	0.68193	0.43475
H	-0.67260	0.03474	3.07996
N	-1.98320	0.15541	0.49468
Br	2.53403	-0.75568	-0.81237

^{6}FeTMCpyCl
Charge: 2+
Energy: -1721170.8711245

Fe	-0.40642	0.13729	-0.09570
N	0.96763	1.19676	-1.49214
N	-0.08722	-1.58904	-1.48081
N	-1.83595	-1.02466	1.24069
N	-0.76525	1.72183	1.36799
C	0.63158	0.50931	-2.78385
C	0.69698	-1.01354	-2.63956
C	-1.45624	-2.05663	-1.91210
C	-2.37718	-2.55193	-0.78050
C	-2.88478	-1.57281	0.29414
C	-2.43170	0.00750	2.17771
C	-2.18536	1.46676	1.78359
C	-0.65217	3.07932	0.72242
C	0.60709	3.31670	-0.12726
C	0.64303	2.66559	-1.52090
C	2.40772	1.01333	-1.15996
C	0.68057	-2.76121	-0.97053
C	-1.35801	-2.15717	2.08566
C	0.13762	1.64906	2.54612
H	1.33829	0.81717	-3.56577
H	-0.36050	0.83231	-3.08752
H	1.73688	-1.31570	-2.49622
H	0.36125	-1.47486	-3.57529
H	-1.31478	-2.88744	-2.61654
H	-1.92622	-1.23820	-2.45352
H	-3.28191	-2.90919	-1.28739
H	-1.95556	-3.44588	-0.31107
H	-3.38656	-0.72642	-0.16690
H	-3.62457	-2.10546	0.90642
H	-3.51187	-0.15419	2.26231
H	-2.01272	-0.17614	3.16803
H	-2.43794	2.10434	2.64119
H	-2.82741	1.75302	0.95484
H	-0.68511	3.82727	1.52489

H	-1.53709	3.22147	0.10222
H	1.51185	3.07642	0.44382
H	0.65471	4.39900	-0.29353
H	-0.32014	2.78698	-2.01442
H	1.39690	3.16711	-2.14129
H	2.96235	0.70817	-2.05442
H	2.83198	1.97879	-0.86824
H	0.76556	-3.52368	-1.75464
H	0.18001	-3.20483	-0.11402
H	1.67929	-2.45391	-0.66712
H	-2.21134	-2.67703	2.53840
H	-0.73242	-1.78555	2.89599
H	-0.78826	-2.87235	1.49742
H	-0.15870	2.38989	3.29856
H	1.16499	1.83867	2.23922
C	2.66483	0.04421	-0.03840
C	1.86547	-1.14262	1.78037
C	3.96866	-0.38419	0.22399
C	3.13122	-1.59759	2.11509
H	1.01018	-1.42823	2.37026
C	4.21078	-1.21662	1.31265
H	4.78086	-0.05622	-0.41787
H	3.26509	-2.23823	2.97996
H	5.21720	-1.55826	1.53395
H	0.09429	0.65616	2.99285
N	1.61836	-0.33978	0.72073
Cl	-2.14090	1.03324	-1.36020

^{6}FeTMCpyF
Charge: 2+
Energy: -1495061.4562221

Fe	-0.39417	0.17069	-0.15975
N	1.14022	0.78923	-1.63729
N	-0.32559	-1.79173	-1.23715
N	-2.10811	-0.51562	1.15759
N	-0.67342	2.06812	0.89134
C	0.75504	-0.09558	-2.78261
C	0.66046	-1.55271	-2.34783
C	-1.71399	-1.98242	-1.78623
C	-2.82594	-2.12197	-0.73490
C	-3.16010	-0.90643	0.14327
C	-2.53702	0.72684	1.89467
C	-2.14202	2.01524	1.18685
C	-0.40724	3.22427	-0.03059
C	0.92286	3.18143	-0.79326
C	0.95264	2.23191	-1.99828
C	2.52597	0.53017	-1.17085
C	0.11873	-3.01071	-0.51120
C	-1.97155	-1.60429	2.16347
C	0.13179	2.19703	2.13071
H	1.48928	-0.00471	-3.59387
H	-0.20548	0.26037	-3.15160
H	1.63464	-1.89652	-1.99086
H	0.40087	-2.17646	-3.21221
H	-1.70884	-2.88711	-2.40935
H	-1.92674	-1.12701	-2.42674
H	-3.74000	-2.32670	-1.30524
H	-2.67701	-3.01631	-0.12265
H	-3.34065	-0.03773	-0.48762
H	-4.08171	-1.12645	0.69846
H	-3.62397	0.71380	2.04142
H	-2.08650	0.69193	2.88815
H	-2.43001	2.87253	1.80956
H	-2.66042	2.09773	0.23228
H	-0.45758	4.14336	0.56754
H	-1.22478	3.24977	-0.75225
H	1.76496	2.99890	-0.11518
H	1.08483	4.19177	-1.18543
H	0.00797	2.30366	-2.53799
H	1.75707	2.52105	-2.68715
H	3.09621	0.00276	-1.94484
H	3.03877	1.48630	-1.02685
H	0.19304	-3.85944	-1.20287
H	-0.58681	-3.27311	0.27231
H	1.09393	-2.83363	-0.05738
H	-2.95074	-1.85200	2.59254
H	-1.32240	-1.28132	2.97791
H	-1.55062	-2.50090	1.71647
H	-0.15780	3.09575	2.68928
H	1.18932	2.25862	1.87481
C	2.59536	-0.23247	0.13159
C	1.51693	-1.00310	2.04026
C	3.81840	-0.71782	0.59981
C	2.69486	-1.49954	2.57546
H	0.58030	-1.10173	2.57032
C	3.87340	-1.35848	1.83486
H	4.71462	-0.58508	0.00124
H	2.68891	-1.98751	3.54402
H	4.81597	-1.73981	2.21541
H	-0.00731	1.32231	2.76636
N	1.45629	-0.38230	0.84001
F	-1.53782	0.85143	-1.38523

^{6}FeTMCpyN$_3$
Charge: 2+
Energy: -1535436.7370803

Fe	0.32955	0.00846	0.04297
N	-0.47892	-1.72786	-1.08572
N	-0.09202	1.13228	-1.85219
N	1.17725	1.85945	1.08375
N	0.75661	-0.94317	1.96989
C	-0.06719	-1.35069	-2.47564
C	-0.51836	0.06766	-2.82996
C	1.22106	1.74980	-2.25127
C	1.81490	2.76440	-1.25503
C	2.27226	2.30452	0.14221
C	1.75841	1.33310	2.37489
C	1.96882	-0.18114	2.41428
C	1.11009	-2.38851	1.75782
C	0.12623	-3.20397	0.90260
C	0.18282	-2.99128	-0.62004
C	-1.95664	-1.86155	-0.98584
C	-1.14896	2.18070	-1.85388
C	0.35675	3.05487	1.42803
C	-0.33101	-0.83182	2.97391
H	-0.50104	-2.04985	-3.20315
H	1.01444	-1.44368	-2.54734
H	-1.60964	0.09382	-2.87263
H	-0.15909	0.31807	-3.83555
H	1.07514	2.26715	-3.20967
H	1.92423	0.93545	-2.42229
H	2.72017	3.14756	-1.74174
H	1.16074	3.63721	-1.17009
H	2.98171	1.48391	0.05701
H	2.79379	3.14724	0.61618
H	2.71481	1.82782	2.58249
H	1.07999	1.62404	3.17832
H	2.23915	-0.46947	3.43907
H	2.79221	-0.46561	1.76176
H	1.19890	-2.86093	2.74479
H	2.09948	-2.42273	1.29831
H	-0.89795	-3.08806	1.27532
H	0.37574	-4.25708	1.07539
H	1.22076	-2.97535	-0.95390
H	-0.29552	-3.84000	-1.12612
H	-2.39336	-1.99965	-1.98185
H	-2.19497	-2.77528	-0.43273
H	-1.25293	2.61612	-2.85584
H	-0.89909	2.97713	-1.15801
H	-2.10265	1.74876	-1.55435
H	0.99901	3.87063	1.78355
H	-0.34294	2.81386	2.22763
H	-0.20558	3.40523	0.56598
H	-0.00333	-1.22482	3.94448
H	-1.20381	-1.38939	2.63604
C	-2.62816	-0.71139	-0.27901
C	-2.46177	1.10873	1.14062
C	-4.01850	-0.58263	-0.32254
C	-3.83597	1.29283	1.16238
H	-1.81160	1.76178	1.70119
C	-4.63514	0.43170	0.40482
H	-4.60517	-1.27904	-0.91416
H	-4.26676	2.09360	1.75354
H	-5.71446	0.54687	0.38565
H	-0.62641	0.21004	3.09443
N	-1.85240	0.13298	0.43136
N	2.05633	-0.53115	-0.52404
N	2.98310	-1.17587	-0.96220
N	3.86004	-1.79200	-1.37927

^{6}FeTMCpyNCS
Charge: 2+
Energy: -1740546.9209269

Fe	0.12526	0.09664	0.09632
N	-0.27629	-1.82975	-0.93023
N	-0.26353	0.98681	-1.92518
N	0.56889	2.13183	1.03409
N	0.50509	-0.62466	2.13047
C	0.21455	-1.49721	-2.30629
C	-0.41837	-0.20787	-2.83112
C	0.97648	1.77179	-2.25867
C	1.30080	2.94347	-1.31211
C	1.67422	2.67386	0.15774
C	1.08843	1.80890	2.41493
C	1.53131	0.35833	2.60763
C	1.10079	-2.00434	2.08764
C	0.35041	-3.03414	1.22748
C	0.52924	-2.92557	-0.29639
C	-1.71624	-2.19833	-0.94885
C	-1.46143	1.84762	-2.12508
C	-0.45895	3.19928	1.18944
C	-0.68515	-0.61519	3.01747
H	-0.02161	-2.31474	-3.00068
H	1.29748	-1.40691	-2.26105
H	-1.49075	-0.36489	-2.96881

H	-0.00423	0.01915	-3.82104
H	0.85494	2.18216	-3.27080
H	1.80810	1.06936	-2.28621
H	2.18364	3.42730	-1.74758
H	0.51654	3.70419	-1.36870
H	2.50844	1.97871	0.21587
H	2.00557	3.62513	0.59625
H	1.92749	2.47054	2.66144
H	0.29256	2.04198	3.12393
H	1.73938	0.19540	3.67381
H	2.45023	0.16600	2.05789
H	1.15882	-2.37581	3.11907
H	2.12354	-1.90921	1.72046
H	-0.71147	-3.06667	1.49779
H	0.74769	-4.01439	1.51477
H	1.57824	-2.74711	-0.53232
H	0.24996	-3.87685	-0.76794
H	-2.02081	-2.48760	-1.96152
H	-1.86312	-3.09069	-0.33259
H	-1.52964	2.16739	-3.17270
H	-1.40558	2.73492	-1.49992
H	-2.36357	1.29687	-1.86265
H	0.00817	4.13440	1.52377
H	-1.19203	2.90936	1.94154
H	-0.97584	3.38452	0.25096
H	-0.40166	-0.86701	4.04706
H	-1.41781	-1.33737	2.65923
C	-2.63108	-1.12273	-0.41905
C	-2.90504	0.80698	0.82970
C	-4.01197	-1.23126	-0.60043
C	-4.28554	0.76028	0.70904
H	-2.42911	1.60206	1.38197
C	-4.85426	-0.27959	-0.03222
H	-4.41564	-2.06056	-1.17356
H	-4.89740	1.52230	1.17943
H	-5.93013	-0.34797	-0.16021
H	-1.15381	0.36851	3.00888
N	-2.07772	-0.10656	0.27473
N	1.98354	-0.22175	-0.27744
C	3.11844	-0.57080	-0.49242
S	4.60605	-1.03109	-0.77162

^{6}FeTMCpyOH
Charge: 2+
Energy: -1479968.5747664

Fe	-0.43696	0.19158	-0.21511
O	-1.63964	0.82278	-1.44513
N	1.17331	0.86981	-1.59878
N	-0.21578	-1.76239	-1.28014
N	-2.11546	-0.59100	1.10381
N	-0.74554	2.03913	0.93067
C	0.85100	0.00628	-2.77912
C	0.76386	-1.46703	-2.38444
C	-1.58587	-2.05195	-1.83441
C	-2.69755	-2.25170	-0.78897
C	-3.13028	-1.06224	0.08603
C	-2.62227	0.62970	1.83139
C	-2.21986	1.95511	1.18994
C	-0.45276	3.23097	0.06758
C	0.90078	3.22201	-0.66037
C	1.00479	2.32529	-1.90496
C	2.54539	0.60735	-1.09182
C	0.29440	-2.95150	-0.54654
C	-1.93285	-1.66633	2.11793
C	0.01684	2.13308	2.19968
H	1.61762	0.12304	-3.55699
H	-0.09873	0.34648	-3.18697
H	1.74377	-1.80863	-2.04233
H	0.51475	-2.06285	-3.27110
H	-1.51792	-2.96550	-2.44109
H	-1.84665	-1.22172	-2.48919
H	-3.58946	-2.52239	-1.36707
H	-2.49373	-3.13130	-0.17089
H	-3.37395	-0.20939	-0.54408
H	-4.03383	-1.35689	0.63674
H	-3.71560	0.58998	1.90713
H	-2.23868	0.58474	2.85202
H	-2.53335	2.77655	1.84831
H	-2.72194	2.07229	0.23145
H	-0.51347	4.12761	0.69831
H	-1.25570	3.30407	-0.66838
H	1.71705	3.01343	0.04060
H	1.07183	4.24933	-1.00158
H	0.10642	2.43473	-2.51489
H	1.84800	2.65266	-2.52735
H	3.14817	0.11392	-1.86333
H	3.04321	1.56242	-0.89714
H	0.39364	-3.80623	-1.22773
H	-0.38642	-3.23065	0.25310
H	1.26788	-2.72902	-0.11064
H	-2.90420	-1.98114	2.52006
H	-1.33259	-1.30050	2.95078
H	-1.43797	-2.53235	1.68571
H	-0.29494	3.01364	2.77544
H	1.08275	2.20304	1.98476
C	2.57686	-0.19487	0.18567
C	1.46193	-0.97339	2.06040
C	3.78347	-0.72050	0.65358
C	2.62132	-1.50982	2.59984
H	0.52069	-1.05873	2.58174
C	3.81071	-1.38805	1.87518
H	4.68850	-0.59695	0.06636
H	2.59098	-2.01400	3.55961
H	4.73891	-1.80208	2.25674
H	-0.14372	1.23974	2.80247
N	1.42428	-0.33033	0.87250
H	-1.76836	1.54821	-2.07261

^{6}FeMeTPENBrB
Charge: 2+
Energy: -3091785.7328057

Fe	0.06625	-0.01013	-0.18875
N	0.51972	-1.99459	0.70759
N	-1.87363	-0.92825	-0.09021
N	-0.58638	2.00320	-0.19136
N	2.18646	0.02180	-0.02239
N	-0.13396	0.51403	2.03434
C	0.56079	-1.84807	2.19960
C	-0.40623	-0.78077	2.70953
C	1.06172	1.18399	2.60670
C	-0.47677	2.82404	-1.26006
C	-1.14931	2.46372	0.95431
C	-0.92118	4.14041	-1.22424
C	-1.61262	3.77036	1.05645
C	-1.49905	4.62109	-0.04718
C	-1.28066	1.45229	2.07248
C	-1.89133	-2.25542	0.15188
C	-3.02952	-0.28298	-0.34555
C	-3.08538	-2.97103	0.19520
C	-4.25646	-0.93331	-0.33591
C	-4.28501	-2.30124	-0.05014
C	-0.54252	-2.92906	0.24734
C	2.93579	1.13021	-0.17144
C	4.32340	1.09310	-0.12003
C	4.94954	-0.13679	0.10006
C	4.16882	-1.28567	0.24653
C	2.78368	-1.17466	0.16461
C	1.86072	-2.37139	0.17726
H	0.34348	-2.81082	2.67707
H	1.58367	-1.58126	2.47192
H	-0.30514	-0.68729	3.79905
H	-1.43715	-1.06802	2.49829
H	1.93191	0.53337	2.54374
H	0.88584	1.45029	3.65664
H	1.27421	2.09174	2.03944
H	-0.03044	2.39046	-2.14776
H	-0.81613	4.76923	-2.10163
H	-2.05277	4.11807	1.98558
H	-1.85406	5.64533	0.01435
H	-1.35869	1.95369	3.04543
H	-2.20073	0.87773	1.92720
H	-2.94481	0.77518	-0.56674
H	-3.07310	-4.03634	0.40279
H	-5.16517	-0.38117	-0.54921
H	-5.22701	-2.84035	-0.02732
H	-0.27836	-3.25670	-0.76394
H	-0.58517	-3.82167	0.88296
H	2.39194	2.05528	-0.33329
H	4.89690	2.00459	-0.24791
H	6.03187	-0.20172	0.15353
H	4.62778	-2.25563	0.40936
H	2.29169	-3.20573	0.74385
H	1.72854	-2.69872	-0.85917
Br	0.21663	-0.49492	-2.56506

^{6}FeMeTPENBrC
Charge: 2+
Energy: -3091773.8209566

N	1.14557	-0.35322	1.75973
Fe	-0.21585	-0.21221	0.05055
N	1.60713	-0.88019	-0.89985
N	-2.02077	0.34376	-0.90665
N	-1.45712	0.67130	1.73061
C	0.27664	-0.74076	2.91233
C	-0.93428	0.19848	3.05591
C	1.84156	0.95310	1.95838
C	-1.51267	2.16039	1.69651
N	0.82231	1.67715	-0.15054
C	1.81323	1.86365	0.74479
C	2.72293	2.91112	0.61107
C	2.59578	3.78891	-0.46674
C	1.55805	3.59752	-1.38243
C	0.69621	2.52510	-1.18801
C	-3.09324	0.36465	-0.07974
C	-4.38197	0.52794	-0.57755

C	-4.56971	0.64990	-1.95605
C	-3.45980	0.61192	-2.80379
C	-2.20160	0.45606	-2.23714
C	1.86867	-0.84793	-2.21681
C	3.08529	-1.27192	-2.73935
C	4.06468	-1.73087	-1.85594
C	3.79127	-1.75630	-0.48657
C	2.54358	-1.33118	-0.03902
C	2.11172	-1.43511	1.40497
C	-2.80613	0.13816	1.38902
H	0.85052	-0.75501	3.84784
H	-0.06668	-1.75514	2.70962
H	-1.71802	-0.32492	3.61166
H	-0.67393	1.07878	3.64783
H	2.87628	0.78071	2.27359
H	1.35869	1.47925	2.78743
H	-2.23788	2.52812	2.43275
H	-1.80700	2.49555	0.70199
H	-0.53394	2.57881	1.92293
H	3.51466	3.04106	1.34257
H	3.29502	4.61043	-0.58834
H	1.42046	4.26153	-2.22884
H	-0.12805	2.32988	-1.86605
H	-5.22616	0.55226	0.10397
H	-5.56889	0.77190	-2.36253
H	-3.56528	0.69730	-3.87968
H	-1.30736	0.40525	-2.85118
H	1.07496	-0.47770	-2.85852
H	3.25763	-1.24127	-3.80961
H	5.02842	-2.06519	-2.22718
H	4.53091	-2.11232	0.22350
H	1.59660	-2.39192	1.53312
H	2.97244	-1.42415	2.08369
H	-3.57798	0.60412	2.01453
H	-2.81009	-0.93843	1.58472
Br	-0.96241	-2.54915	0.09542

^{6}FeMeTPENClB
Charge: 2+
Energy: -1765257.2749541

Fe	0.07897	-0.03172	-0.40658
N	0.53193	-2.05758	0.37791
N	-1.87099	-0.93902	-0.31501
N	-0.56918	1.97257	-0.29253
N	2.20498	-0.01265	-0.25844
N	-0.08201	0.37996	1.84835
C	0.60002	-1.99227	1.87448
C	-0.35100	-0.94793	2.45810
C	1.12627	1.01258	2.43676
C	-0.47959	2.83278	-1.33119
C	-1.10638	2.38458	0.88289
C	-0.91789	4.14801	-1.23169
C	-1.56134	3.68751	1.04835
C	-1.46674	4.58177	-0.02264
C	-1.22161	1.32238	1.95510
C	-1.89057	-2.27782	-0.15144
C	-3.02672	-0.27614	-0.51909
C	-3.08679	-2.99089	-0.13298
C	-4.25625	-0.92189	-0.53073
C	-4.28673	-2.30369	-0.32284
C	-0.54314	-2.96006	-0.11633
C	2.96011	1.09654	-0.36124
C	4.34833	1.04522	-0.34461
C	4.96751	-0.20045	-0.21088
C	4.17983	-1.35000	-0.11492
C	2.79431	-1.22287	-0.15860
C	1.86000	-2.41015	-0.20075
H	0.38383	-2.97812	2.30277
H	1.62940	-1.74693	2.14251
H	-0.23000	-0.91398	3.54904
H	-1.38725	-1.21782	2.25011
H	1.99180	0.36233	2.32565
H	0.96797	1.22339	3.50198
H	1.33487	1.94833	1.91540
H	-0.05580	2.43013	-2.24458
H	-0.83070	4.81221	-2.08462
H	-1.98095	3.99892	1.99960
H	-1.81539	5.60404	0.08839
H	-1.27650	1.77721	2.95215
H	-2.14856	0.76125	1.80123
H	-2.94050	0.79268	-0.67993
H	-3.07627	-4.06652	0.01208
H	-5.16533	-0.35544	-0.70047
H	-5.23064	-2.83989	-0.31790
H	-0.29703	-3.23085	-1.14868
H	-0.57847	-3.88698	0.46854
H	2.42113	2.03374	-0.45564
H	4.92740	1.95789	-0.43278
H	6.05012	-0.27702	-0.18590
H	4.63339	-2.33154	-0.02102
H	2.29340	-3.28198	0.30414
H	1.70417	-2.67038	-1.25272
Cl	0.19234	-0.35449	-2.61617

^{6}FeMeTPENClC
Charge: 2+
Energy: -1765246.0941598

N	-1.11908	0.37493	-1.78076
Fe	0.25464	-0.37076	-0.24794
N	-1.61207	-1.26619	0.37519
N	2.10256	-0.44409	0.78755
N	1.55979	1.09545	-1.38594
C	-0.27898	0.49594	-3.01129
C	0.98803	1.32789	-2.75399
C	-1.72261	1.66726	-1.34126
C	1.75599	2.39188	-0.67885
N	-0.62037	1.29432	0.81813
C	-1.59779	1.93660	0.14731
C	-2.40768	2.88110	0.77584
C	-2.19300	3.17196	2.12388
C	-1.16959	2.51172	2.80885
C	-0.40971	1.57656	2.11745
C	3.16638	-0.14664	0.00391
C	4.46781	-0.34385	0.45433
C	4.67445	-0.87928	1.72754
C	3.57147	-1.19861	2.52338
C	2.30068	-0.96597	2.01373
C	-1.87092	-1.81202	1.57453
C	-3.11362	-2.35130	1.88795
C	-4.12108	-2.30481	0.92202
C	-3.84956	-1.72985	-0.32160
C	-2.57572	-1.22591	-0.56890
C	-2.15145	-0.69536	-1.91865
C	2.84965	0.34888	-1.39125
H	-0.85403	0.93718	-3.83550
H	-0.00174	-0.51928	-3.29414
H	1.72741	1.08869	-3.52447
H	0.77727	2.39515	-2.85115
H	-2.77510	1.70904	-1.64172
H	-1.22481	2.48233	-1.87548
H	2.50846	2.99643	-1.19999
H	2.08612	2.20835	0.34360
H	0.81873	2.94443	-0.64278
H	-3.19024	3.38505	0.21685
H	-2.81389	3.90408	2.63094
H	-0.96596	2.71463	3.85460
H	0.39989	1.03681	2.59737
H	5.30643	-0.08808	-0.18521
H	5.68314	-1.04544	2.09285
H	3.69129	-1.62118	3.51486
H	1.40931	-1.20745	2.58525
H	-1.05478	-1.81557	2.29066
H	-3.28424	-2.79353	2.86334
H	-5.10554	-2.71066	1.13310
H	-4.61155	-1.68376	-1.09313
H	-1.69661	-1.52016	-2.47505
H	-3.00999	-0.33253	-2.49560
H	3.66094	0.98037	-1.77486
H	2.74297	-0.51504	-2.05395
Cl	0.77079	-2.27107	-1.35309

^{6}FeMeTPENFB
Charge: 2+
Energy: -1539131.8600034

Fe	0.08760	-0.03101	-0.52167
N	0.59347	-2.07509	0.21647
N	-1.82947	-1.00090	-0.45518
N	-0.63256	1.93788	-0.33783
N	2.21485	0.01323	-0.39400
N	-0.05939	0.32915	1.75628
C	0.68663	-2.02557	1.71317
C	-0.28608	-1.02148	2.33212
C	1.13841	0.97767	2.34972
C	-0.59149	2.79732	-1.37871
C	-1.15331	2.32445	0.85061
C	-1.06066	4.10071	-1.26187
C	-1.63647	3.61462	1.03449
C	-1.58771	4.51464	-0.03555
C	-1.22169	1.23919	1.90451
C	-1.82681	-2.34059	-0.29912
C	-2.99834	-0.35557	-0.64341
C	-3.01089	-3.07371	-0.27748
C	-4.21717	-1.02142	-0.65072
C	-4.22328	-2.40511	-0.45388
C	-0.46794	-3.00120	-0.26356
C	2.94497	1.14092	-0.47356
C	4.33427	1.11946	-0.47335
C	4.98116	-0.11576	-0.38109
C	4.21948	-1.28448	-0.30830
C	2.83118	-1.18549	-0.33329
C	1.91954	-2.39081	-0.38716
H	0.51048	-3.02388	2.13096
H	1.71243	-1.75111	1.96605
H	-0.15648	-1.01615	3.42270
H	-1.31670	-1.31441	2.12525

H	2.02059	0.35613	2.20773
H	0.98999	1.15315	3.42274
H	1.31386	1.93388	1.85333
H	-0.18371	2.39670	-2.30090
H	-1.01465	4.77154	-2.11282
H	-2.04346	3.91161	1.99578
H	-1.95802	5.52774	0.08889
H	-1.27375	1.67074	2.91191
H	-2.13632	0.65724	1.75049
H	-2.93096	0.71598	-0.79374
H	-2.98182	-4.14989	-0.13898
H	-5.13689	-0.46867	-0.80782
H	-5.15821	-2.95684	-0.44541
H	-0.22141	-3.28819	-1.29157
H	-0.48717	-3.92108	0.33317
H	2.38448	2.06829	-0.53591
H	4.89286	2.04646	-0.54182
H	6.06538	-0.16952	-0.36935
H	4.69512	-2.25804	-0.24563
H	2.37795	-3.26334	0.09431
H	1.75531	-2.63909	-1.44114
F	0.15025	-0.02882	-2.28848

^{2}FeMeTPENFC
Charge: 2+
Energy: -1539125.2081897

N	1.23392	-0.80512	-1.53173
Fe	-0.16834	0.06794	-0.41385
N	1.29741	1.40030	-0.08469
N	-1.89614	0.76614	0.37893
N	-1.40916	-1.49187	-0.89365
C	0.43257	-1.50267	-2.59596
C	-0.70272	-2.29564	-1.95457
C	2.06157	-1.72952	-0.68779
C	-1.82251	-2.40481	0.21318
N	0.58624	-0.95978	1.10776
C	1.64350	-1.72762	0.76810
C	2.31446	-2.49213	1.72137
C	1.89070	-2.44661	3.04931
C	0.79985	-1.64089	3.39141
C	0.17027	-0.91610	2.38970
C	-2.95002	0.29679	-0.33889
C	-4.24235	0.76389	-0.12932
C	-4.46456	1.75205	0.83138
C	-3.38226	2.22868	1.57060
C	-2.11890	1.70917	1.31095
C	1.40408	2.29355	0.91277
C	2.47629	3.17254	1.01488
C	3.48494	3.11273	0.05256
C	3.38908	2.16697	-0.96987
C	2.28097	1.32810	-1.01344
C	2.04845	0.31359	-2.09931
C	-2.62257	-0.75833	-1.37152
H	1.07202	-2.16087	-3.19572
H	0.03060	-0.72114	-3.23793
H	-1.41144	-2.63162	-2.71897
H	-0.31117	-3.19133	-1.46662
H	3.11394	-1.43715	-0.75823
H	1.99987	-2.74621	-1.09013
H	-2.53010	-3.14904	-0.16914
H	-2.30024	-1.82943	1.00583
H	-0.95243	-2.91661	0.62077
H	3.15708	-3.10995	1.42622
H	2.40299	-3.03176	3.80675
H	0.44057	-1.58015	4.41286
H	-0.69286	-0.29202	2.58759
H	-5.06288	0.35856	-0.71259
H	-5.46537	2.13528	1.00381
H	-3.50654	2.99011	2.33264
H	-1.25697	2.05730	1.86484
H	0.61380	2.29233	1.65044
H	2.51579	3.88229	1.83379
H	4.33736	3.78297	0.10208
H	4.16120	2.08212	-1.72776
H	1.45729	0.78077	-2.88880
H	2.98310	-0.05752	-2.53278
H	-3.45710	-1.45434	-1.51369
H	-2.39051	-0.27915	-2.32270
F	-0.64465	0.97222	-1.86467

^{6}FeMeTPENN$_3$B
Charge: 2+
Energy: -1579519.7179335

Fe	-0.07853	-0.01920	0.32493
N	-0.55259	-2.01883	-0.55735
N	1.87624	-0.97754	0.20413
N	0.61368	1.99339	0.26454
N	-2.22883	0.02302	0.12782
N	0.12162	0.46406	-1.92169
C	-0.59879	-1.89329	-2.04965
C	0.37515	-0.84221	-2.58046
C	-1.06489	1.13937	-2.50700
C	0.52391	2.83527	1.31575
C	1.17362	2.42262	-0.89177
C	0.98574	4.14468	1.25486
C	1.65526	3.72113	-1.02322
C	1.56176	4.59412	0.06407
C	1.27973	1.38607	-1.98983
C	1.86449	-2.30571	-0.02846
C	3.05113	-0.35324	0.41484
C	3.04379	-3.04422	-0.10275
C	4.26724	-1.02472	0.37287
C	4.26277	-2.39490	0.09890
C	0.50105	-2.95804	-0.09315
C	-2.98743	1.12924	0.23026
C	-4.37449	1.08637	0.14804
C	-4.99118	-0.15060	-0.05521
C	-4.20206	-1.29883	-0.15359
C	-2.81898	-1.17852	-0.04263
C	-1.89317	-2.37566	-0.01874
H	-0.39282	-2.86436	-2.51598
H	-1.62006	-1.62027	-2.32222
H	0.26818	-0.76527	-3.67098
H	1.40428	-1.13821	-2.37242
H	-1.94316	0.50060	-2.43476
H	-0.88659	1.38793	-3.56112
H	-1.26755	2.05818	-1.95385
H	0.07271	2.42450	2.21219
H	0.89509	4.79288	2.11965
H	2.09306	4.04475	-1.96215
H	1.93002	5.61205	-0.01980
H	1.35787	1.86677	-2.97347
H	2.19367	0.80302	-1.83974
H	2.99315	0.71032	0.62149
H	3.00629	-4.11022	-0.30401
H	5.19204	-0.48641	0.54940
H	5.19385	-2.95087	0.04895
H	0.24293	-3.26778	0.92550
H	0.52465	-3.86448	-0.71068
H	-2.45180	2.06233	0.37567
H	-4.95366	1.99897	0.23698
H	-6.07155	-0.22148	-0.13446
H	-4.65310	-2.27443	-0.30490
H	-2.32844	-3.22590	-0.55862
H	-1.76193	-2.67851	1.02539
N	-0.18842	-0.29493	2.16656
N	-0.26299	-0.50378	3.35778
N	-0.33348	-0.70372	4.48634

^{2}FeMeTPENN$_3$C
Charge: 2+
Energy: -1579509.7818105

N	1.24926	-0.72385	-1.64048
Fe	-0.16745	-0.05897	-0.38426
N	1.18766	1.39095	0.07286
N	-1.89184	0.33974	0.64843
N	-1.27078	-1.64416	-1.03987
C	0.47908	-1.25860	-2.81326
C	-0.66046	-2.15935	-2.32411
C	2.07947	-1.78122	-0.97685
C	-1.38295	-2.76848	-0.06026
N	0.83021	-1.13399	0.99493
C	1.92821	-1.76069	0.52369
C	2.82212	-2.40593	1.37502
C	2.56554	-2.41125	2.74653
C	1.42125	-1.76860	3.22710
C	0.58279	-1.13528	2.31890
C	-2.95345	-0.21914	0.00561
C	-4.26113	-0.01261	0.43265
C	-4.49966	0.80075	1.54118
C	-3.41185	1.36954	2.20344
C	-2.13243	1.11142	1.72595
C	1.21922	2.25733	1.09967
C	2.27081	3.14413	1.30357
C	3.34498	3.12408	0.41464
C	3.31966	2.22337	-0.65150
C	2.22477	1.37886	-0.80337
C	2.06754	0.47426	-1.99950
C	-2.62934	-1.04599	-1.21637
H	1.13917	-1.80808	-3.49509
H	0.07371	-0.39622	-3.33797
H	-1.42583	-2.24011	-3.10137
H	-0.30214	-3.17293	-2.13307
H	3.12982	-1.67575	-1.26604
H	1.75924	-2.76081	-1.34590
H	-2.05121	-3.54107	-0.45672
H	-1.78217	-2.39536	0.88300
H	-0.40159	-3.20268	0.12234
H	3.70065	-2.89798	0.96948
H	3.24762	-2.90835	3.42927
H	1.18358	-1.75436	4.28516
H	-0.31649	-0.62262	2.63683
H	-5.08125	-0.48220	-0.10098
H	-5.51385	0.98039	1.88376
H	-3.54487	2.00395	3.07280

H	-1.26782	1.52956	2.22326
H	0.37487	2.23978	1.77303
H	2.24167	3.82994	2.14308
H	4.18655	3.79693	0.54600
H	4.13415	2.18391	-1.36775
H	1.51832	1.02459	-2.76776
H	3.03569	0.18066	-2.41858
H	-3.37895	-1.82980	-1.37623
H	-2.60208	-0.39952	-2.09672
N	-0.79351	1.06652	-1.77078
N	-1.18922	2.18053	-1.42537
N	-1.56008	3.22592	-1.14678

^{6}FeMeTPENNCSB
Charge: 2+
Energy: -1784628.2161517

Fe	-0.07171	-0.01070	0.12690
N	-0.56190	-1.80798	-1.10475
N	1.85752	-1.00225	-0.07406
N	0.68912	1.94759	0.45413
N	-2.20843	0.14180	-0.13575
N	0.24086	0.85194	-1.98829
C	-0.54221	-1.42121	-2.55199
C	0.48453	-0.32969	-2.85394
C	-0.89865	1.66100	-2.49087
C	0.58530	2.58501	1.63926
C	1.30728	2.55652	-0.58574
C	1.09085	3.86514	1.83346
C	1.83406	3.83796	-0.46177
C	1.72546	4.50135	0.76372
C	1.42713	1.72929	-1.84834
C	1.81989	-2.26895	-0.53466
C	3.03708	-0.46796	0.29732
C	2.97980	-3.02703	-0.68129
C	4.23374	-1.16717	0.19637
C	4.20444	-2.46831	-0.31238
C	0.44404	-2.85045	-0.77356
C	-2.94001	1.23780	0.13518
C	-4.32397	1.25447	0.00656
C	-4.96611	0.09162	-0.42621
C	-4.20528	-1.04735	-0.69935
C	-2.82419	-0.99282	-0.52874
C	-1.93270	-2.20605	-0.68277
H	-0.34629	-2.30238	-3.17492
H	-1.54267	-1.06701	-2.80790
H	0.42841	-0.06243	-3.91792
H	1.49419	-0.69487	-2.66043
H	-1.79775	1.05179	-2.56318
H	-0.66838	2.08166	-3.47821
H	-1.09768	2.47697	-1.79371
H	0.08939	2.03246	2.42991
H	0.98862	4.34825	2.79905
H	2.31862	4.31008	-1.31047
H	2.12850	5.50285	0.87949
H	1.56054	2.37459	-2.72613
H	2.31674	1.09609	-1.77240
H	2.99858	0.54500	0.68383
H	2.92239	-4.04014	-1.06678
H	5.16298	-0.70257	0.50754
H	5.12055	-3.04171	-0.41471
H	0.13040	-3.32758	0.16131
H	0.47250	-3.63221	-1.54271
H	-2.38496	2.11374	0.45660
H	-4.88129	2.15614	0.23578
H	-6.04464	0.07048	-0.54800
H	-4.67690	-1.96710	-1.03060
H	-2.36922	-2.93517	-1.37682
H	-1.85106	-2.68743	0.29738
N	-0.27939	-0.60477	1.90142
C	-0.41606	-1.00644	3.03359
S	-0.59488	-1.53161	4.51392

^{6}FeMeTPENOHB
Charge: 2+
Energy: -1524047.6616347

Fe	0.10657	-0.02518	-0.55410
O	0.19967	-0.15158	-2.35450
N	0.55401	-2.07505	0.21018
N	-1.86714	-0.96301	-0.47123
N	-0.57982	1.97110	-0.35621
N	2.23605	-0.01323	-0.38015
N	-0.09069	0.32641	1.73680
C	0.62010	-2.03742	1.70671
C	-0.34340	-1.01657	2.31469
C	1.11125	0.95576	2.34158
C	-0.48274	2.85698	-1.37017
C	-1.12743	2.34763	0.82349
C	-0.92697	4.16795	-1.24235
C	-1.59147	3.64423	1.01884
C	-1.49069	4.56621	-0.02738
C	-1.23588	1.25644	1.86902
C	-1.87091	-2.30187	-0.30731
C	-3.03685	-0.31093	-0.62226
C	-3.06019	-3.02602	-0.24866
C	-4.26192	-0.96644	-0.59142
C	-4.27266	-2.34956	-0.39175
C	-0.51603	-2.97385	-0.29470
C	2.99812	1.09346	-0.44399
C	4.38621	1.03649	-0.40970
C	4.99805	-0.21460	-0.29809
C	4.20392	-1.36225	-0.24091
C	2.81949	-1.22725	-0.30057
C	1.88232	-2.41254	-0.37335
H	0.41711	-3.03407	2.11702
H	1.64620	-1.78431	1.98024
H	-0.22308	-1.01140	3.40661
H	-1.37666	-1.29462	2.10102
H	1.98280	0.31600	2.21618
H	0.95263	1.14272	3.41152
H	1.31373	1.90422	1.84064
H	-0.04160	2.47328	-2.28414
H	-0.83239	4.85687	-2.07465
H	-2.02020	3.92951	1.97426
H	-1.84456	5.58384	0.10730
H	-1.29654	1.68750	2.87668
H	-2.15948	0.69352	1.70084
H	-2.96658	0.76183	-0.76874
H	-3.03530	-4.10141	-0.10313
H	-5.18191	-0.40625	-0.71824
H	-5.21102	-2.89408	-0.35220
H	-0.27136	-3.23037	-1.33107
H	-0.54552	-3.91200	0.27314
H	2.46446	2.03554	-0.52091
H	4.97023	1.94852	-0.46602
H	6.07981	-0.29684	-0.25857
H	4.65208	-2.34765	-0.16262
H	2.31757	-3.29646	0.10913
H	1.72876	-2.64804	-1.43144
H	-0.46824	-0.28721	-3.04652

^{2}FeMeTPENOHC
Charge: 2+
Energy: -1524040.1426029

N	1.16510	-1.29541	-1.24426
Fe	-0.21242	-0.06785	-0.47232
N	1.27899	1.31190	-0.53496
N	-1.91933	0.88370	0.13875
N	-1.45593	-1.68359	-0.46081
O	-0.65361	0.34431	-2.16976
C	0.36342	-2.22540	-2.10845
C	-0.83500	-2.75804	-1.32141
C	1.91329	-2.00603	-0.15683
C	-1.76471	-2.24917	0.88726
N	0.61132	-0.55875	1.30325
C	1.65201	-1.41103	1.20797
C	2.41215	-1.75819	2.32352
C	2.08096	-1.21370	3.56424
C	0.99827	-0.33378	3.65552
C	0.29251	-0.02814	2.49970
C	-3.00412	0.19088	-0.30342
C	-4.29988	0.66118	-0.11365
C	-4.49837	1.88041	0.53562
C	-3.38636	2.58710	0.99439
C	-2.12171	2.05210	0.77697
C	1.41076	2.47748	0.12033
C	2.54539	3.27405	0.01563
C	3.59843	2.83542	-0.78766
C	3.47611	1.61384	-1.45097
C	2.30387	0.87689	-1.31037
C	2.06199	-0.41271	-2.05173
C	-2.71456	-1.10583	-1.02435
H	0.98360	-3.05246	-2.47431
H	0.02113	-1.63718	-2.95704
H	-1.57882	-3.17318	-2.00842
H	-0.53293	-3.57039	-0.65699
H	2.98603	-1.99916	-0.37433
H	1.61316	-3.05887	-0.14771
H	-2.49675	-3.05887	0.79129
H	-2.17343	-1.46826	1.52883
H	-0.85666	-2.63884	1.34400
H	3.24710	-2.44440	2.22062
H	2.65903	-1.47076	4.44644
H	0.70763	0.10793	4.60239
H	-0.55751	0.64377	2.51033
H	-5.14165	0.07649	-0.47058
H	-5.50177	2.26568	0.68753
H	-3.48997	3.53466	1.51162
H	-1.23856	2.57179	1.12418
H	0.58453	2.77257	0.75184
H	2.59847	4.21164	0.55802
H	4.50202	3.42825	-0.88951
H	4.27854	1.23548	-2.07615
H	1.53426	-0.17803	-2.97824
H	2.99843	-0.92267	-2.30147
H	-3.54484	-1.81370	-0.91831

H	-2.54565	-0.90262	-2.08335
H	-0.97133	1.26164	-2.23001

^{5}FeMe3tacnClacacBr
Charge: 2+
Energy: -3239544.7076776

C	2.97794	0.54007	2.61036
C	2.16751	0.53294	1.35507
C	2.83500	0.43671	0.03642
Cl	4.49547	0.10493	0.00851
O	0.92112	0.61507	1.42065
Fe	-0.48581	-0.03789	0.00848
N	-1.44390	1.96710	0.20604
C	-0.46248	3.07598	0.09279
O	0.91960	0.80620	-1.31077
C	2.16630	0.74345	-1.25064
C	2.98059	0.98445	-2.48061
N	-2.08084	-0.57788	1.36424
C	-1.53797	-1.28643	2.56054
N	-2.00795	-0.27102	-1.50835
C	-1.52764	-1.12656	-2.63386
C	-2.89642	-1.49765	0.50826
C	-3.22512	-0.86726	-0.85030
C	-2.83917	0.64807	1.79127
C	-2.00406	1.90841	1.58692
C	-2.22802	1.12475	-2.00102
C	-2.49521	2.09601	-0.85544
H	3.77968	1.28596	2.57203
H	3.46272	-0.43804	2.73712
H	2.32366	0.73081	3.46179
H	2.32510	1.30841	-3.28989
H	3.48591	0.05371	-2.77382
H	3.76670	1.72782	-2.30712
H	-3.11365	0.56195	2.84670
H	-3.77571	0.69872	1.23532
H	-2.60445	2.80158	1.80460
H	-1.15037	1.90208	2.27046
H	-2.51029	3.11814	-1.24656
H	-3.47788	1.92623	-0.41499
H	-1.31304	1.41201	-2.52625
H	-3.05446	1.14759	-2.72270
H	-3.98611	-0.09269	-0.74957
H	-3.65212	-1.63503	-1.50181
H	-3.82409	-1.77509	1.02483
H	-2.30427	-2.40403	0.36669
H	-2.35695	-1.60983	3.21298
H	-0.88394	-0.60157	3.10437
H	-0.95822	-2.15229	2.24351
H	-0.94320	4.03874	0.30370
H	-0.05360	3.09083	-0.91848
H	0.34737	2.91753	0.80537
H	-2.23821	-1.08410	-3.46739
H	-1.42205	-2.15423	-2.28883
H	-0.55148	-0.76548	-2.96294
Br	0.61218	-2.22524	-0.15187

^{5}FeMe3tacnClacacCl
Charge: 2+
Energy: -1913017.0127959

C	-3.05537	2.56372	0.42022
C	-2.24086	1.31238	0.35532
C	-2.89954	0.00471	0.12718
Cl	-4.53971	0.00550	-0.29217
O	-1.00085	1.37082	0.50377
Fe	0.43303	0.01013	-0.21471
N	1.33612	0.05520	1.82131
C	0.32241	-0.14498	2.88852
O	-1.00059	-1.36922	0.48376
C	-2.24148	-1.30496	0.35242
C	-3.06103	-2.55257	0.43153
N	2.03436	1.40582	-0.60430
C	1.48523	2.64239	-1.23275
N	1.96490	-1.47986	-0.51895
C	1.49063	-2.52075	-1.47742
C	2.86957	0.62343	-1.57051
C	3.19239	-0.77674	-1.03558
C	2.75998	1.74180	0.66707
C	1.89325	1.43763	1.88619
C	2.15098	-2.08118	0.83709
C	2.38784	-1.01166	1.89938
H	-3.88883	2.46847	1.12529
H	-3.49741	2.76506	-0.56543
H	-2.41320	3.39803	0.70471
H	-2.41954	-3.38826	0.71371
H	-3.51410	-2.75732	-0.54838
H	-3.88671	-2.45019	1.14465
H	3.02987	2.80203	0.66827
H	3.69809	1.18703	0.69893
H	2.46923	1.58533	2.80912
H	1.03751	2.11820	1.91110
H	2.37688	-1.47780	2.88956
H	3.37289	-0.55769	1.78920
H	1.23090	-2.62890	1.05887
H	2.97932	-2.80094	0.82517
H	3.93437	-0.73127	-0.23763
H	3.63992	-1.36858	-1.83926
H	3.79935	1.16242	-1.79252
H	2.29266	0.54699	-2.49438
H	2.30010	3.32211	-1.50660
H	0.82336	3.13315	-0.51612
H	0.91190	2.37736	-2.12032
H	0.77280	-0.00730	3.87873
H	-0.08217	-1.15533	2.81323
H	-0.48575	0.57542	2.75975
H	2.19626	-3.35913	-1.50138
H	1.39890	-2.08229	-2.47027
H	0.50819	-2.87454	-1.15922
Cl	-0.48992	0.02122	-2.26871

^{5}FeMe3tacnClacacF
Charge: 2+
Energy: -1686893.8603369

C	-3.08598	2.56684	0.25833
C	-2.27391	1.31159	0.23511
C	-2.92970	0.00397	-0.00238
Cl	-4.55879	0.00627	-0.46462
O	-1.04093	1.36600	0.43173
Fe	0.40686	0.00665	-0.26369
N	1.37037	0.06599	1.72862
C	0.38021	-0.12618	2.82057
O	-1.04152	-1.36881	0.40809
C	-2.27677	-1.30645	0.23113
C	-3.09617	-2.55684	0.26904
N	1.98108	1.39769	-0.71924
C	1.35983	2.59959	-1.34227
N	1.91654	-1.48155	-0.60948
C	1.36263	-2.48311	-1.56307
C	2.76307	0.60616	-1.72019
C	3.11994	-0.78373	-1.18236
C	2.75296	1.75364	0.51434
C	1.93391	1.44860	1.77014
C	2.15393	-2.08283	0.73553
C	2.42297	-1.00328	1.78454
H	-3.93093	2.48561	0.95184
H	-3.51252	2.75270	-0.73668
H	-2.44697	3.40407	0.54133
H	-2.45971	-3.39613	0.55192
H	-3.53200	-2.74674	-0.72122
H	-3.93483	-2.46638	0.96892
H	3.01167	2.81682	0.49688
H	3.69696	1.20755	0.51448
H	2.54493	1.59895	2.66947
H	1.07984	2.12995	1.82647
H	2.44271	-1.46102	2.77846
H	3.40450	-0.55106	1.63927
H	1.24383	-2.63233	0.99262
H	2.98358	-2.80011	0.69838
H	3.89105	-0.72305	-0.41365
H	3.53908	-1.38479	-1.99484
H	3.67403	1.14550	-2.00855
H	2.12678	0.51085	-2.60297
H	2.13223	3.27662	-1.72459
H	0.76126	3.11472	-0.58817
H	0.70843	2.27880	-2.15628
H	0.84951	0.01184	3.80174
H	-0.03146	-1.13488	2.75496
H	-0.42906	0.59615	2.70487
H	2.07109	-3.30674	-1.70700
H	1.15732	-1.99056	-2.51379
H	0.42539	-2.87289	-1.16108
F	-0.25371	0.03518	-1.90859

^{3}FeTp2Cl
Charge: 1+
Energy: -1963610.7625034

Fe	0.31635	-0.00372	-0.09495
N	1.53452	1.18008	-1.11644
N	1.43340	-1.49611	-0.78756
N	1.50042	0.15531	1.42428
B	3.42368	-0.14066	-0.14499
H	4.61748	-0.18363	-0.14133
B	-2.88342	0.24418	1.11831
H	-3.74597	0.36189	1.94038
N	2.84740	0.06444	1.27620
N	2.88065	1.01823	-1.01133
N	2.78742	-1.42699	-0.70659
N	-4.32898	-0.96375	-0.53675
N	-3.52795	0.07687	-0.29567
N	-0.79371	-1.24030	0.95243
N	-2.04032	-0.99606	1.44764
N	-0.73831	1.54485	0.58652
N	-1.99233	1.49310	1.12143
C	1.23904	0.35311	2.72837
H	0.21797	0.44931	3.06555

C	2.43828	0.39125	3.43966
H	2.57124	0.53336	4.50150
C	3.43226	0.20563	2.47812
H	4.50833	0.16713	2.56850
C	1.31483	2.17159	-1.99498
H	0.30403	2.45646	-2.24249
C	2.53508	2.66926	-2.46027
H	2.69480	3.46537	-3.17159
C	3.50115	1.90483	-1.81242
H	4.58000	1.92821	-1.86704
C	1.12222	-2.64175	-1.41212
H	0.08794	-2.89575	-1.58848
C	2.29492	-3.33474	-1.73544
H	2.37976	-4.28645	-2.23775
C	3.32633	-2.52534	-1.27455
H	4.39902	-2.64915	-1.31111
C	-4.66680	-0.90753	-1.86177
H	-5.32420	-1.66044	-2.27314
C	-4.07145	0.17183	-2.47635
H	-4.13360	0.49598	-3.50466
C	-3.31001	0.79389	-1.43080
H	-2.82301	1.75671	-1.40742
C	-0.39361	-2.42297	1.45738
H	0.58866	-2.80267	1.22795
C	-1.39392	-2.96526	2.26355
H	-1.37417	-3.90144	2.80046
C	-2.41900	-2.02837	2.22856
H	-3.39243	-2.02250	2.69637
C	-0.27671	2.78992	0.78731
H	0.72131	3.05221	0.47458
C	-1.24131	3.56592	1.43820
H	-1.16522	4.60112	1.73461
C	-2.30979	2.70444	1.63354
H	-3.27189	2.85853	2.10038
Cl	-1.00182	-0.19924	-2.01285

^{3}FeTp2F
Charge: 1+
Energy: -1737484.5961854

Fe	0.21751	-0.00511	-0.07879
N	1.45609	0.84793	-1.35461
N	1.26061	-1.64713	-0.37178
N	1.44207	0.49130	1.35358
B	3.31659	-0.26896	-0.12015
H	4.50775	-0.36160	-0.12374
B	-2.99307	0.52137	0.76365
H	-3.99329	0.81525	1.35011
N	2.78212	0.31152	1.21120
N	2.79590	0.65758	-1.24587
N	2.61678	-1.62833	-0.33422
N	-4.06263	-1.20099	-0.72270
N	-3.34160	-0.08509	-0.64245
N	-0.93662	-0.89907	1.23883
N	-2.20985	-0.53388	1.55432
N	-0.80075	1.68163	0.18123
N	-2.11024	1.75893	0.55458
C	1.22508	1.01736	2.57084
H	0.21704	1.23590	2.89011
C	2.44348	1.18315	3.23102
H	2.60985	1.57939	4.22132
C	3.40386	0.72331	2.32996
H	4.47980	0.66336	2.40969
C	1.23566	1.57273	-2.45961
H	0.22699	1.83446	-2.74003
C	2.45486	1.87191	-3.07754
H	2.61639	2.44273	-3.97944
C	3.41710	1.26691	-2.27469
H	4.49322	1.22778	-2.36279
C	0.87485	-2.88205	-0.71418
H	-0.17642	-3.10962	-0.80669
C	2.00445	-3.69179	-0.89211
H	2.03112	-4.73652	-1.16265
C	3.08649	-2.85399	-0.64708
H	4.15042	-3.04023	-0.67291
C	-4.04600	-1.59506	-2.04732
H	-4.59431	-2.47979	-2.33864
C	-3.29189	-0.73606	-2.80178
H	-3.07464	-0.76061	-3.85933
C	-2.81770	0.23937	-1.85681
H	-2.34711	1.19340	-2.03127
C	-0.58553	-1.88577	2.08089
H	0.40470	-2.31032	2.02719
C	-1.64516	-2.18084	2.94169
H	-1.67310	-2.92316	3.72484
C	-2.65547	-1.30273	2.56973
H	-3.65957	-1.17338	2.94626
C	-0.32996	2.93644	0.12412
H	0.70324	3.10981	-0.13465
C	-1.34184	3.84661	0.45025
H	-1.27309	4.92301	0.49451
C	-2.45134	3.05745	0.71762
H	-3.45585	3.32048	1.01620
F	-0.84388	-0.48690	-1.49576

^{3}FeTp2NCS
Charge: 1+
Energy: -1982993.8857870

Fe	0.47288	-0.05885	-0.00284
N	1.40307	1.22811	1.18001
N	1.40863	0.84313	-1.49613
N	1.97317	-1.25733	0.18675
B	3.47693	0.72441	-0.11733
H	4.63844	1.00126	-0.15273
B	-2.43951	-1.78630	0.21706
H	-3.16339	-2.73647	0.35101
N	3.24827	-0.79003	0.10962
N	2.73283	1.45787	1.02290
N	2.73912	1.10004	-1.41894
N	-3.64935	-0.14303	-1.30556
N	-3.31386	-0.51154	-0.00778
N	-0.37380	-1.33740	-1.22379
N	-1.52767	-2.02054	-0.98904
N	-0.42363	-0.93061	1.54214
N	-1.58956	-1.63074	1.48971
C	2.03232	-2.58432	0.39514
H	1.12075	-3.15599	0.48369
C	3.36657	-2.98621	0.45508
H	3.74946	-3.98350	0.61038
C	4.10254	-1.81524	0.26963
H	5.16931	-1.64543	0.24208
C	0.96481	2.03405	2.15969
H	-0.07530	2.01579	2.44863
C	2.02829	2.79576	2.65367
H	2.00223	3.53196	3.44274
C	3.12993	2.39877	1.90116
H	4.16178	2.71801	1.92929
C	0.95891	1.35389	-2.65067
H	-0.08458	1.25724	-2.91199
C	2.02022	1.94895	-3.34395
H	1.98624	2.44159	-4.30387
C	3.12852	1.76823	-2.52404
H	4.16001	2.06549	-2.64652
C	-4.51171	0.83918	-1.18036
H	-4.93200	1.31832	-2.05464
C	-4.75792	1.15240	0.20467
H	-5.46742	1.85319	0.61937
C	-3.96596	0.22274	0.89719
H	-3.83077	0.07149	1.95857
C	0.13268	-1.79642	-2.38217
H	1.07173	-1.41344	-2.74867
C	-0.70774	-2.77282	-2.91805
H	-0.57752	-3.32485	-3.83638
C	-1.74748	-2.88075	-2.00342
H	-2.63090	-3.50189	-2.00374
C	0.05774	-1.05032	2.78943
H	0.99858	-0.59147	3.04999
C	-0.80844	-1.82532	3.56740
H	-0.69634	-2.10059	4.60516
C	-1.83497	-2.17645	2.70268
H	-2.71728	-2.78126	2.85523
N	-0.96970	1.20752	-0.16804
C	-1.71365	2.11711	-0.11157
S	-2.82598	3.30203	-0.00652

^{6}FeCDOCABr
Charge: 0
Energy: -4099190.9574167

Fe	-2.68977	-0.04367	0.19731
O	-3.55682	1.29212	1.49105
C	-3.08821	1.85110	2.55075
O	-1.89055	1.84983	2.90841
C	-4.12660	2.57741	3.39909
H	-3.66365	3.02796	4.27923
H	-4.90505	1.87071	3.70683
H	-4.61368	3.35397	2.79803
N	-1.48228	1.58908	-0.69661
C	-0.93691	2.57099	0.01104
N	-0.15807	3.34339	-0.78002
C	-1.02390	1.73563	-1.99303
C	-0.19135	2.81913	-2.05979
H	-1.06295	2.71689	1.07473
H	0.47651	4.05795	-0.44085
H	-1.30198	1.02603	-2.75594
H	0.38971	3.23836	-2.86529
N	-4.36835	0.29694	-1.12833
C	-4.66953	-0.31287	-2.26179
N	-5.83425	0.17451	-2.75513
C	-5.37638	1.20776	-0.87724
C	-6.30051	1.14558	-1.88382
H	-4.07109	-1.08397	-2.72444
H	-6.28329	-0.12990	-3.60624
H	-5.34023	1.81068	0.01619
H	-7.22063	1.68081	-2.05924
O	1.97084	1.83241	1.40152
C	2.39589	1.59333	0.14076

C	2.28903	0.35112	-0.49502
C	2.73124	0.18222	-1.80810
C	3.29967	1.25316	-2.49425
C	3.42338	2.49741	-1.86570
C	2.97650	2.68175	-0.55388
S	3.02798	4.22894	0.34398
C	3.83927	5.34305	-0.85278
H	1.64655	1.00101	1.85068
H	1.87551	-0.48552	0.05435
H	2.63526	-0.78685	-2.28390
H	3.65014	1.13004	-3.51489
H	3.87085	3.32047	-2.41204
H	3.90312	6.31543	-0.35755
H	3.25690	5.45244	-1.77270
H	4.85052	5.00291	-1.09464
N	1.56247	-3.16987	-1.87079
C	2.31619	-3.13967	-0.74595
N	3.60333	-3.33236	-1.01731
C	3.66594	-3.49397	-2.38723
C	2.40903	-3.38928	-2.93404
H	0.56424	-2.93814	-1.91649
H	1.89083	-2.99301	0.23843
H	4.60454	-3.67758	-2.89197
H	2.04751	-3.44751	-3.94914
N	4.04411	-2.52357	1.84219
C	4.52929	-1.32895	1.48498
N	4.29576	-0.25493	2.26693
N	5.31459	-1.24880	0.39366
C	5.87755	0.00530	-0.08650
H	3.16226	-2.57198	2.39218
H	4.15691	-3.26039	1.15095
H	3.40811	-0.32366	2.78815
H	4.40370	0.65187	1.83018
H	5.11876	-1.98395	-0.28671
H	6.51459	-0.21561	-0.94477
H	6.50178	0.45634	0.69190
H	5.10704	0.71865	-0.40162
S	-2.94559	-2.91195	1.78237
C	-1.12619	-2.76876	1.73563
C	-0.59069	-1.44796	2.29592
N	-0.88433	-0.30944	1.40536
C	0.93456	-1.55008	2.58515
O	1.56828	-0.44985	2.65839
O	1.43796	-2.69028	2.71220
H	-0.75796	-3.60451	2.33782
H	-0.80229	-2.90469	0.69981
H	-1.08249	-1.23138	3.25226
H	-0.14049	-0.19000	0.72074
H	-0.94717	0.55162	1.97379
O	-3.51530	-1.63103	1.06422
Br	-1.52961	-1.75350	-1.76173

^{6}FeCDOCACl
Charge: 0
Energy: -2772659.8949427

Fe	-2.77086	0.00945	-0.26798
O	-2.55941	-1.32408	-1.82544
C	-1.51709	-1.70935	-2.46921
O	-0.35250	-1.28003	-2.30862
C	-1.77181	-2.79689	-3.50805
H	-0.85572	-3.03690	-4.05164
H	-2.54764	-2.46587	-4.20665
H	-2.14790	-3.69691	-3.00723
N	-1.57065	-1.34251	1.04236
C	-0.34656	-1.78106	0.78561
N	0.17480	-2.39368	1.87394
C	-1.84494	-1.68561	2.35181
C	-0.76582	-2.33736	2.88749
H	0.16582	-1.67920	-0.15872
H	1.15184	-2.65310	1.95889
H	-2.78351	-1.40833	2.80514
H	-0.58393	-2.75854	3.86420
N	-4.60872	-1.04339	0.22070
C	-5.50523	-0.69797	1.12779
N	-6.55452	-1.55655	1.09297
C	-5.09545	-2.15980	-0.42813
C	-6.31066	-2.49593	0.10393
H	-5.40864	0.14523	1.79577
H	-7.37474	-1.50571	1.67898
H	-4.52446	-2.60306	-1.22861
H	-7.00819	-3.28806	-0.11964
O	2.16609	-0.05361	-0.29641
C	2.83410	-1.01441	-0.97805
C	2.80246	-1.09849	-2.37601
C	3.53080	-2.08942	-3.03241
C	4.28419	-3.00992	-2.30242
C	4.30463	-2.94140	-0.90667
C	3.58764	-1.94625	-0.23166
S	3.58359	-1.71896	1.54850
C	4.75523	-3.00496	2.10226
H	1.83813	0.63729	-0.94048
H	2.17085	-0.40175	-2.91623
H	3.49477	-2.14802	-4.11657
H	4.84821	-3.78781	-2.80881
H	4.89035	-3.66756	-0.35419
H	4.82045	-2.90329	3.18896
H	5.74967	-2.85191	1.67200
H	4.40374	-4.01260	1.86227
N	0.02850	1.43229	2.76855
C	0.91005	2.26817	2.16392
N	2.14498	2.07672	2.61094
C	2.04438	1.07199	3.54852
C	0.73769	0.66078	3.65933
H	-0.98404	1.39237	2.58252
H	0.62311	2.98653	1.40643
H	2.91120	0.70761	4.08265
H	0.25619	-0.09350	4.26000
N	3.44682	3.00493	0.26107
C	4.25706	2.13794	-0.33506
N	4.27233	2.04693	-1.68585
N	5.12755	1.42307	0.41086
C	6.07299	0.46526	-0.14305
H	2.66898	3.41858	-0.28052
H	3.22511	2.84083	1.25577
H	3.33600	2.23528	-2.08195
H	4.68167	1.20240	-2.06599
H	4.88395	1.32965	1.38799
H	6.68342	0.08145	0.67630
H	6.73822	0.96501	-0.85537
H	5.58056	-0.38400	-0.63021
S	-3.47556	2.95487	-1.50856
C	-1.76122	3.26154	-0.93721
C	-0.77707	2.22692	-1.48384
N	-0.86239	0.96013	-0.72345
C	0.69332	2.71380	-1.45827
O	1.52519	1.89682	-1.98655
O	0.98131	3.78222	-0.87940
H	-1.51095	4.26316	-1.30131
H	-1.75165	3.27121	0.15614
H	-1.02334	1.97724	-2.52122
H	-0.34853	1.03259	0.15485
H	-0.43284	0.20396	-1.28663
O	-3.74206	1.41412	-1.29951
Cl	-3.03377	1.45122	1.84063

^{6}FeCDOCAF
Charge: 0
Energy: -2546536.7297766

Fe	-2.61106	-0.32689	0.01932
O	-3.25483	0.83237	1.57656
C	-2.66791	1.18951	2.66333
O	-1.46019	1.01283	2.93637
C	-3.56895	1.90117	3.66734
H	-3.00600	2.19891	4.55441
H	-4.38925	1.23430	3.95487
H	-4.01886	2.78337	3.19777
N	-1.48029	1.45229	-0.69822
C	-0.77999	2.27524	0.06330
N	-0.15195	3.20149	-0.70065
C	-1.29404	1.85951	-2.00195
C	-0.46087	2.94809	-2.02436
H	-0.70179	2.21337	1.13822
H	0.53672	3.85074	-0.34333
H	-1.76475	1.32563	-2.81300
H	-0.06603	3.54647	-2.83060
N	-4.31981	0.38344	-1.11925
C	-4.55791	-0.01527	-2.35354
N	-5.71312	0.53784	-2.80475
C	-5.34926	1.21881	-0.75113
C	-6.23300	1.32851	-1.79238
H	-3.91692	-0.68694	-2.90417
H	-6.12703	0.38434	-3.71230
H	-5.35934	1.65764	0.23478
H	-7.15625	1.87450	-1.90907
O	2.70433	0.21199	0.45923
C	2.41195	1.38220	1.08319
C	1.68300	1.43117	2.27608
C	1.37222	2.65639	2.86630
C	1.81531	3.84314	2.28275
C	2.56137	3.80090	1.09726
C	2.85779	2.57917	0.47767
S	3.71375	2.41570	-1.08192
C	4.39723	4.09134	-1.32046
H	2.28593	-0.54837	0.95308
H	1.33746	0.50091	2.71296
H	0.75840	2.66590	3.76073
H	1.59044	4.80245	2.74036
H	2.90892	4.73231	0.66168
H	5.03343	4.03183	-2.20768
H	5.00608	4.40066	-0.46571
H	3.61615	4.83630	-1.50350
N	0.60703	-1.14921	-2.21305
C	1.48124	-2.13816	-1.89394
N	2.68650	-1.91979	-2.41009
C	2.57399	-0.72516	-3.09163
C	1.29560	-0.23783	-2.97984

H	-0.41525	-1.12135	-1.98971
H	1.20506	-2.98318	-1.27836
H	3.41771	-0.28508	-3.60545
H	0.83024	0.66560	-3.33802
N	3.68548	-3.64675	0.03966
C	4.40949	-2.54267	0.24004
N	4.52352	-2.04015	1.49352
N	5.07266	-2.00665	-0.80129
C	5.86487	-0.78961	-0.66814
H	2.87342	-3.85726	0.66115
H	3.57447	-3.93080	-0.92584
H	3.69210	-2.24165	2.06053
H	4.72620	-1.04716	1.51595
H	4.50972	-2.09143	-1.65954
H	6.37429	-0.61268	-1.61788
H	6.62893	-0.92546	0.10395
H	5.24609	0.08533	-0.43677
S	-3.08576	-3.40954	0.76780
C	-1.28956	-3.32017	0.45276
C	-0.55299	-2.36065	1.40339
N	-0.73766	-0.95050	1.00155
C	0.95057	-2.74186	1.51957
O	1.74806	-1.81555	1.87716
O	1.27729	-3.92368	1.26202
H	-0.91310	-4.33747	0.58855
H	-1.15075	-3.00645	-0.58439
H	-0.97488	-2.46535	2.41060
H	0.02575	-0.65481	0.39378
H	-0.73707	-0.31835	1.81646
O	-3.58849	-1.90090	0.66221
F	-1.97525	-1.16101	-1.64501

$^{6}FeCDOCAN_{3}$
Charge: 0
Energy: -2586917.3113454

Fe	-2.58431	-0.34379	0.33119
O	-3.72562	0.84500	1.55725
C	-3.37213	1.63449	2.50858
O	-2.19776	1.91393	2.83379
C	-4.53186	2.26987	3.26936
H	-5.17096	1.48368	3.68560
H	-5.14814	2.85482	2.57655
H	-4.16483	2.91491	4.07022
N	-2.07636	1.55342	-0.73197
C	-1.56303	2.62841	-0.15310
N	-1.29756	3.57764	-1.08141
C	-2.13631	1.82338	-2.08659
C	-1.64821	3.07977	-2.32296
H	-1.38499	2.74592	0.90471
H	-0.83710	4.45571	-0.89362
H	-2.50518	1.09304	-2.78862
H	-1.51903	3.64893	-3.23010
N	-4.31112	-0.48737	-0.99743
C	-4.51314	-1.30419	-2.01546
N	-5.69728	-1.02067	-2.61239
C	-5.40340	0.35313	-0.92910
C	-6.27984	0.03523	-1.93083
H	-3.84008	-2.08079	-2.34272
H	-6.07936	-1.49724	-3.41603
H	-5.45409	1.09813	-0.15077
H	-7.23755	0.44233	-2.21515
O	1.25127	2.43754	1.17819
C	2.42371	2.65699	0.50977
C	3.44170	3.41695	1.08681
C	4.63048	3.66406	0.39208
C	4.79284	3.15508	-0.89695
C	3.77685	2.39342	-1.48803
C	2.59045	2.12544	-0.79171
S	1.24119	1.14130	-1.38614
C	1.79554	0.61212	-3.03730
H	1.35764	1.61835	1.74650
H	3.28145	3.80116	2.08960
H	5.41848	4.25047	0.85560
H	5.70672	3.34850	-1.45246
H	3.92019	2.00577	-2.49116
H	0.94324	0.07264	-3.45990
H	2.65420	-0.06382	-2.98630
H	2.02113	1.47211	-3.67558
N	1.35153	-2.60500	-1.36679
C	2.37139	-2.77500	-0.49020
N	3.49544	-3.11766	-1.10937
C	3.16970	-3.16255	-2.45220
C	1.84370	-2.84593	-2.63039
H	0.40427	-2.27486	-1.14056
H	2.24541	-2.64881	0.57520
H	3.90348	-3.42528	-3.20208
H	1.21701	-2.75877	-3.50473
N	4.47860	-2.09974	1.82798
C	4.84102	-1.09810	1.01757
N	4.51857	0.16085	1.34237
N	5.58899	-1.40010	-0.07278
C	5.99495	-0.37816	-1.02796
H	3.62636	-1.99255	2.42254
H	4.66648	-3.03709	1.49615
H	3.70935	0.27315	1.97489
H	4.57684	0.87026	0.62284
H	5.24315	-2.26663	-0.50450
H	6.69392	-0.83173	-1.73422
H	6.51228	0.43684	-0.51387
H	5.14699	0.03982	-1.58455
S	-2.25258	-2.98976	2.19832
C	-0.50659	-2.51906	1.97897
C	-0.17033	-1.08383	2.41374
N	-0.73214	-0.07549	1.49547
C	1.37424	-0.94216	2.58457
O	1.89724	0.19456	2.37513
O	2.00132	-1.97977	2.91223
H	0.06166	-3.22663	2.58887
H	-0.24433	-2.67193	0.92977
H	-0.61449	-0.90622	3.40101
H	-0.03169	0.20389	0.80959
H	-1.01442	0.76267	2.03146
O	-3.07991	-1.94899	1.33401
N	-1.37351	-1.45466	-1.13042
N	-1.36866	-1.28244	-2.32217
N	-1.34685	-1.15323	-3.48060

$^{4}FeCDOCAOH$
Charge: 0
Energy: -2531443.3657160

Fe	-2.28205	-0.27286	-0.09325
O	-3.01681	0.20361	1.75244
C	-2.46524	0.65190	2.82524
O	-1.25288	0.91933	2.97510
C	-3.42940	0.86407	3.98851
H	-2.90367	1.24496	4.86657
H	-3.92275	-0.08354	4.23130
H	-4.21527	1.56664	3.68924
N	-1.56849	1.67198	-0.54932
C	-0.99177	2.51768	0.29074
N	-0.57333	3.61782	-0.37762
C	-1.49814	2.23478	-1.80625
C	-0.87125	3.45028	-1.71920
H	-0.85615	2.34543	1.34975
H	0.01485	4.33045	0.03211
H	-1.88978	1.70377	-2.66000
H	-0.62866	4.19679	-2.45953
N	-4.34205	0.15015	-0.82378
C	-5.17287	-0.70097	-1.39595
N	-6.34136	-0.08074	-1.70807
C	-4.99392	1.36178	-0.76018
C	-6.24378	1.24060	-1.30762
H	-4.96404	-1.74747	-1.57352
H	-7.14060	-0.51444	-2.14613
H	-4.51136	2.22214	-0.32218
H	-7.05001	1.94408	-1.44695
O	2.51250	0.16310	0.90823
C	2.29609	1.46332	1.21997
C	1.79741	1.88027	2.45709
C	1.64959	3.24286	2.72588
C	2.01832	4.19046	1.76860
C	2.48771	3.77156	0.51580
C	2.59189	2.40996	0.21176
S	3.01154	1.72340	-1.37821
C	2.92622	3.18760	-2.45808
H	2.18457	-0.47491	1.61203
H	1.49646	1.13224	3.18410
H	1.25247	3.55500	3.68708
H	1.94972	5.25251	1.99031
H	2.75657	4.51612	-0.22697
H	3.05852	2.80779	-3.47478
H	3.71437	3.91731	-2.24773
H	1.94389	3.66445	-2.38549
N	0.84015	-1.10195	-2.57299
C	1.80076	-1.73801	-1.86719
N	2.99058	-1.67617	-2.46298
C	2.77005	-0.95285	-3.61723
C	1.44479	-0.58938	-3.69544
H	-0.18659	-1.03445	-2.29788
H	1.59583	-2.26136	-0.94450
H	3.57104	-0.74304	-4.31343
H	0.89188	-0.02581	-4.43189
N	3.86709	-3.24063	0.03327
C	4.49810	-2.13775	0.45344
N	4.57039	-1.88374	1.78228
N	5.11782	-1.36006	-0.44914
C	5.80935	-0.13578	-0.07474
H	3.09044	-3.61380	0.61199
H	3.74737	-3.31969	-0.97205
H	3.73677	-2.20765	2.29483
H	4.76052	-0.91463	2.00548
H	4.65071	-1.39058	-1.36595
H	6.22302	0.31095	-0.97971
H	6.63496	-0.36355	0.60826
H	5.13482	0.59760	0.38345
S	-2.85956	-2.67876	0.41813

C	-1.08208	-3.14480	0.54429
C	-0.35057	-2.17915	1.47964
N	-0.38802	-0.81134	0.92143
C	1.10403	-2.64849	1.75331
O	1.83355	-1.84314	2.42206
O	1.46869	-3.74031	1.26171
H	-1.00789	-4.17811	0.88990
H	-0.69515	-3.07643	-0.47572
H	-0.86728	-2.12667	2.44630
H	0.38292	-0.64372	0.27704
H	-0.33933	-0.12100	1.68143
O	-3.37540	-3.32254	-0.88131
O	-1.70629	-0.97492	-1.81161
H	-2.19969	-1.76508	-2.08978

^{6}FeCDODMBr
Charge: 0
Energy: -4099174.4482262

Fe	-2.60852	-0.14791	0.06167
N	-3.57040	0.78177	1.84740
C	-3.75486	0.13870	2.98840
N	-4.36447	0.94857	3.88906
C	-4.08950	2.05332	2.01053
C	-4.58913	2.17241	3.27965
H	-3.47118	-0.88439	3.18113
H	-4.61866	0.69490	4.83249
H	-4.07821	2.75800	1.19002
H	-5.07363	2.98805	3.79352
O	-2.10819	1.64179	-0.59002
C	-2.45957	2.86128	-0.85749
O	-3.62370	3.28875	-0.81967
C	-1.30316	3.77710	-1.22988
H	-1.64991	4.80809	-1.32902
H	-0.86537	3.43823	-2.17468
H	-0.50854	3.70534	-0.47975
N	-4.45829	-0.29915	-0.97080
C	-4.96719	-1.45626	-1.35582
N	-6.06876	-1.24390	-2.11158
C	-5.25133	0.70301	-1.49767
C	-6.26426	0.12639	-2.21381
H	-4.54717	-2.42119	-1.11923
H	-6.62920	-1.96151	-2.54693
H	-4.99436	1.74101	-1.32440
H	-7.08277	0.54658	-2.77696
O	1.66348	2.80155	0.80555
C	2.81105	2.76083	0.06046
C	3.93888	3.45277	0.50518
C	5.13054	3.42457	-0.22867
C	5.18620	2.69155	-1.41650
C	4.05673	2.00702	-1.87798
C	2.85234	2.04540	-1.16098
S	1.32856	1.28658	-1.66875
C	1.78673	0.44882	-3.21895
H	1.53097	1.89509	1.18923
H	3.85791	4.00207	1.43834
H	5.99850	3.97759	0.12053
H	6.10177	2.66528	-2.00215
H	4.11707	1.45764	-2.81063
H	0.87923	-0.07986	-3.52111
H	2.58813	-0.27815	-3.06180
H	2.06837	1.17146	-3.99046
N	1.95033	-2.39443	-1.39220
C	2.43583	-3.54569	-1.93896
N	3.72737	-3.69731	-1.71206
C	4.08928	-2.58181	-0.98726
C	3.00537	-1.75892	-0.77508
H	0.99810	-2.03600	-1.50168
H	1.80324	-4.22860	-2.48972
H	5.11410	-2.42604	-0.67643
H	2.87496	-0.81880	-0.26287
N	4.68658	-1.78186	2.31612
C	5.24417	-0.75283	1.65255
N	4.63611	0.42568	1.61676
N	6.44485	-0.93351	1.05730
C	7.08052	0.04680	0.18818
H	3.70568	-1.66320	2.65765
H	4.87597	-2.70496	1.94571
H	3.60922	0.46734	1.81272
H	5.05140	1.22480	1.15451
H	6.95645	-1.76683	1.30636
H	7.91886	-0.43461	-0.31821
H	7.45831	0.91198	0.74816
H	6.37162	0.39741	-0.56766
S	-2.07867	-2.92275	1.72670
C	-0.35042	-2.35554	1.57925
C	-0.10525	-0.91273	2.03884
N	-0.64815	0.04297	1.05947
C	1.41226	-0.70291	2.30066
O	1.93228	0.36517	1.83908
O	2.01168	-1.59844	2.93077
H	0.22390	-3.03423	2.21699
H	-0.02458	-2.48378	0.54385
H	-0.62538	-0.74979	2.99076
H	-0.01972	0.11009	0.25383
H	-0.67031	0.98625	1.44491
O	-2.96276	-1.85472	0.90939
Br	-1.32690	-1.42586	-1.97893

^{6}FeCDODMCl
Charge: 0
Energy: -2772656.6392040

Fe	-2.34679	-0.27271	-0.14185
N	-3.42142	0.49527	1.64920
C	-3.77746	-0.30293	2.64264
N	-4.36758	0.41289	3.63123
C	-3.80435	1.77600	2.00382
C	-4.39584	1.74093	3.23813
H	-3.63184	-1.37156	2.66381
H	-4.73135	0.03685	4.49458
H	-3.64221	2.59835	1.32104
H	-4.82738	2.51239	3.85676
O	-1.51853	1.52295	-0.53503
C	-1.87744	2.76018	-0.67222
O	-3.04257	3.18487	-0.61070
C	-0.72397	3.72773	-0.90880
H	-1.09421	4.75232	-0.98151
H	-0.19658	3.46043	-1.82923
H	0.00523	3.65137	-0.09604
N	-4.09449	-0.13425	-1.35033
C	-4.58699	-1.19517	-1.96564
N	-5.62416	-0.82951	-2.75347
C	-4.83289	0.96186	-1.75484
C	-5.79427	0.54252	-2.63305
H	-4.19955	-2.19685	-1.86627
H	-6.16097	-1.44878	-3.34249
H	-4.56840	1.94673	-1.39341
H	-6.56027	1.07365	-3.17603
O	2.19828	0.70526	0.25630
C	2.39490	2.04670	0.27459
C	2.26992	2.78194	1.46348
C	2.50782	4.15731	1.46395
C	2.86729	4.81175	0.28478
C	2.97621	4.08047	-0.90004
C	2.74602	2.69984	-0.92760
S	2.97495	1.77881	-2.44192
C	1.27048	1.16242	-2.77801
H	1.99652	0.37963	1.18352
H	1.97775	2.26146	2.37154
H	2.40493	4.71517	2.39097
H	3.04707	5.88267	0.28114
H	3.23608	4.57905	-1.82909
H	1.35625	0.19764	-3.28159
H	0.73262	1.86182	-3.42248
H	0.71028	1.02203	-1.85352
N	1.85849	-2.63262	-2.09462
C	2.83372	-1.91356	-1.49176
N	3.97003	-2.60219	-1.42698
C	3.69896	-3.82001	-2.02139
C	2.39129	-3.85594	-2.43954
H	0.88906	-2.31164	-2.20982
H	2.68228	-0.91040	-1.11821
H	4.45638	-4.58642	-2.11013
H	1.80667	-4.61540	-2.93547
N	4.17126	-2.13527	1.58155
C	4.66057	-0.91114	1.34898
N	4.49237	0.05364	2.28487
N	5.37538	-0.69552	0.23604
C	5.86967	0.61814	-0.15137
H	3.43340	-2.27434	2.28923
H	4.15141	-2.76312	0.78377
H	3.62165	-0.06058	2.82150
H	4.62390	1.00633	1.96807
H	5.22729	-1.39986	-0.50025
H	6.39207	0.51331	-1.10317
H	6.58179	0.99563	0.59116
H	5.05851	1.34223	-0.28882
S	-2.14565	-3.34276	1.01666
C	-0.39844	-2.84485	1.22556
C	-0.21426	-1.52753	1.98267
N	-0.53247	-0.39393	1.09705
C	1.21895	-1.42920	2.59278
O	1.72554	-0.25389	2.64096
O	1.76605	-2.47972	2.97392
H	0.06234	-3.65593	1.79717
H	0.07756	-2.78506	0.24149
H	-0.91931	-1.48972	2.82337
H	0.17157	-0.30450	0.36162
H	-0.47970	0.48295	1.61380
O	-2.90873	-2.06324	0.42583
Cl	-1.07616	-1.35813	-2.02822

^{6}FeCDODMF
Charge: 0
Energy: -2546537.8930035

Fe	-2.14221	0.08892	-0.38242

N	-3.23217	0.22748	1.58206
C	-4.34427	-0.43973	1.82614
N	-4.73205	-0.25777	3.11285
C	-2.87684	0.86156	2.75815
C	-3.80049	0.56556	3.72478
H	-4.86003	-1.06125	1.11208
H	-5.53721	-0.67855	3.55257
H	-1.97860	1.46084	2.80440
H	-3.88319	0.85395	4.76112
O	-0.21336	2.11302	1.67423
C	-0.74276	2.62112	0.66464
O	-1.61333	2.04185	-0.09023
C	-0.33768	4.03564	0.27119
H	-0.55396	4.71841	1.10002
H	-0.85436	4.37028	-0.63139
H	0.74545	4.05724	0.11073
N	-3.91926	0.80761	-1.38254
C	-4.80649	0.04650	-1.99546
N	-5.72337	0.82215	-2.62540
C	-4.26286	2.11939	-1.62564
C	-5.39068	2.14895	-2.40098
H	-4.78810	-1.03289	-1.99473
H	-6.49855	0.48819	-3.17916
H	-3.65363	2.91510	-1.22621
H	-5.97206	2.96177	-2.80738
O	2.29078	0.50217	0.20523
C	2.80354	1.72119	0.49484
C	2.94937	2.15148	1.82297
C	3.51990	3.39141	2.09727
C	3.94574	4.22342	1.05784
C	3.77883	3.80644	-0.26276
C	3.21144	2.56001	-0.56494
S	3.06321	2.04507	-2.27248
C	1.24038	2.03572	-2.49731
H	2.03431	0.02772	1.05084
H	2.57537	1.51416	2.61807
H	3.62069	3.71277	3.13065
H	4.38780	5.19228	1.27152
H	4.08567	4.44739	-1.08426
H	1.05974	1.78058	-3.54565
H	0.82878	3.02701	-2.29381
H	0.74388	1.29667	-1.87016
N	0.58673	-1.95002	-2.36320
C	1.88767	-1.73568	-2.05483
N	2.60272	-2.85521	-2.14222
C	1.70419	-3.83217	-2.52747
C	0.44923	-3.28623	-2.66468
H	-0.16115	-1.22656	-2.30960
H	2.26661	-0.76797	-1.75554
H	2.01465	-4.85654	-2.68226
H	-0.50469	-3.71465	-2.93238
N	3.45085	-3.12818	0.77204
C	4.20976	-2.03388	0.63392
N	4.42728	-1.24482	1.71141
N	4.80232	-1.80035	-0.54741
C	5.53162	-0.57311	-0.83887
H	2.83419	-3.22533	1.59323
H	3.11368	-3.54309	-0.09107
H	3.61016	-1.21742	2.34071
H	4.78730	-0.31885	1.51618
H	4.37152	-2.30432	-1.33148
H	5.87508	-0.62321	-1.87310
H	6.41167	-0.48650	-0.19172
H	4.90061	0.31596	-0.73262
S	-2.63687	-3.02634	0.39579
C	-0.87236	-2.97091	0.85882
C	-0.43044	-1.73521	1.64653
N	-0.45341	-0.53928	0.79041
C	0.98942	-1.96624	2.25437
O	1.74577	-0.93947	2.33963
O	1.30385	-3.12988	2.57460
H	-0.71525	-3.86085	1.47584
H	-0.26036	-3.07896	-0.04412
H	-1.13017	-1.55684	2.47140
H	0.28078	-0.60736	0.08543
H	-0.23225	0.31101	1.33785
O	-2.88515	-1.69542	-0.51967
F	-1.10240	0.01080	-1.96485

$^{6}FeCDODMN_3$
Charge: 0
Energy: -2586919.7478769

Fe	1.97740	-0.18492	0.21860
N	3.26607	-0.70851	-1.54493
C	3.58499	-1.91153	-1.99163
N	4.47106	-1.81207	-3.01458
C	3.97944	0.20551	-2.29961
C	4.73565	-0.46803	-3.22086
H	3.20058	-2.84443	-1.60481
H	4.86101	-2.58524	-3.53328
H	3.90867	1.26489	-2.09127
H	5.41967	-0.12867	-3.98311
O	1.72323	1.57255	-0.65491
C	2.14903	2.77542	-0.91072
O	3.33997	3.08571	-1.04573
C	1.04047	3.80328	-1.05165
H	1.44623	4.77386	-1.34490
H	0.51513	3.89065	-0.09567
H	0.30401	3.46374	-1.78557
N	3.84041	0.24552	1.24555
C	4.32277	-0.54664	2.18623
N	5.45387	-0.01104	2.70559
C	4.68485	1.33520	1.14684
C	5.69880	1.18842	2.05458
H	3.87637	-1.48208	2.48617
H	6.01248	-0.41521	3.44258
H	4.48012	2.11737	0.42635
H	6.54853	1.80767	2.29604
O	-2.59889	0.57683	-0.57200
C	-2.51052	1.87357	-0.99115
C	-2.35212	2.20168	-2.34100
C	-2.29936	3.54132	-2.73243
C	-2.39967	4.55073	-1.77613
C	-2.55047	4.22218	-0.42606
C	-2.60608	2.88619	-0.01448
S	-2.80797	2.34647	1.67334
C	-2.45920	3.86335	2.62158
H	-2.38041	-0.03853	-1.33738
H	-2.26494	1.39721	-3.06574
H	-2.17410	3.78859	-3.78288
H	-2.35275	5.59504	-2.07070
H	-2.61804	5.01868	0.30646
H	-2.46752	3.56227	3.67241
H	-3.22270	4.63117	2.46624
H	-1.46426	4.23963	2.37340
N	-0.99969	-1.52861	2.56475
C	-2.22856	-1.36455	2.02316
N	-2.99041	-2.44076	2.20880
C	-2.19703	-3.33354	2.90574
C	-0.95698	-2.78285	3.12791
H	-0.23116	-0.83997	2.46742
H	-2.50942	-0.47193	1.48461
H	-2.56508	-4.30689	3.19923
H	-0.06634	-3.16599	3.60054
N	-3.88888	-3.04156	-0.62623
C	-4.57752	-1.89312	-0.65063
N	-4.77561	-1.26702	-1.83357
N	-5.11968	-1.44084	0.48987
C	-5.71353	-0.11545	0.61986
H	-3.32175	-3.30310	-1.44344
H	-3.53980	-3.32461	0.28619
H	-3.97620	-1.35834	-2.47719
H	-5.10788	-0.31362	-1.77314
H	-4.72497	-1.87564	1.33177
H	-6.01845	0.01551	1.65905
H	-6.60769	-0.02885	-0.00768
H	-4.99782	0.67594	0.37007
S	1.52664	-3.44636	0.38153
C	-0.08440	-3.10162	-0.39762
C	-0.08366	-2.05681	-1.52023
N	0.18871	-0.71197	-0.98093
C	-1.44217	-2.15991	-2.28352
O	-2.06887	-1.07073	-2.51956
O	-1.84790	-3.30541	-2.56092
H	-0.40082	-4.05956	-0.82112
H	-0.80561	-2.81738	0.37413
H	0.71657	-2.29175	-2.23107
H	-0.57560	-0.41120	-0.37246
H	0.20445	-0.02457	-1.73468
O	2.08308	-1.99060	0.86088
N	0.87609	0.45848	1.83182
N	0.77784	1.64249	2.07711
N	0.69096	2.76272	2.33684

$^{6}FeCDODMNCS$
Charge: 0
Energy: -2792026.1933421

Fe	1.97264	-0.29904	0.07286
N	3.21724	-1.13508	-1.56945
C	3.54043	-2.39662	-1.79959
N	4.39823	-2.47533	-2.84720
C	3.89742	-0.36520	-2.49627
C	4.63932	-1.18815	-3.29990
H	3.17639	-3.24776	-1.24293
H	4.78514	-3.32596	-3.22905
H	3.81318	0.71369	-2.48182
H	5.29953	-0.98655	-4.12904
O	1.72770	1.24510	-1.11015
C	2.11539	2.44782	-1.43301
O	3.27694	2.73953	-1.74051
C	1.00549	3.48169	-1.41018
H	1.35620	4.43628	-1.80823
H	0.67271	3.61348	-0.37445
H	0.14491	3.12440	-1.98161
N	3.81389	0.31445	1.02011
C	4.25161	-0.24247	2.13590

N	5.34232	0.42187	2.58556
C	4.64635	1.38049	0.73442
C	5.60693	1.45947	1.70561
H	3.79978	-1.09913	2.61124
H	5.85588	0.20849	3.42779
H	4.47023	1.99484	-0.13863
H	6.42846	2.14222	1.85544
O	-2.58320	0.44322	-0.69855
C	-2.50271	1.64634	-1.34094
C	-2.36952	1.73145	-2.72971
C	-2.32518	2.98162	-3.35168
C	-2.41503	4.14305	-2.58607
C	-2.53851	4.05712	-1.19624
C	-2.57626	2.81461	-0.55425
S	-2.70763	2.57825	1.20730
C	-2.40151	4.25226	1.85801
H	-2.40929	-0.29879	-1.35310
H	-2.29467	0.81198	-3.30350
H	-2.21713	3.04018	-4.43102
H	-2.37858	5.11938	-3.06043
H	-2.59342	4.97027	-0.61446
H	-2.35059	4.14055	2.94355
H	-3.20722	4.94699	1.60240
H	-1.43612	4.62490	1.50752
N	-0.97765	-1.19884	2.70800
C	-2.21113	-1.04685	2.17195
N	-3.02741	-2.02783	2.54972
C	-2.26718	-2.84254	3.36867
C	-0.99052	-2.34339	3.47150
H	-0.17834	-0.58908	2.48319
H	-2.45604	-0.23594	1.50232
H	-2.68357	-3.72807	3.82839
H	-0.11102	-2.69692	3.98618
N	-4.01721	-3.05877	-0.12670
C	-4.65986	-1.90286	-0.33804
N	-4.86004	-1.48220	-1.60850
N	-5.15759	-1.23793	0.71472
C	-5.70821	0.10892	0.62063
H	-3.47463	-3.48024	-0.89225
H	-3.66451	-3.19918	0.81654
H	-4.08163	-1.72200	-2.23863
H	-5.14891	-0.51814	-1.70996
H	-4.76140	-1.53519	1.61332
H	-5.98774	0.42861	1.62541
H	-6.61163	0.11449	0.00050
H	-4.97416	0.82103	0.22734
S	1.47103	-3.47124	0.83477
C	-0.15741	-3.23708	0.04799
C	-0.17365	-2.39637	-1.23329
N	0.13672	-0.98593	-0.93744
C	-1.55883	-2.59073	-1.92957
O	-2.15652	-1.54048	-2.34548
O	-2.00664	-3.75268	-1.98094
H	-0.49581	-4.24760	-0.19977
H	-0.85497	-2.81683	0.77793
H	0.60048	-2.76352	-1.91702
H	-0.60235	-0.56843	-0.36710
H	0.13495	-0.43804	-1.79834
O	2.07966	-1.97513	1.01706
N	0.89874	0.67155	1.60366
C	0.96262	1.77379	2.06214
S	1.06240	3.25200	2.70297

[6]FeCDODMOH
Charge: 0
Energy: -2531447.5734180

Fe	1.96996	-0.32075	0.14443
N	3.90815	0.47271	-0.92998
C	5.06360	-0.12240	-0.70103
N	6.05800	0.48359	-1.40052
C	4.15976	1.49838	-1.82117
C	5.49526	1.51997	-2.12670
H	5.18732	-0.98398	-0.06370
H	7.02928	0.20913	-1.40695
H	3.35548	2.11344	-2.19493
H	6.08217	2.15157	-2.77555
O	0.97196	2.01135	-2.18977
C	1.02723	2.37501	-1.00429
O	1.33233	1.61547	0.00028
C	0.72603	3.82124	-0.62741
H	1.57129	4.24416	-0.07205
H	-0.15069	3.85372	0.02685
H	0.52835	4.41683	-1.52017
N	2.93728	0.30266	2.00435
C	3.50012	-0.52938	2.85891
N	3.82338	0.12816	4.00179
C	2.88376	1.53916	2.60889
C	3.43404	1.45065	3.85987
H	3.66424	-1.57925	2.66767
H	4.25249	-0.28243	4.81800
H	2.43720	2.37109	2.08762
H	3.58121	2.17834	4.64271
O	-1.74609	0.60831	-0.18582
C	-2.19956	1.84252	-0.49947
C	-2.21998	2.29809	-1.82803
C	-2.74023	3.55577	-2.12776
C	-3.23598	4.38137	-1.11560
C	-3.18357	3.94368	0.20811
C	-2.66780	2.68216	0.53643
S	-2.64111	2.14753	2.24376
C	-0.83466	2.18545	2.59050
H	-1.45846	0.11274	-1.00926
H	-1.78634	1.67033	-2.59912
H	-2.74402	3.89369	-3.16057
H	-3.63953	5.36201	-1.34993
H	-3.53967	4.58134	1.01205
H	-0.68380	1.67991	3.54867
H	-0.48488	3.21905	2.66449
H	-0.27029	1.66539	1.81573
N	-1.66537	-2.45534	1.79243
C	-2.77741	-1.71336	2.00947
N	-3.85751	-2.46966	2.17584
C	-3.40116	-3.77157	2.06030
C	-2.04461	-3.77611	1.81495
H	-0.74707	-2.03077	1.52996
H	-2.76123	-0.63191	1.99221
H	-4.06836	-4.61608	2.17179
H	-1.33824	-4.57814	1.66157
N	-3.73558	-2.53696	-0.99881
C	-4.28612	-1.32331	-0.99839
N	-4.03363	-0.49725	-2.03993
N	-5.14616	-0.97403	-0.02272
C	-5.69110	0.37068	0.10328
H	-2.92666	-2.74261	-1.62158
H	-3.81189	-3.10452	-0.16256
H	-3.11337	-0.66121	-2.47702
H	-4.21496	0.48747	-1.89199
H	-5.06363	-1.52727	0.83721
H	-6.35644	0.38383	0.96822
H	-6.28118	0.63133	-0.78236
H	-4.91125	1.12782	0.25546
S	2.91543	-3.22221	-0.74259
C	1.15311	-3.18251	-1.22609
C	0.78989	-2.08981	-2.25106
N	1.44982	-0.80715	-1.94099
C	-0.74617	-1.94661	-2.31656
O	-1.23726	-0.76710	-2.36923
O	-1.39307	-3.01395	-2.33347
H	0.88752	-4.16596	-1.62254
H	0.59190	-3.01555	-0.30399
H	1.10538	-2.43221	-3.24663
H	0.90347	0.00162	-2.26603
H	2.35432	-0.75398	-2.40507
O	2.99902	-1.95558	0.30787
O	0.33931	-0.88828	0.91482
H	-0.31275	-0.17770	0.76759

[6]FeTauDBr
Charge: 0
Energy: -2979368.7577559

Fe	0.09379	0.38041	-0.22976
N	0.00778	-1.09061	1.28831
C	0.43637	-2.33462	1.14005
N	0.32162	-2.99041	2.31898
C	-0.20134	-2.11765	3.25983
C	-0.39102	-0.93526	2.59909
H	0.84683	-2.74073	0.22080
H	0.60135	-3.94665	2.48164
H	-0.37633	-2.41214	4.28271
H	-0.76092	0.01566	2.94857
N	-1.99648	-0.25815	-0.68788
C	-3.08942	0.02525	-0.00343
N	-4.15869	-0.60775	-0.54820
C	-3.71546	-1.33540	-1.63956
C	-2.36740	-1.10705	-1.70883
H	-3.12411	0.66695	0.86309
H	-5.11001	-0.55225	-0.21492
H	-4.38387	-1.92686	-2.24562
H	-1.62816	-1.48060	-2.39941
O	-0.43199	2.24893	-0.87594
C	-0.92551	2.60593	0.24829
O	-0.99768	1.75878	1.18827
C	-1.36994	4.03197	0.43940
H	-2.05370	4.11257	1.28722
H	-1.83462	4.41097	-0.47453
H	-0.48244	4.64259	0.64326
C	1.68368	-1.40055	-1.99612
O	0.59909	-0.70001	-1.68098
C	2.64461	-0.66429	-2.90165
H	2.10876	-0.24118	-3.75727
H	3.44160	-1.33058	-3.23676
H	3.06790	0.17105	-2.33206
O	1.87532	-2.53831	-1.58740
Br	2.38412	1.10240	0.52384

^{6}FeTauDCl
Charge: 0
Energy: -1652840.2958757

Fe	0.08294	-0.63154	-0.01158
N	0.60501	1.08734	-1.13992
C	1.60655	1.89628	-0.83223
N	1.73386	2.83784	-1.79737
C	0.76815	2.61030	-2.76475
C	0.07243	1.51242	-2.33826
H	2.24003	1.78946	0.04282
H	2.43646	3.56252	-1.81347
H	0.67632	3.23043	-3.64264
H	-0.75050	0.98088	-2.78961
N	-1.38695	0.73562	0.97619
C	-2.52921	1.17655	0.48214
N	-3.10583	2.05032	1.34537
C	-2.27855	2.17044	2.44912
C	-1.21363	1.34704	2.19972
H	-2.94190	0.88323	-0.47044
H	-3.98543	2.52523	1.20466
H	-2.52190	2.81095	3.28244
H	-0.33394	1.14170	2.78856
O	-1.26078	-2.14524	0.34908
C	-1.94233	-1.91552	-0.70700
O	-1.65356	-0.91143	-1.42545
C	-3.04872	-2.86283	-1.09233
H	-3.74079	-2.38429	-1.78874
H	-3.57402	-3.21549	-0.20092
H	-2.60029	-3.73378	-1.58451
C	2.46570	-0.35394	1.70405
O	1.15148	-0.32073	1.50825
C	2.97853	-1.68901	2.19493
H	2.38433	-2.03165	3.04810
H	4.03410	-1.61877	2.46391
H	2.84362	-2.41591	1.38588
O	3.18572	0.61576	1.50416
Cl	1.53520	-1.96115	-1.21032

^{6}FeTauDF
Charge: 0
Energy: -1426715.3152620

Fe	0.01887	-0.76825	-0.21769
N	0.83185	1.00964	-1.07313
C	1.96340	1.56540	-0.67067
N	2.21032	2.67028	-1.41536
C	1.18400	2.81991	-2.33417
C	0.33210	1.77375	-2.10522
H	2.60021	1.17499	0.11706
H	3.02070	3.26508	-1.32290
H	1.16288	3.63078	-3.04541
H	-0.59108	1.49822	-2.59101
N	-1.09218	0.71451	1.10097
C	-2.16360	1.42024	0.79131
N	-2.47253	2.27430	1.80077
C	-1.53828	2.09951	2.80763
C	-0.68729	1.12798	2.35259
H	-2.71020	1.33583	-0.13513
H	-3.24938	2.91863	1.81278
H	-1.57037	2.66586	3.72537
H	0.18680	0.69090	2.80870
O	-1.61695	-2.01787	0.04542
C	-2.27387	-1.47685	-0.90443
O	-1.79835	-0.45903	-1.49644
C	-3.59639	-2.07214	-1.31977
H	-4.15754	-1.37162	-1.94189
H	-4.17495	-2.35492	-0.43584
H	-3.40430	-2.98448	-1.89599
C	2.48686	-1.25810	1.21706
O	1.22322	-0.85319	1.25294
C	2.65827	-2.76167	1.19061
H	2.08248	-3.22415	1.99875
H	3.71292	-3.03313	1.26525
H	2.23820	-3.11317	0.24147
O	3.42595	-0.47049	1.18815
F	0.88429	-1.86988	-1.32270

^{6}FeTauDN$_3$
Charge: 0
Energy: -1467102.3155059

Fe	-0.04417	0.28082	0.58246
N	1.38812	-0.86948	-0.71678
C	2.29132	-0.30889	-1.50494
N	3.16907	-1.24218	-1.94631
C	2.81546	-2.46195	-1.39577
C	1.70663	-2.21303	-0.63315
H	2.32699	0.74090	-1.74726
H	3.97915	-1.05818	-2.51978
H	3.37613	-3.36350	-1.58788
H	1.11947	-2.87260	-0.01499
N	-1.55733	-0.09397	-0.92912
C	-1.60045	-1.07753	-1.80708
N	-2.80314	-1.09127	-2.43372
C	-3.56754	-0.05747	-1.91637
C	-2.77672	0.54985	-0.97929
H	-0.80405	-1.78139	-1.99118
H	-3.08931	-1.74495	-3.14758
H	-4.57278	0.13793	-2.25551
H	-2.96860	1.38814	-0.32856
O	-1.53136	-0.10599	2.01461
C	-1.36371	-1.36791	1.98273
O	-0.52283	-1.86173	1.17647
C	-2.15460	-2.24636	2.92209
H	-2.10035	-3.29198	2.61131
H	-3.19446	-1.90968	2.96238
H	-1.73615	-2.15045	3.93062
C	-0.07987	2.70912	-0.20613
O	-0.89443	2.26050	0.65893
C	-0.07810	4.18099	-0.54602
H	0.38526	4.35155	-1.52046
H	0.50037	4.71601	0.21637
H	-1.09806	4.57399	-0.52892
O	0.74633	1.91909	-0.75318
N	1.42062	0.57715	1.82609
N	2.59239	0.67346	1.54685
N	3.71723	0.76440	1.29676

^{6}FeTauDNCS
Charge: 0
Energy: -1672209.2180929

Fe	-0.15347	0.13351	0.53672
N	0.89720	-0.94845	-1.11564
C	1.85114	-0.38340	-1.83893
N	2.53102	-1.32860	-2.52987
C	1.98848	-2.56480	-2.22045
C	0.97397	-2.30990	-1.33820
H	2.06472	0.67311	-1.85694
H	3.34140	-1.15879	-3.10748
H	2.37178	-3.48181	-2.64001
H	0.31409	-2.98564	-0.81892
N	-1.96146	0.00288	-0.62977
C	-2.10411	-0.28972	-1.90820
N	-3.40123	-0.14633	-2.27520
C	-4.11906	0.26543	-1.16337
C	-3.20571	0.35509	-0.14880
H	-1.30650	-0.59327	-2.56749
H	-3.77436	-0.30924	-3.19886
H	-5.18097	0.45091	-1.20271
H	-3.32077	0.64321	0.88395
O	-1.39671	-0.29924	2.22407
C	-1.20627	-1.55295	2.10966
O	-0.51622	-1.98271	1.13750
C	-1.76925	-2.49836	3.14105
H	-1.81441	-3.51589	2.74680
H	-2.75956	-2.16197	3.45971
H	-1.11346	-2.48826	4.01949
C	-0.22973	2.61367	-0.05819
O	-0.80718	2.12726	0.96364
C	-0.21230	4.10698	-0.27536
H	-0.09596	4.33911	-1.33675
H	0.64238	4.52786	0.26747
H	-1.12351	4.55976	0.12314
O	0.35512	1.83424	-0.87058
N	1.57511	0.32510	1.44247
C	2.74044	0.45780	1.22096
S	4.30845	0.62887	0.89200

^{6}FeTauDOH
Charge: 0
Energy: -1411624.7716869

Fe	0.01600	-0.45436	-0.71273
N	0.78626	1.52927	-0.27939
C	2.07308	1.80666	-0.16475
N	2.24065	3.14127	0.00835
C	0.99220	3.74081	-0.00839
C	0.09929	2.71947	-0.19075
H	2.86512	1.07140	-0.22575
H	3.12776	3.61207	0.10947
H	0.86505	4.80670	0.09924
H	-0.97385	2.74082	-0.29400
N	-1.10391	-0.20450	1.29150
C	-2.21496	0.47669	1.50208
N	-2.57128	0.41099	2.81154
C	-1.62890	-0.36044	3.46944
C	-0.72651	-0.73190	2.50837
H	-2.76755	1.00468	0.74038
H	-3.38524	0.84089	3.22554
H	-1.69280	-0.56707	4.52651
H	0.16146	-1.33929	2.57816
O	-1.62452	-1.59304	-1.30729
C	-2.29585	-0.57105	-1.66479
O	-1.83525	0.59312	-1.45031
C	-3.62026	-0.76413	-2.36353
H	-4.21156	0.15378	-2.33221
H	-4.16822	-1.59493	-1.91055

H	-3.42761	-1.02368	-3.41092
C	2.52170	-1.68731	0.26786
O	1.25324	-1.47649	0.46062
C	3.10906	-2.77590	1.15424
H	2.97318	-2.50758	2.20821
H	4.17060	-2.91519	0.94168
H	2.56712	-3.71273	0.98619
O	3.23448	-1.07489	-0.54272
O	0.99939	-0.60935	-2.23384
H	1.94647	-0.72807	-2.00566

^{5}FeCDOBrC
Charge: 0
Energy: -4097757.3147897

C	-3.12654	1.56025	-2.32087
H	-2.94101	1.94219	-3.32574
H	-4.20739	1.43641	-2.19049
N	-2.62015	2.54048	-1.36590
H	-1.81167	3.08884	-1.65199
C	-2.75017	2.37440	-0.03796
N	-3.50002	1.38527	0.46309
H	-3.43599	1.22238	1.47187
H	-3.77215	0.59457	-0.10465
N	-2.19178	3.24112	0.81779
H	-2.06552	2.89639	1.77577
H	-1.63385	4.02401	0.48389
N	4.31797	-0.97908	3.50506
H	4.97307	-0.58932	4.16685
C	3.32113	-1.89702	3.78642
C	4.17346	-0.59238	2.21203
H	4.77790	0.16275	1.73364
N	3.16699	-1.22942	1.64151
C	2.62226	-2.04172	2.61738
H	1.75840	-2.65512	2.40931
N	1.47729	-4.61951	-0.65969
H	1.82692	-5.56603	-0.63540
C	0.18843	-4.23087	-0.98811
C	2.19062	-3.49787	-0.37702
H	3.22743	-3.49657	-0.07804
N	1.43208	-2.42473	-0.50631
C	0.18215	-2.86588	-0.89283
H	-0.61375	-2.16809	-1.09227
C	-4.17183	-2.11756	-3.13535
H	-5.10733	-2.67706	-3.23011
H	-3.49453	-2.42040	-3.93820
S	-3.29476	-2.49384	-1.58284
N	4.99837	-0.37069	-3.24934
H	5.27317	-0.13597	-4.19194
C	5.78285	-1.00226	-2.30089
C	3.78595	-0.11566	-2.69229
H	2.95325	0.35404	-3.19702
N	3.75297	-0.54708	-1.44477
C	4.99056	-1.10186	-1.18799
H	5.21548	-1.52887	-0.22255
N	1.19507	3.66528	-0.67955
H	1.78089	2.84340	-0.41923
C	0.55158	3.89056	-1.87289
C	0.75159	4.60864	0.19352
H	1.10904	4.64999	1.21298
N	-0.14638	5.42038	-0.34984
C	-0.26722	4.97930	-1.65577
H	-0.91858	5.48163	-2.35977
C	-6.44892	-0.77353	0.42259
C	-5.67803	-1.33294	-0.60028
H	-6.09322	-1.39288	-1.60041
C	-4.38407	-1.80959	-0.34605
C	-3.86576	-1.72881	0.96893
O	-2.60690	-2.17644	1.18556
H	-2.28416	-1.80526	2.06194
C	-5.92993	-0.69294	1.71500
H	-6.51551	-0.24784	2.51447
C	-4.64907	-1.17137	1.99020
H	-4.20307	-1.06872	2.97423
N	0.09903	-0.15544	1.09381
H	-0.34554	-1.07379	1.12959
C	0.04716	0.44232	2.45708
H	0.67175	-0.18294	3.10081
C	0.58888	1.86656	2.42504
H	0.03875	2.45392	1.68741
H	0.43350	2.34021	3.40177
S	2.37336	2.05626	2.07617
C	-1.42314	0.33761	2.95177
O	-1.78621	-0.83279	3.26518
O	-2.15157	1.36861	2.92071
H	-0.48715	0.39334	0.45967
Fe	1.99879	-0.27623	-0.10138
O	2.52107	1.54231	0.49929
H	-2.61422	0.59529	-2.22229
H	3.20879	-2.34470	4.76165
H	-0.58401	-4.93867	-1.24422
H	-4.37090	-1.04540	-3.22972
H	6.79783	-1.30763	-2.50369
H	0.71329	3.25156	-2.72609
H	-7.44515	-0.40148	0.20170
Br	0.35389	0.40786	-2.24166

^{5}FeCDOBrC1
Charge: 0
Energy: -4097754.2879915

C	-6.00025	0.54890	0.61460
H	-6.72513	-0.06836	0.08089
H	-6.54657	1.17383	1.32949
N	-5.31691	1.38321	-0.36126
H	-5.14990	0.99608	-1.30025
C	-4.40308	2.30807	-0.02223
N	-4.13174	2.60343	1.27170
H	-3.17540	2.97203	1.40126
H	-4.33764	1.86533	1.93463
N	-3.80943	3.01184	-0.98982
H	-2.92426	3.52235	-0.80070
H	-3.96796	2.69383	-1.94077
N	4.26968	2.87935	2.35871
H	4.78494	3.74724	2.34149
C	3.27814	2.53239	3.25929
C	4.32998	1.90935	1.40945
H	4.94905	1.94962	0.52719
N	3.45509	0.95097	1.66077
C	2.79039	1.33243	2.81115
H	2.00327	0.72208	3.22992
N	1.24368	-2.60673	3.00568
H	1.39953	-3.02453	3.91108
C	0.06352	-2.64221	2.28220
C	2.15981	-1.91568	2.27399
H	3.17063	-1.71673	2.59588
N	1.63073	-1.50976	1.13532
C	0.32546	-1.96388	1.12156
H	-0.31582	-1.77576	0.27423
C	-4.13230	-3.81419	-0.15260
H	-3.46206	-4.50804	0.36425
H	-4.26451	-4.15441	-1.18299
S	-3.40712	-2.14702	-0.27946
N	5.63842	-2.87419	-1.48840
H	6.00035	-3.52956	-2.16532
C	6.28725	-2.43151	-0.34835
C	4.43210	-2.25293	-1.55570
H	3.69914	-2.39270	-2.33820
N	4.27573	-1.44602	-0.52349
C	5.42271	-1.54401	0.23578
H	5.53790	-0.95685	1.13490
N	-2.11220	-0.62771	-3.16759
H	-1.13372	-0.92440	-3.05717
C	-3.11468	-1.26695	-3.86004
C	-2.66110	0.43750	-2.54767
H	-2.09058	1.10091	-1.91672
N	-3.96085	0.54190	-2.80741
C	-4.25077	-0.52779	-3.63155
H	-5.25026	-0.69454	-4.00921
C	-3.38203	-2.00742	3.84226
C	-3.59308	-2.46780	2.53587
H	-4.07238	-3.42956	2.38839
C	-3.19719	-1.70344	1.43269
C	-2.57958	-0.45019	1.66078
O	-2.20409	0.25502	0.57339
H	-1.83505	1.15263	0.84510
C	-2.77859	-0.76882	4.05534
H	-2.61491	-0.40382	5.06571
C	-2.37905	0.01159	2.96683
H	-1.88787	0.97119	3.10465
N	0.74862	1.12193	0.10104
H	0.41014	0.89312	1.03371
C	0.71469	2.59321	-0.06454
H	1.34581	3.01038	0.73007
C	1.29389	2.97658	-1.42678
H	0.85686	2.34298	-2.20911
H	1.03028	4.01433	-1.65460
S	3.11687	2.90695	-1.54348
C	-0.72827	3.11737	0.16146
O	-1.33593	2.62399	1.18706
O	-1.22799	3.92321	-0.64692
H	0.09320	0.68237	-0.54853
Fe	2.60711	-0.03770	-0.33464
O	3.51826	1.31998	-1.34084
H	-5.31783	-0.11745	1.15608
H	3.02586	3.15210	4.10595
H	-0.83659	-3.09893	2.66264
H	-5.10835	-3.80273	0.34303
H	7.27234	-2.77799	-0.07624
H	-2.92853	-2.15580	-4.44300
H	-3.70072	-2.61760	4.68276
Br	1.08630	-1.34371	-2.33153

^{3}FeCDOClC
Charge: 0
Energy: -2771217.0442229

C	6.70951	-2.25615	-0.92105

H	7.63905	-2.71036	-1.27026
H	6.94722	-1.32507	-0.39842
N	6.06826	-3.18161	0.01153
H	6.24312	-4.16777	-0.11406
C	4.99027	-2.84320	0.75649
N	4.48388	-1.61540	0.66935
H	3.63286	-1.42643	1.22629
H	4.45342	-1.17414	-0.26550
N	4.47300	-3.71590	1.63851
H	3.44013	-3.64424	1.78238
H	4.90214	-4.62483	1.73808
N	-3.12470	-0.61669	2.70735
H	-3.27565	-1.39139	2.02744
C	-2.18880	-0.54061	3.71435
C	-3.52855	0.65747	2.45244
H	-4.23582	0.88190	1.66436
N	-2.93360	1.54468	3.23710
C	-2.09394	0.79602	4.03524
H	-1.48557	1.25703	4.80227
N	-0.93162	3.37007	-0.28185
H	-0.54415	4.12067	0.27808
C	-0.62689	3.09434	-1.59977
C	-1.58671	2.30668	0.23549
H	-1.91510	2.24735	1.26374
N	-1.74175	1.37190	-0.69610
C	-1.15002	1.85533	-1.85265
H	-1.14521	1.25165	-2.74663
C	3.47348	5.24514	-1.17033
H	2.56635	5.83760	-1.32898
H	4.10906	5.33928	-2.05505
S	3.11697	3.46305	-1.00288
N	-6.23682	-0.55882	-1.94247
H	-7.06320	-1.07373	-2.20796
C	-6.00674	0.78866	-2.15991
C	-5.14915	-1.08424	-1.33034
H	-5.01889	-2.11185	-1.03187
N	-4.23948	-0.14165	-1.14361
C	-4.75716	1.03082	-1.65789
H	-4.18588	1.94500	-1.63647
N	1.48620	-0.83186	-2.60274
H	0.49000	-1.09016	-2.71944
C	2.09776	0.28719	-3.11976
C	2.42133	-1.51075	-1.89370
H	2.20451	-2.42733	-1.36103
N	3.59950	-0.89817	-1.93042
C	3.40208	0.23024	-2.69630
H	4.19829	0.93925	-2.87089
C	0.94319	4.40855	2.36848
C	1.72074	4.54287	1.20865
H	1.96633	5.53890	0.85631
C	2.17397	3.41675	0.51149
C	1.84789	2.12896	1.00278
O	2.26573	1.06911	0.28267
H	2.04994	0.21868	0.75362
C	0.63628	3.13635	2.85189
H	0.03283	3.01741	3.74626
C	1.09844	2.00316	2.18067
H	0.88952	1.00835	2.56371
N	-0.55888	-0.87935	0.39148
H	-0.36581	-0.12329	1.04893
C	-0.23934	-2.16573	1.06075
H	-0.75523	-2.14793	2.02624
C	-0.77097	-3.33771	0.23865
H	-0.57855	-3.16513	-0.82575
H	-0.27227	-4.25778	0.55470
S	-2.55823	-3.61554	0.50266
C	1.27054	-2.28127	1.39396
O	1.89725	-1.18862	1.59814
O	1.75911	-3.42933	1.48314
H	0.09918	-0.72740	-0.37587
Fe	-2.41208	-0.56361	-0.45647
O	-3.20737	-2.07177	0.43580
H	6.06282	-2.02395	-1.77419
H	-1.71186	-1.42052	4.11927
H	-0.05408	3.77372	-2.20999
H	4.01712	5.63123	-0.30263
H	-6.73272	1.42799	-2.63704
H	1.55619	1.00787	-3.71179
H	0.60125	5.29644	2.89269
Cl	-1.60213	-1.41365	-2.71127

^{5}FeCDOClC1
Charge: 0
Energy: -2771231.7546387

C	-6.03745	-0.21908	0.16337
H	-6.60792	-0.40233	1.07549
H	-6.73838	0.11785	-0.60861
N	-5.40566	-1.47189	-0.22975
H	-5.16430	-2.13716	0.51780
C	-4.62031	-1.58102	-1.31438
N	-4.54941	-0.60108	-2.24648
H	-3.62200	-0.56301	-2.70003
H	-4.86903	0.31104	-1.94814
N	-3.95069	-2.71933	-1.52210
H	-3.19042	-2.74483	-2.22491
H	-3.83517	-3.32190	-0.71374
N	5.13755	-0.46875	-3.19401
H	5.52398	-1.08826	-3.89126
C	5.53003	0.83373	-2.94785
C	4.15027	-0.78692	-2.31403
H	3.66882	-1.75544	-2.25708
N	3.88364	0.24052	-1.52708
C	4.73979	1.25560	-1.90966
H	4.73423	2.21080	-1.40491
N	0.24913	3.60462	0.20983
H	-0.58217	4.09034	0.52409
C	0.84473	3.75953	-1.02498
C	0.81319	2.52646	0.81265
H	0.50843	2.12907	1.76807
N	1.74886	1.99277	0.04293
C	1.77527	2.75819	-1.11072
H	2.44211	2.52003	-1.92382
C	-2.15803	1.50007	2.86591
H	-1.49949	2.29077	3.23652
H	-1.62807	0.88865	2.13706
S	-3.68982	2.21104	2.15012
N	5.18101	0.26237	3.58843
H	5.34823	0.18712	4.58080
C	6.13595	0.47669	2.60966
C	3.97491	0.13602	2.97811
H	3.04054	-0.06049	3.48339
N	4.10361	0.26416	1.66942
C	5.44672	0.47315	1.42700
H	5.81800	0.59273	0.42130
N	-1.60579	-2.49974	2.12793
H	-0.75011	-1.93995	2.26548
C	-1.79350	-3.83354	2.41057
C	-2.75549	-2.02828	1.59276
H	-2.87065	-1.00694	1.25749
N	-3.68095	-2.98109	1.51441
C	-3.08277	-4.11612	2.02767
H	-3.61340	-5.05628	2.08794
C	-2.88540	4.78042	-0.90507
C	-3.21580	4.23741	0.34029
H	-3.57930	4.87910	1.13804
C	-3.10742	2.86086	0.58983
C	-2.62783	2.01412	-0.43963
O	-2.49890	0.69264	-0.19543
H	-2.14829	0.22305	-1.01925
C	-2.43825	3.93087	-1.92038
H	-2.18404	4.33334	-2.89770
C	-2.30261	2.56301	-1.69228
H	-1.93708	1.89815	-2.46836
N	0.59162	-0.41916	-1.02232
H	0.43809	0.41797	-1.58203
C	0.29842	-1.60654	-1.84448
H	0.99723	-1.60179	-2.69119
C	0.53601	-2.88585	-1.03271
H	0.01538	-2.81215	-0.06954
H	0.11607	-3.73305	-1.58403
S	2.28709	-3.32354	-0.75248
C	-1.13241	-1.59364	-2.44743
O	-1.78116	-0.48363	-2.39386
O	-1.57260	-2.65047	-2.93797
H	-0.08600	-0.35978	-0.25937
Fe	2.47458	-0.22996	0.24980
O	2.92453	-2.08693	0.12274
H	-5.30143	0.56605	0.37539
H	6.30916	1.31934	-3.51499
H	0.54361	4.53580	-1.70967
H	-2.45866	0.86640	3.70439
H	7.18180	0.60294	2.84330
H	-1.01126	-4.44094	2.83912
H	-2.98887	5.84749	-1.07932
Cl	0.76833	-0.40896	2.31221

^{5}FeCDOFC
Charge: 0
Energy: -2545094.6480069

C	-7.12270	-1.53909	1.32167
H	-7.80489	-2.31180	1.68176
H	-7.61338	-0.56029	1.39926
N	-6.77343	-1.85542	-0.06395
H	-7.43832	-2.39834	-0.59470
C	-5.85029	-1.16717	-0.77791
N	-5.04940	-0.30033	-0.17210
H	-4.27439	0.12245	-0.71676
H	-4.90042	-0.35879	0.83820
N	-5.77100	-1.32718	-2.11335
H	-4.82390	-1.17123	-2.54059
H	-6.31102	-2.07423	-2.52797
N	4.17734	-3.14231	-2.72519
H	4.47203	-4.03566	-3.09074
C	4.49974	-1.89838	-3.24128
C	3.33931	-2.95355	-1.67139
H	2.89468	-3.73172	-1.07075

N	3.11893	-1.66580	-1.48090
C	3.83518	-0.99653	-2.45158
H	3.81853	0.08157	-2.50910
N	4.31238	2.50944	0.18067
H	5.12378	2.95357	0.58442
C	3.47525	3.05158	-0.77733
C	3.82730	1.27943	0.50731
H	4.27805	0.62153	1.23364
N	2.73877	1.00643	-0.18646
C	2.50814	2.10434	-0.99044
H	1.65222	2.17049	-1.64325
C	1.05052	2.92658	2.18481
H	0.71660	1.94591	1.83706
H	1.08481	2.92895	3.27977
S	-0.10567	4.27667	1.71354
N	3.45823	-2.03086	3.92737
H	3.29977	-2.10882	4.92112
C	4.50233	-2.60070	3.21846
C	2.65249	-1.38763	3.04207
H	1.73690	-0.86403	3.27302
N	3.12578	-1.50818	1.81612
C	4.27521	-2.26289	1.90940
H	4.84336	-2.51893	1.02694
N	-1.90234	-0.07196	2.31355
H	-0.89036	-0.17109	2.05716
C	-2.52851	1.11455	2.61739
C	-2.84986	-1.04026	2.32891
H	-2.62568	-2.07756	2.12078
N	-4.05512	-0.55705	2.62149
C	-3.85172	0.80021	2.81122
H	-4.67129	1.46140	3.05877
C	0.59826	4.96958	-2.24457
C	0.59858	5.03942	-0.84959
H	1.16469	5.81481	-0.34089
C	-0.11553	4.12283	-0.06956
C	-0.86129	3.10741	-0.71337
O	-1.53440	2.22258	0.04059
H	-2.01021	1.55806	-0.53615
C	-0.14297	3.96577	-2.87359
H	-0.16610	3.90128	-3.95884
C	-0.86835	3.04317	-2.12088
H	-1.47321	2.27944	-2.60007
N	-0.07048	-0.32820	-1.15834
H	0.20962	0.40226	-1.81031
C	-1.02739	-1.23205	-1.82254
H	-0.58954	-1.56112	-2.76909
C	-1.29232	-2.48014	-0.95554
H	-1.61155	-2.15877	0.04375
H	-2.11197	-3.04424	-1.41359
S	0.07574	-3.66956	-0.77656
C	-2.41330	-0.60960	-2.11400
O	-2.75396	0.45586	-1.49423
O	-3.16260	-1.26722	-2.87277
H	-0.53358	0.16191	-0.39150
Fe	1.63623	-1.05084	0.15328
O	1.13147	-2.95523	0.26906
H	-6.23090	-1.53619	1.95653
H	5.15022	-1.78055	-4.09439
H	3.61772	4.03922	-1.18541
H	2.05102	3.13481	1.79638
H	5.27758	-3.17625	3.70052
H	-1.99670	2.05368	2.60980
H	1.15756	5.69420	-2.82991
F	0.60280	-0.10743	1.59654

^{5}FeCDOFC1
Charge: 0
Energy: -2545094.6324070

C	-7.12146	-1.52927	1.32624
H	-7.80517	-2.29991	1.68785
H	-7.60997	-0.54930	1.40248
N	-6.77383	-1.84841	-0.05917
H	-7.43892	-2.39282	-0.58810
C	-5.84953	-1.16396	-0.77503
N	-5.04558	-0.29833	-0.17141
H	-4.27145	0.12306	-0.71821
H	-4.89556	-0.35570	0.83873
N	-5.77199	-1.32597	-2.11034
H	-4.82446	-1.17451	-2.53827
H	-6.31529	-2.07139	-2.52361
N	4.17168	-3.14974	-2.72490
H	4.46539	-4.04370	-3.08973
C	4.49538	-1.90660	-3.24201
C	3.33476	-2.95924	-1.67058
H	2.88971	-3.73647	-1.06903
N	3.11609	-1.67108	-1.48078
C	3.83248	-1.00335	-2.45248
H	3.81713	0.07473	-2.51076
N	4.31488	2.50736	0.16988
H	5.12789	2.95143	0.57047
C	3.47493	3.04896	-0.78597
C	3.83033	1.27781	0.49916
H	4.28346	0.62050	1.22453
N	2.73947	1.00460	-0.19084
C	2.50677	2.10188	-0.99508
H	1.64879	2.16776	-1.64520
C	1.05471	2.92906	2.17974
H	0.72228	1.94699	1.83450
H	1.09241	2.93345	3.27459
S	-0.10717	4.27493	1.70975
N	3.46870	-2.00388	3.93237
H	3.31537	-2.07122	4.92769
C	4.50970	-2.58041	3.22434
C	2.65782	-1.37095	3.04425
H	1.74342	-0.84498	3.27444
N	3.12508	-1.50428	1.81737
C	4.27563	-2.25690	1.91285
H	4.83960	-2.52190	1.03036
N	-1.90103	-0.07238	2.31447
H	-0.88917	-0.17150	2.05725
C	-2.52698	1.11486	2.61604
C	-2.84861	-1.04062	2.33283
H	-2.62468	-2.07842	2.12691
N	-4.05364	-0.55671	2.62507
C	-3.85003	0.80103	2.81159
H	-4.66946	1.46281	3.05803
C	0.59657	4.96858	-2.24816
C	0.59652	5.03825	-0.85322
H	1.16204	5.81390	-0.34426
C	-0.11731	4.12121	-0.07338
C	-0.86237	3.10544	-0.71740
O	-1.53513	2.21993	0.03611
H	-2.01048	1.55540	-0.54108
C	-0.14407	3.96445	-2.87742
H	-0.16693	3.90006	-3.96267
C	-0.86908	3.04140	-2.12498
H	-1.47323	2.27723	-2.60433
N	-0.07046	-0.33214	-1.15874
H	0.21048	0.39550	-1.81350
C	-1.02811	-1.23771	-1.81941
H	-0.59008	-1.57173	-2.76416
C	-1.29436	-2.48205	-0.94722
H	-1.61089	-2.15626	0.05143
H	-2.11606	-3.04596	-1.40175
S	0.07132	-3.67396	-0.76640
C	-2.41321	-0.61535	-2.11460
O	-2.75266	0.45470	-1.50209
O	-3.16327	-1.27689	-2.86923
H	-0.53273	0.16131	-0.39353
Fe	1.63536	-1.05368	0.15436
O	1.13104	-2.95756	0.27379
H	-6.22929	-1.52740	1.96061
H	5.14554	-1.79009	-4.09555
H	3.61645	4.03619	-1.19537
H	2.05326	3.13985	1.78768
H	5.28774	-3.15038	3.70853
H	-1.99505	2.05389	2.60633
H	1.15559	5.69355	-2.83334
F	0.60313	-0.10418	1.59479

^{5}FeCDON$_3$C
Charge: 0
Energy: -2585474.0971282

C	-8.57796	-0.35851	0.07952
H	-9.59343	-0.69073	0.30255
H	-8.63241	0.45502	-0.65721
N	-7.81494	-1.50054	-0.40225
H	-8.32636	-2.24934	-0.84603
C	-6.47548	-1.46708	-0.63684
N	-5.77569	-0.35912	-0.42692
H	-4.71663	-0.38937	-0.46525
H	-6.23658	0.51431	-0.22494
N	-5.86143	-2.56472	-1.09092
H	-4.80243	-2.56964	-1.17546
H	-6.31118	-3.45768	-0.94412
N	2.29918	-3.83963	-2.95768
H	2.44078	-4.82251	-3.13747
C	1.80818	-2.90453	-3.85419
C	2.47517	-3.21828	-1.76133
H	2.81420	-3.70062	-0.85912
N	2.14203	-1.94478	-1.84828
C	1.72338	-1.73450	-3.14554
H	1.40362	-0.75468	-3.46756
N	3.48162	2.74839	-2.27464
H	4.27550	3.35757	-2.40333
C	2.15498	3.09567	-2.44255
C	3.51820	1.52040	-1.69502
H	4.42566	1.02161	-1.39431
N	2.29693	1.04718	-1.52066
C	1.43664	2.02694	-1.97860
H	0.36543	1.92147	-1.92476
C	0.60570	5.16246	1.64192
H	1.43936	4.85371	1.00632
H	0.97242	5.24740	2.66830
S	-0.66955	3.85932	1.69026
N	5.72632	-1.29330	1.86790

H	6.19378	-1.35158	2.76062
C	6.18239	-1.81236	0.66845
C	4.51721	-0.71714	1.64182
H	3.89921	-0.24995	2.39424
N	4.17816	-0.83297	0.37215
C	5.20466	-1.51721	-0.24558
H	5.15616	-1.75805	-1.29765
N	-0.11180	-0.03213	3.13881
H	0.60535	0.48007	2.60436
C	-1.40020	0.37520	3.40964
C	0.04469	-1.27048	3.68683
H	0.95152	-1.83978	3.54066
N	-1.05711	-1.68884	4.28915
C	-1.96320	-0.66161	4.11905
H	-2.96689	-0.72671	4.52079
C	-1.13231	4.37193	-2.36655
C	-0.74430	4.59002	-1.03923
H	-0.13423	5.45487	-0.80393
C	-1.11641	3.70405	-0.02368
C	-1.91040	2.58119	-0.35885
O	-2.27877	1.76290	0.65491
H	-2.59449	0.88911	0.29538
C	-1.89681	3.25349	-2.69268
H	-2.19483	3.06983	-3.72163
C	-2.28515	2.35804	-1.69063
H	-2.87777	1.47845	-1.92235
N	-0.32554	-0.53809	-0.21035
H	-0.56347	0.13092	-0.94131
C	-1.06258	-1.79529	-0.43615
H	-0.62430	-2.29057	-1.30823
C	-0.92992	-2.72628	0.78357
H	-1.23423	-2.19470	1.69192
H	-1.60762	-3.57616	0.64530
S	0.70408	-3.50655	1.01903
C	-2.56637	-1.61523	-0.72384
O	-3.11139	-0.48551	-0.46056
O	-3.17696	-2.61231	-1.17370
H	-0.63411	-0.10497	0.66090
Fe	1.92700	-0.68094	0.00665
O	1.78991	-2.27504	1.13604
H	-8.13922	0.02356	1.00706
H	1.57924	-3.15572	-4.87839
H	1.84721	4.04201	-2.85627
H	0.19764	6.12983	1.33165
H	7.12968	-2.32289	0.58635
H	-1.77609	1.32496	3.06393
H	-0.83206	5.07804	-3.13652
N	1.92141	0.97230	1.41708
N	2.51370	2.00542	1.25542
N	3.10202	2.99614	1.08738

^{5}FeCDON$_{3}$C1
Charge: 0
Energy: -2585474.0961053

C	-8.57836	-0.35688	0.07855
H	-9.59378	-0.68901	0.30198
H	-8.63299	0.45627	-0.65859
N	-7.81540	-1.49913	-0.40276
H	-8.32680	-2.24801	-0.84644
C	-6.47583	-1.46605	-0.63679
N	-5.77593	-0.35809	-0.42722
H	-4.71684	-0.38859	-0.46503
H	-6.23679	0.51570	-0.22676
N	-5.86179	-2.56411	-1.08987
H	-4.80277	-2.56911	-1.17457
H	-6.31158	-3.45693	-0.94232
N	2.29670	-3.84083	-2.95708
H	2.43723	-4.82390	-3.13670
C	1.80590	-2.90552	-3.85348
C	2.47352	-3.21947	-1.76085
H	2.81256	-3.70196	-0.85873
N	2.14117	-1.94576	-1.84780
C	1.72212	-1.73535	-3.14493
H	1.40291	-0.75535	-3.46692
N	3.48271	2.74630	-2.27647
H	4.27704	3.35463	-2.40640
C	2.15621	3.09479	-2.44294
C	3.51880	1.51826	-1.69691
H	4.42614	1.01867	-1.39716
N	2.29728	1.04618	-1.52116
C	1.43740	2.02675	-1.97815
H	0.36618	1.92220	-1.92309
C	0.60700	5.16219	1.64139
H	1.44057	4.85299	1.00587
H	0.97370	5.24721	2.66776
S	-0.66875	3.85954	1.69002
N	5.72728	-1.29200	1.86709
H	6.19544	-1.34916	2.75951
C	6.18263	-1.81213	0.66784
C	4.51778	-0.71650	1.64131
H	3.90017	-0.24877	2.39372
N	4.17784	-0.83376	0.37202
C	5.20410	-1.51829	-0.24576
H	5.15491	-1.76021	-1.29756
N	-0.11177	-0.03085	3.13889
H	0.60516	0.48131	2.60413
C	-1.40023	0.37623	3.40983
C	0.04504	-1.26913	3.68697
H	0.95196	-1.83827	3.54071
N	-1.05659	-1.68765	4.28948
C	-1.96291	-0.66061	4.11944
H	-2.96651	-0.72584	4.52138
C	-1.13128	4.37139	-2.36689
C	-0.74328	4.58969	-1.03960
H	-0.13300	5.45443	-0.80445
C	-1.11564	3.70401	-0.02388
C	-1.90989	2.58126	-0.35883
O	-2.27855	1.76329	0.65507
H	-2.59438	0.88944	0.29570
C	-1.89600	3.25305	-2.69282
H	-2.19398	3.06922	-3.72175
C	-2.28460	2.35791	-1.69059
H	-2.87740	1.47839	-1.92216
N	-0.32574	-0.53805	-0.21007
H	-0.56358	0.13073	-0.94126
C	-1.06303	-1.79517	-0.43546
H	-0.62488	-2.29081	-1.30740
C	-0.93058	-2.72580	0.78456
H	-1.23476	-2.19384	1.69274
H	-1.60846	-3.57559	0.64660
S	0.70322	-3.50642	1.02025
C	-2.56677	-1.61489	-0.72320
O	-3.11169	-0.48519	-0.45959
O	-3.17746	-2.61178	-1.17333
H	-0.63421	-0.10458	0.66105
Fe	1.92679	-0.68146	0.00695
O	1.78943	-2.27519	1.13674
H	-8.13942	0.02569	1.00578
H	1.57637	-3.15666	-4.87756
H	1.84890	4.04142	-2.85641
H	0.19929	6.12965	1.33092
H	7.13001	-2.32246	0.58557
H	-1.77639	1.32586	3.06406
H	-0.83082	5.07726	-3.13700
N	1.92152	0.97255	1.41643
N	2.51445	2.00525	1.25434
N	3.10345	2.99549	1.08588

^{5}FeCDONCSC
Charge: 0
Energy: -2790606.3064693

C	5.43965	-1.24449	-1.15803
H	5.84568	-1.31450	-2.16890
H	6.27276	-1.30468	-0.45131
N	4.52904	-2.36656	-0.96163
H	3.97237	-2.67157	-1.77000
C	3.98128	-2.66774	0.22356
N	4.34624	-2.04347	1.35647
H	3.72945	-2.21019	2.16267
H	4.71517	-1.10297	1.27809
N	3.10427	-3.68627	0.30451
H	2.50627	-3.69434	1.13876
H	2.71121	-4.02477	-0.56314
N	-4.29511	0.00436	3.55181
H	-4.69595	-0.33435	4.41408
C	-4.11844	1.33002	3.19920
C	-3.82340	-0.76925	2.54016
H	-3.80752	-1.84951	2.54042
N	-3.36339	-0.00446	1.56316
C	-3.54044	1.30652	1.95962
H	-3.20001	2.12897	1.35134
N	-0.12298	2.82293	1.52324
H	0.45216	2.47658	0.76220
C	-0.07360	2.37157	2.82619
C	-1.09207	3.77730	1.45733
H	-1.33374	4.28276	0.53161
N	-1.67199	3.96928	2.63159
C	-1.03861	3.09532	3.48856
H	-1.30938	3.03761	4.53489
C	2.51308	3.63888	-2.84527
H	2.91459	4.48998	-2.28779
H	1.59235	3.94190	-3.35061
S	2.00477	2.30458	-1.71280
N	-5.54558	0.34116	-3.04502
H	-6.05556	0.98800	-3.62877
C	-5.75899	-1.02272	-2.95062
C	-4.50314	0.66108	-2.23614
H	-4.10265	1.65902	-2.13547
N	-4.04668	-0.42024	-1.62846
C	-4.81792	-1.47820	-2.06605
H	-4.60611	-2.47830	-1.72088
N	0.03254	-2.37554	-2.21615
H	-0.91392	-2.57442	-1.83216
C	0.57930	-1.11271	-2.29492
C	1.03933	-3.26250	-2.41888
H	0.88197	-4.33320	-2.41189

N	2.19993	-2.65146	-2.63698
C	1.91386	-1.30100	-2.55934
H	2.67340	-0.54390	-2.69179
C	5.79361	2.32831	-0.08149
C	4.74416	2.53124	-0.98655
H	4.93950	3.04878	-1.92025
C	3.45132	2.08233	-0.69649
C	3.22725	1.39690	0.51874
O	1.97060	0.95554	0.74108
H	1.90897	0.39338	1.58060
C	5.55358	1.68506	1.13298
H	6.35690	1.55227	1.85253
C	4.26846	1.22319	1.43852
H	4.03886	0.75526	2.39290
N	-0.43126	-0.73080	0.98642
H	-0.41921	0.14314	1.51218
C	-0.13377	-1.85018	1.90377
H	-0.83549	-1.75941	2.74254
C	-0.37858	-3.19087	1.20668
H	0.29236	-3.29336	0.34673
H	-0.15045	-4.00602	1.89999
S	-2.08809	-3.49018	0.62611
C	1.31082	-1.76232	2.49297
O	1.76443	-0.60665	2.75008
O	1.94640	-2.83637	2.66556
H	0.31892	-0.63411	0.29972
Fe	-2.33537	-0.58790	-0.22627
O	-2.23306	-2.48975	-0.70399
H	4.94190	-0.27523	-1.04284
H	-4.38314	2.14777	3.85010
H	0.61865	1.60436	3.14182
H	3.24111	3.29929	-3.58813
H	-6.53378	-1.52303	-3.51053
H	-0.01335	-0.22046	-2.15395
H	6.78888	2.68831	-0.32531
N	-1.61641	1.19934	-0.96715
C	-1.56818	2.20363	-1.59938
S	-1.53307	3.58497	-2.45841

^{5}FeCDONCSC1
Charge: 0
Energy: -2790599.5722761

C	-5.41392	-0.29005	1.19843
H	-5.84368	0.18815	2.08053
H	-6.23168	-0.56457	0.52600
N	-4.69369	-1.47988	1.63669
H	-4.19257	-1.40799	2.53314
C	-4.15484	-2.35019	0.77354
N	-4.40606	-2.30064	-0.54417
H	-3.78471	-2.87848	-1.12723
H	-4.68357	-1.41441	-0.95205
N	-3.40166	-3.36630	1.24424
H	-2.75904	-3.77679	0.55603
H	-3.07409	-3.28628	2.19786
N	4.21340	-3.72839	-1.25541
H	4.59514	-4.63616	-1.03312
C	3.71536	-3.32860	-2.48388
C	4.01129	-2.71521	-0.37399
H	4.26320	-2.76367	0.67350
N	3.43248	-1.68800	-0.96951
C	3.23961	-2.05950	-2.28587
H	2.76636	-1.38513	-2.98347
N	3.19779	2.56898	-3.15183
H	3.87332	3.09824	-3.68300
C	1.82853	2.77428	-3.13588
C	3.47502	1.55692	-2.28819
H	4.47145	1.19890	-2.07662
N	2.36658	1.10467	-1.73214
C	1.32851	1.85989	-2.24908
H	0.30665	1.71152	-1.93270
C	-2.81603	4.23650	0.63740
H	-3.31239	4.97825	0.00377
H	-1.98064	4.70598	1.16328
S	-2.04840	2.90439	-0.33786
N	5.51002	2.13866	1.91536
H	5.81670	2.90172	2.50130
C	6.31843	1.26948	1.20648
C	4.21641	1.79680	1.68320
H	3.37123	2.32337	2.09866
N	4.15156	0.75880	0.86794
C	5.45572	0.41995	0.56461
H	5.67173	-0.40948	-0.09153
N	-0.55957	-0.37594	2.93069
H	0.41229	-0.53607	2.59647
C	-1.30630	0.77264	2.80613
C	-1.38877	-1.34441	3.39945
H	-1.03782	-2.34961	3.59130
N	-2.62603	-0.89534	3.58566
C	-2.57197	0.43958	3.22079
H	-3.44528	1.07564	3.27636
C	-5.80814	1.83642	-1.65194
C	-4.78276	2.54779	-1.01635
H	-5.03298	3.43211	-0.44008
C	-3.44967	2.12932	-1.10923
C	-3.15268	0.97560	-1.87434
O	-1.85433	0.61240	-1.96377
H	-1.76978	-0.34476	-2.26894
C	-5.50731	0.69678	-2.39744
H	-6.29520	0.14464	-2.90307
C	-4.17895	0.26804	-2.51233
H	-3.91098	-0.60928	-3.09562
N	0.35401	-1.01442	-0.81868
H	0.36886	-0.72254	-1.79477
C	-0.01609	-2.44593	-0.78876
H	0.77395	-2.99038	-1.32122
C	-0.09446	-2.95442	0.64980
H	-0.87738	-2.39802	1.17364
H	-0.38813	-4.00878	0.63176
S	1.42460	-2.92020	1.65978
C	-1.36677	-2.71421	-1.53415
O	-1.69122	-1.91724	-2.45931
O	-2.05415	-3.70639	-1.16134
H	-0.39479	-0.45731	-0.40167
Fe	2.20758	-0.18143	0.18417
O	1.81193	-1.31108	1.76870
H	-4.76047	0.42762	0.68987
H	3.75043	-3.96611	-3.35366
H	1.35367	3.53926	-3.72987
H	-3.52559	3.83768	1.36992
H	7.39533	1.33462	1.23072
H	-0.88695	1.68975	2.43107
H	-6.83441	2.18205	-1.56461
N	1.19255	1.54372	0.93285
C	1.09095	2.69362	1.19512
S	0.97320	4.27480	1.60758

^{5}FeCDOOHC
Charge: 0
Energy: -2530008.4437602

C	-5.02575	-4.78244	1.36479
H	-5.46938	-5.74038	1.64218
H	-5.71181	-3.97866	1.64949
N	-4.83030	-4.77182	-0.08442
H	-4.84991	-5.65080	-0.57860
C	-4.42088	-3.67915	-0.76789
N	-4.08858	-2.57726	-0.10085
H	-3.78296	-1.76313	-0.65704
H	-3.65433	-2.66347	0.82931
N	-4.41101	-3.68157	-2.10983
H	-3.72584	-3.05875	-2.59612
H	-4.75978	-4.48728	-2.60797
N	5.83203	0.24584	-1.33183
H	6.67607	-0.30697	-1.26959
C	5.71834	1.58488	-1.00617
C	4.58626	-0.27284	-1.41037
H	4.37629	-1.31142	-1.60643
N	3.67544	0.66060	-1.17885
C	4.37596	1.83159	-0.93154
H	3.84874	2.74120	-0.69142
N	-0.22459	4.10474	-0.43901
H	-0.98919	4.63048	-0.03079
C	0.10915	4.09410	-1.77749
C	0.47350	3.11640	0.17392
H	0.40771	2.85419	1.21809
N	1.24613	2.48470	-0.69524
C	1.02989	3.08753	-1.91962
H	1.55239	2.75512	-2.80495
C	-1.69468	2.43135	3.05112
H	-1.42461	1.67154	2.31920
H	-1.74485	1.97240	4.04236
S	-3.36511	3.08697	2.67332
N	4.61129	-1.63278	1.26063
H	3.62743	-1.80121	0.97630
C	5.69011	-2.44017	0.98192
C	5.11084	-0.44483	1.70718
H	4.46151	0.38851	1.94329
N	6.43294	-0.44267	1.75357
C	6.80336	-1.69204	1.30127
H	7.84379	-1.98966	1.25826
N	-0.10163	-2.15312	1.82386
H	0.83457	-2.16288	1.35397
C	-0.69856	-0.99758	2.28252
C	-1.06857	-3.10033	1.75228
H	-0.87512	-4.10639	1.40514
N	-2.24978	-2.63683	2.15033
C	-2.02207	-1.31359	2.48381
H	-2.82237	-0.66721	2.81523
C	-3.49788	4.98199	-0.92868
C	-3.45835	4.70377	0.44170
H	-3.60596	5.50019	1.16596
C	-3.24901	3.40039	0.91758
C	-3.05783	2.35192	-0.01668
O	-2.82341	1.10784	0.44473
H	-2.75464	0.46396	-0.31393
C	-3.32802	3.93624	-1.84016
H	-3.36778	4.13062	-2.90892

C	-3.10513	2.63584	-1.39257
H	-2.98794	1.81465	-2.09356
N	-0.15086	-0.11660	-0.94729
H	-0.55802	0.76487	-1.25920
C	-0.42259	-1.14217	-1.97508
H	0.06020	-0.81686	-2.90293
C	0.14642	-2.51505	-1.57864
H	-0.42152	-2.90959	-0.72999
H	-0.01144	-3.19959	-2.41736
S	1.92543	-2.61290	-1.19092
C	-1.94203	-1.34145	-2.23108
O	-2.76190	-0.62706	-1.56133
O	-2.25942	-2.25340	-3.02596
H	-0.67831	-0.35484	-0.10299
Fe	1.83897	0.36928	-0.07899
O	2.05684	-1.75464	0.23829
H	-4.08592	-4.64120	1.90972
H	6.58213	2.20999	-0.84623
H	-0.33842	4.77888	-2.47980
H	-0.94891	3.23135	3.06899
H	5.56763	-3.44854	0.61417
H	-0.11449	-0.09165	2.37653
H	-3.67394	5.99660	-1.27416
O	1.79986	0.88172	1.74648
H	2.14269	0.23531	2.38135

^{5}FeCDOOHC1
Charge: 0
Energy: -2530013.3128447

C	6.54682	-2.23686	-1.31256
H	7.44176	-2.67693	-1.75750
H	6.83024	-1.32374	-0.78109
N	5.98945	-3.19483	-0.35914
H	6.14769	-4.17584	-0.53623
C	4.97532	-2.88365	0.48274
N	4.46469	-1.65561	0.47795
H	3.66315	-1.48852	1.10990
H	4.35414	-1.18113	-0.43658
N	4.53182	-3.78632	1.37539
H	3.51044	-3.72275	1.59612
H	4.96547	-4.69815	1.40435
N	-3.34765	-0.97830	2.21876
H	-3.48268	-1.65699	1.42916
C	-2.57789	-1.16986	3.34464
C	-3.44935	0.36836	2.04543
H	-3.96816	0.79523	1.19831
N	-2.81455	1.05326	2.98592
C	-2.26559	0.08986	3.80859
H	-1.69595	0.35832	4.68870
N	-0.86042	3.42237	-0.29617
H	-0.45004	4.13184	0.29949
C	-0.62465	3.24657	-1.64506
C	-1.50091	2.32272	0.16843
H	-1.77723	2.18984	1.20539
N	-1.71277	1.46190	-0.81748
C	-1.17364	2.03123	-1.95886
H	-1.21016	1.49351	-2.89422
C	3.52881	5.31724	-0.73414
H	2.62656	5.91175	-0.91236
H	4.21174	5.46174	-1.57579
S	3.17951	3.52685	-0.67895
N	-6.54054	-0.24750	-1.49272
H	-7.46112	-0.66170	-1.50675
C	-6.23269	1.07116	-1.78434
C	-5.38825	-0.88944	-1.17487
H	-5.29230	-1.92579	-0.88576
N	-4.36545	-0.05437	-1.24715
C	-4.87610	1.17080	-1.62678
H	-4.22509	2.02196	-1.75543
N	1.23465	-0.59747	-2.50046
H	0.20141	-0.81118	-2.57480
C	1.86491	0.52251	-2.99254
C	2.18907	-1.35746	-1.91161
H	1.97402	-2.29862	-1.42303
N	3.39290	-0.79782	-1.99860
C	3.19346	0.38587	-2.67439
H	4.00669	1.07199	-2.86330
C	0.81335	4.27968	2.61132
C	1.65222	4.48172	1.50542
H	1.90314	5.49710	1.21740
C	2.15974	3.39684	0.77966
C	1.82577	2.08360	1.18910
O	2.29356	1.06437	0.44118
H	2.08895	0.19008	0.87379
C	0.49861	2.98135	3.01436
H	-0.15828	2.80998	3.86166
C	1.01569	1.88976	2.31555
H	0.79756	0.87304	2.62764
N	-0.59707	-0.90576	0.56635
H	-0.76488	-0.30045	1.36964
C	-0.18688	-2.25057	1.03940
H	-0.69815	-2.42634	1.99051
C	-0.64534	-3.33037	0.05242
H	-0.42759	-3.00229	-0.97302
H	-0.09942	-4.25741	0.25072
S	-2.41172	-3.77633	0.18548
C	1.32663	-2.35255	1.36337
O	1.95466	-1.26967	1.60291
O	1.82203	-3.50283	1.40388
H	0.17813	-0.46750	0.06588
Fe	-2.27532	-0.70066	-0.92669
O	-1.41360	-1.01018	-2.62580
O	-3.21286	-2.34094	-0.10226
H	5.82782	-1.97543	-2.09665
H	-2.34447	-2.15858	3.70957
H	-0.08354	3.97223	-2.23118
H	4.01949	5.66134	0.18157
H	-6.98758	1.78807	-2.06788
H	1.31835	1.30939	-3.48699
H	0.42713	5.13644	3.15630
H	-1.68387	-1.82945	-3.06750

^{5}FeH3BueaBr
Charge: 0
Energy: -3308992.4044812

Fe	-0.46448	-0.36220	0.38146
O	2.93352	-2.21814	1.71111
O	0.34718	3.13300	1.74165
O	-4.23383	-1.32374	0.72755
N	-1.02760	-0.35395	2.83612
N	1.35150	-0.63661	1.31157
N	-0.91311	1.48333	0.70456
N	-1.93566	-1.57822	0.51170
N	2.98569	-1.08274	-0.30278
N	0.91439	2.40907	-0.36480
N	-3.17281	-0.62374	-1.18890
C	0.23798	-0.68077	3.47979
C	1.41331	-0.10676	2.66063
C	2.50639	-1.38309	0.91355
C	4.03219	-1.86410	-1.01300
C	4.25433	-1.15206	-2.35535
C	3.52691	-3.29976	-1.24420
C	5.32807	-1.85677	-0.18720
C	-1.49290	1.02866	3.05742
C	-1.94857	1.64743	1.72368
C	0.13220	2.41604	0.75318
C	2.18765	3.13798	-0.52416
C	1.94878	4.65616	-0.43116
C	3.18879	2.68071	0.55417
C	2.72315	2.77336	-1.91728
C	-2.07426	-1.39004	2.94097
C	-1.94974	-2.35161	1.75295
C	-3.20845	-1.19053	0.05015
C	-4.30805	0.04164	-1.85532
C	-5.43529	-0.97167	-2.12831
C	-4.81870	1.19726	-0.97505
C	-3.76116	0.59861	-3.17852
H	2.35944	-0.53753	-0.88921
H	0.57663	1.86569	-1.15035
H	-2.31552	-0.73109	-1.71823
H	0.35266	-1.76747	3.51670
H	0.29771	-0.29306	4.50848
H	1.30001	0.98410	2.58540
H	2.36827	-0.34028	3.13741
H	3.33189	-1.12661	-2.94668
H	5.01640	-1.68369	-2.93355
H	4.59849	-0.12302	-2.20017
H	3.34177	-3.79826	-0.28874
H	4.27537	-3.87660	-1.79887
H	2.59691	-3.28731	-1.82264
H	5.66644	-0.82893	-0.01549
H	6.11295	-2.39266	-0.73189
H	5.17964	-2.34270	0.77973
H	-0.66559	1.63095	3.43594
H	-2.30234	1.05412	3.80050
H	-2.85387	1.14770	1.36680
H	-2.17353	2.70813	1.87883
H	1.24810	4.97914	-1.20932
H	2.89217	5.19744	-0.56900
H	1.52997	4.91296	0.54405
H	2.80397	2.91048	1.55068
H	4.14719	3.19601	0.42399
H	3.36479	1.60146	0.47795
H	2.88681	1.69383	-2.00990
H	3.67632	3.28103	-2.09584
H	2.02201	3.07923	-2.70274
H	-3.05018	-0.90790	2.86859
H	-2.01883	-1.91876	3.90395
H	-1.01099	-2.91595	1.81096
H	-2.78457	-3.05995	1.75626
H	-5.79275	-1.39891	-1.18884
H	-5.07109	-1.78414	-2.76729
H	-6.27195	-0.47972	-2.63829
H	-4.01098	1.91380	-0.78732
H	-5.18377	0.81647	-0.01824
H	-5.63864	1.72124	-1.47914

H	-3.38078	-0.20637	-3.81876
H	-2.94476	1.30725	-2.99761
H	-4.55633	1.11816	-3.72265
Br	0.21341	-0.55812	-2.12057

^{5}FeH3BueaCl
Charge: 0
Energy: -1982465.0362621

Fe	-0.45190	-0.41478	0.20291
O	3.16201	-2.25436	1.28849
O	0.34709	2.86582	2.02679
O	-4.19735	-1.43851	0.39374
N	-0.99533	-0.76531	2.63288
N	1.38387	-0.82167	1.06493
N	-0.91751	1.35926	0.79615
N	-1.89743	-1.67127	0.16267
N	2.85772	-1.14377	-0.71230
N	0.88253	2.44063	-0.16852
N	-3.12110	-0.51509	-1.41709
C	0.27790	-1.17974	3.20614
C	1.44462	-0.48234	2.47136
C	2.55768	-1.47151	0.55594
C	3.95665	-1.75258	-1.50025
C	3.93711	-1.05586	-2.86875
C	3.69758	-3.26185	-1.66466
C	5.29895	-1.49776	-0.79456
C	-1.45851	0.56794	3.06340
C	-1.93780	1.37156	1.84179
C	0.12249	2.28744	0.95336
C	2.18315	3.13456	-0.23344
C	2.00329	4.63001	0.08328
C	3.17430	2.48752	0.75328
C	2.69398	2.95471	-1.67118
C	-2.04236	-1.80594	2.59766
C	-1.91855	-2.59961	1.29226
C	-3.16651	-1.22611	-0.25462
C	-4.23555	0.26921	-1.98130
C	-5.39644	-0.66266	-2.37535
C	-4.70455	1.31582	-0.95345
C	-3.67518	0.97605	-3.22485
H	2.13248	-0.65195	-1.23296
H	0.56463	1.95619	-1.00002
H	-2.24758	-0.52750	-1.93018
H	0.39417	-2.25988	3.08215
H	0.34937	-0.94862	4.28014
H	1.31135	0.60599	2.54950
H	2.40390	-0.76630	2.90874
H	2.97375	-1.19617	-3.37189
H	4.72208	-1.47339	-3.50693
H	4.11827	0.01993	-2.76373
H	3.67797	-3.75481	-0.68941
H	4.49083	-3.71418	-2.27037
H	2.73894	-3.43244	-2.16702
H	5.46742	-0.42204	-0.67259
H	6.11571	-1.90963	-1.39728
H	5.31933	-1.96985	0.19028
H	-0.62550	1.11222	3.51130
H	-2.25407	0.48039	3.81676
H	-2.84717	0.92364	1.42974
H	-2.16265	2.39759	2.15210
H	1.30963	5.08859	-0.63027
H	2.96578	5.15046	0.01428
H	1.60098	4.75608	1.09061
H	2.80528	2.57999	1.77769
H	4.15062	2.98132	0.69002
H	3.30898	1.42650	0.51387
H	2.81071	1.89267	-1.91613
H	3.66641	3.44360	-1.78759
H	1.99986	3.39811	-2.39476
H	-3.01745	-1.31667	2.58942
H	-1.98854	-2.45814	3.48205
H	-0.98295	-3.17201	1.27650
H	-2.75675	-3.29813	1.20040
H	-5.76418	-1.19747	-1.49698
H	-5.06127	-1.39607	-3.11748
H	-6.21803	-0.08129	-2.81023
H	-3.87209	1.97338	-0.67842
H	-5.07986	0.82400	-0.05270
H	-5.50806	1.92873	-1.37743
H	-3.32453	0.24881	-3.96708
H	-2.83528	1.62875	-2.95968
H	-4.45434	1.58770	-3.69078
Cl	0.15496	-0.19000	-2.11228

^{5}FeH3BueaF
Charge: 0
Energy: -1756342.6408619

Fe	-0.41398	-0.82369	-0.23846
O	3.52917	-2.05256	0.17434
O	0.12782	1.06680	3.31426
O	-4.23124	-0.77899	-0.82781
N	-1.24737	-2.48003	1.24991
N	1.24358	-1.70269	0.21181
N	-0.98452	0.32846	1.40384
N	-2.01690	-1.39903	-1.14064
N	2.64982	-0.45001	-1.20097
N	0.71596	1.84981	1.21543
N	-2.70172	0.76759	-1.58357
C	-0.12212	-3.43517	1.27590
C	1.21479	-2.70562	1.28136
C	2.55205	-1.42863	-0.25302
C	3.86502	-0.19903	-2.00328
C	3.48368	0.86968	-3.04022
C	4.29937	-1.48630	-2.73126
C	5.00730	0.31928	-1.10967
C	-1.48385	-1.77902	2.51287
C	-1.95814	-0.32350	2.23823
C	-0.00511	1.10936	2.09278
C	1.92946	2.61443	1.56862
C	1.58531	3.69634	2.60652
C	2.99633	1.64436	2.11732
C	2.41892	3.25953	0.26494
C	-2.47689	-3.01569	0.62045
C	-2.40449	-2.78486	-0.89592
C	-3.08187	-0.47998	-1.17484
C	-3.49539	1.99493	-1.38446
C	-4.77558	1.93928	-2.23673
C	-3.84664	2.16743	0.10647
C	-2.59978	3.15678	-1.84189
H	1.80104	0.03414	-1.47670
H	0.54840	1.65531	0.22570
H	-1.71722	0.89381	-1.79715
H	-0.18876	-4.03135	0.36102
H	-0.19987	-4.12170	2.13330
H	1.39682	-2.22239	2.25292
H	2.02495	-3.42663	1.14419
H	2.67167	0.51813	-3.68831
H	4.34662	1.10268	-3.67221
H	3.15856	1.79848	-2.55736
H	4.55020	-2.26594	-2.00909
H	5.17719	-1.28944	-3.35770
H	3.49036	-1.84992	-3.37568
H	4.72106	1.25813	-0.62343
H	5.90447	0.50469	-1.71203
H	5.24378	-0.41591	-0.33796
H	-0.55414	-1.72499	3.08240
H	-2.23946	-2.28740	3.12870
H	-2.90075	-0.35182	1.68079
H	-2.08110	0.19415	3.19374
H	0.82427	4.37817	2.21094
H	2.48323	4.27850	2.84131
H	1.20818	3.24480	3.52645
H	2.63902	1.16126	3.03017
H	3.91482	2.19490	2.35025
H	3.23176	0.87372	1.37685
H	2.63929	2.49204	-0.48405
H	3.33439	3.82989	0.44944
H	1.66498	3.94183	-0.14499
H	-3.33591	-2.45405	0.99241
H	-2.61884	-4.07557	0.87807
H	-1.64610	-3.43243	-1.35040
H	-3.37527	-3.01010	-1.34818
H	-5.38861	1.08623	-1.93840
H	-4.52114	1.83310	-3.29706
H	-5.35624	2.86044	-2.10895
H	-2.92977	2.20965	0.70618
H	-4.45757	1.32959	0.45172
H	-4.40823	3.09559	0.26177
H	-2.32947	3.05024	-2.89912
H	-1.67569	3.19246	-1.25147
H	-3.12369	4.10969	-1.71716
F	0.13378	0.68574	-1.26586

^{5}FeH3BueaN_3
Charge: 0
Energy: -1796726.9528113

Fe	-0.30735	-0.10719	-0.65870
O	3.64385	-0.22221	-2.05195
O	0.41445	-3.23367	1.37956
O	-4.10445	1.18922	-1.47535
N	-0.88288	-1.92195	-2.16342
N	1.44971	-0.53965	-1.37971
N	-0.89233	-1.45804	0.63488
N	-1.90725	0.48143	-1.44924
N	2.71457	1.25925	-0.57139
N	0.89334	-1.08435	2.04829
N	-3.07348	0.77203	0.53866
C	0.38794	-2.14966	-2.85490
C	1.54852	-1.90505	-1.88281
C	2.69795	0.16355	-1.36242
C	3.84322	2.20808	-0.47042
C	3.39125	3.30639	0.50500
C	4.13845	2.82426	-1.85098
C	5.08875	1.48927	0.07943
C	-1.28099	-3.00863	-1.24992

C	-1.82584	-2.42063	0.06413
C	0.16654	-2.02167	1.37084
C	2.18295	-1.33080	2.72270
C	1.97897	-2.29024	3.90886
C	3.20369	-1.91364	1.72657
C	2.67015	0.03749	3.22183
C	-1.98168	-1.37259	-2.98906
C	-1.96871	0.15542	-2.87423
C	-3.11965	0.84126	-0.82137
C	-4.18336	1.13830	1.44074
C	-4.57315	2.60950	1.21662
C	-5.38944	0.21013	1.20537
C	-3.64030	0.95211	2.86620
H	1.85563	1.48605	-0.07387
H	0.56557	-0.12701	1.98865
H	-2.30051	0.25736	0.94957
H	0.46739	-1.43482	-3.67931
H	0.44763	-3.16624	-3.27171
H	1.48288	-2.60289	-1.03602
H	2.51285	-2.05513	-2.37186
H	2.49853	3.82397	0.13321
H	4.18658	4.04844	0.62509
H	3.16306	2.89172	1.49374
H	4.42981	2.04764	-2.56132
H	4.95316	3.55278	-1.77007
H	3.25156	3.34046	-2.23615
H	4.88270	1.06647	1.06866
H	5.91965	2.19774	0.17228
H	5.38939	0.68057	-0.59033
H	-0.40474	-3.60961	-1.00402
H	-2.02236	-3.66521	-1.72699
H	-2.77145	-1.89996	-0.11746
H	-2.00332	-3.24280	0.76516
H	1.26330	-1.86721	4.62291
H	2.92930	-2.45844	4.42888
H	1.59328	-3.24862	3.55434
H	2.84579	-2.86592	1.32852
H	4.16329	-2.08464	2.22757
H	3.37130	-1.22022	0.89661
H	2.79603	0.73054	2.38250
H	3.63511	-0.06696	3.72766
H	1.95895	0.47588	3.93262
H	-2.93006	-1.73937	-2.58688
H	-1.90179	-1.71170	-4.03109
H	-1.08356	0.56653	-3.37533
H	-2.86022	0.60256	-3.32254
H	-4.95225	2.75472	0.20292
H	-3.70226	3.25820	1.35758
H	-5.35112	2.90253	1.93094
H	-5.11038	-0.83467	1.38875
H	-5.74024	0.30508	0.17497
H	-6.21052	0.47009	1.88348
H	-2.77926	1.60745	3.04319
H	-3.32798	-0.08601	3.03824
H	-4.41433	1.19802	3.59982
N	0.05599	1.46201	0.50168
N	-0.51688	2.53811	0.44721
N	-1.03327	3.56343	0.43763

^{5}FeH3BueaNCS
Charge: 0
Energy: -2001833.7610084

Fe	-0.31268	-0.58128	-0.49957
O	3.65570	-1.32126	-1.76607
O	0.58295	-2.18136	2.82745
O	-4.13174	-0.07254	-1.92197
N	-0.80057	-2.96103	-0.79487
N	1.48863	-1.30398	-0.93703
N	-0.80126	-1.07403	1.32070
N	-1.92014	-0.58569	-1.48921
N	2.67729	0.68581	-1.23283
N	0.98756	0.01823	2.29198
N	-3.14797	0.71370	-0.00199
C	0.47394	-3.48616	-1.28282
C	1.63632	-2.71756	-0.63523
C	2.71011	-0.65893	-1.34056
C	3.76454	1.59505	-1.65830
C	3.27330	3.01987	-1.35832
C	4.01767	1.43150	-3.16884
C	5.04353	1.29230	-0.85695
C	-1.16376	-3.39880	0.56603
C	-1.71754	-2.20834	1.36989
C	0.28750	-1.15008	2.20972
C	2.28655	0.19409	2.97015
C	2.12044	-0.02288	4.48470
C	3.32559	-0.78714	2.39489
C	2.72207	1.63860	2.68249
C	-1.91550	-2.97939	-1.76855
C	-1.95283	-1.63652	-2.50505
C	-3.15383	0.02789	-1.17762
C	-4.28317	1.49158	0.53639
C	-4.67449	2.60057	-0.45598
C	-5.47593	0.55829	0.81351
C	-3.78035	2.11560	1.84753
H	1.80831	1.10695	-0.91252
H	0.62363	0.79815	1.75855
H	-2.33385	0.62216	0.59300
H	0.52087	-3.33769	-2.36573
H	0.58224	-4.56216	-1.07931
H	1.59629	-2.83947	0.45796
H	2.60345	-3.08364	-0.98552
H	2.35019	3.24787	-1.90372
H	4.03434	3.74535	-1.66150
H	3.08040	3.15984	-0.28869
H	4.33521	0.41144	-3.39625
H	4.80168	2.12519	-3.49252
H	3.10610	1.65338	-3.73517
H	4.86351	1.41907	0.21594
H	5.84108	1.98094	-1.15706
H	5.37827	0.26828	-1.03732
H	-0.26998	-3.75605	1.07916
H	-1.88887	-4.22434	0.53020
H	-2.67350	-1.87733	0.95218
H	-1.87503	-2.52795	2.40536
H	1.39232	0.68652	4.89370
H	3.07764	0.12858	4.99707
H	1.76832	-1.03779	4.68236
H	3.00423	-1.81898	2.55480
H	4.29354	-0.64386	2.88824
H	3.46228	-0.61727	1.32200
H	2.82381	1.80319	1.60377
H	3.68950	1.84224	3.15194
H	1.99406	2.35820	3.07601
H	-2.85177	-3.09233	-1.21509
H	-1.82690	-3.83007	-2.45880
H	-1.07483	-1.53552	-3.15598
H	-2.85284	-1.53990	-3.11838
H	-5.00710	2.16642	-1.40144
H	-3.81765	3.25476	-0.64905
H	-5.48842	3.20477	-0.03891
H	-5.19478	-0.21752	1.53602
H	-5.80132	0.07655	-0.11145
H	-6.31498	1.12760	1.22981
H	-2.93198	2.78425	1.66097
H	-3.46802	1.33985	2.55874
H	-4.57938	2.69957	2.31482
N	0.00993	1.39061	-0.32324
C	-0.34000	2.53802	-0.31393
S	-0.76154	4.08218	-0.27362

^{5}FeH3BueaOH
Charge: 0
Energy: -1741254.1475234

Fe	0.33774	-0.68085	-0.02701
O	-0.13139	0.38810	1.45504
O	-3.63585	-1.96457	-0.30263
O	-0.19973	1.63573	-3.03705
O	4.05649	-1.47998	1.47517
N	0.95986	-2.09326	-1.88257
N	-1.40244	-1.39423	-0.52422
N	1.00000	0.68265	-1.28871
N	1.93242	-1.48730	0.57466
N	-2.65209	-0.67158	1.31872
N	-0.73413	2.14406	-0.85286
N	2.93060	0.51718	1.16820
C	-0.29853	-2.78731	-2.16959
C	-1.47691	-1.83940	-1.90879
C	-2.66292	-1.36325	0.15824
C	-3.81245	-0.55472	2.22508
C	-3.34974	0.31997	3.40062
C	-4.22008	-1.94944	2.73819
C	-4.99335	0.11817	1.50045
C	1.37101	-1.12877	-2.91993
C	1.93529	0.14309	-2.26284
C	-0.00624	1.51127	-1.82089
C	-2.02068	2.82796	-1.08757
C	-1.80209	4.06547	-1.97540
C	-3.03088	1.86590	-1.74348
C	-2.53280	3.25379	0.29657
C	2.06226	-2.93232	-1.35573
C	2.04307	-2.88930	0.17661
C	3.06519	-0.85370	1.09743
C	4.03932	1.42571	1.53495
C	4.47999	1.15096	2.98182
C	5.22319	1.25889	0.56288
C	3.46390	2.84683	1.42401
H	-1.76814	-0.23789	1.60394
H	-0.51439	1.88224	0.10555
H	2.27304	0.91138	0.49548
H	-0.38382	-3.64262	-1.49268
H	-0.32989	-3.16033	-3.20420
H	-1.41150	-0.96485	-2.57164
H	-2.43457	-2.33015	-2.09410
H	-2.50286	-0.13991	3.92391
H	-4.16690	0.44400	4.11817
H	-3.04220	1.31448	3.05781

H	-4.52008	-2.58851	1.90492
H	-5.05971	-1.86246	3.43737
H	-3.38206	-2.42315	3.26234
H	-4.71069	1.11616	1.14932
H	-5.84199	0.22080	2.18637
H	-5.30648	-0.47851	0.64111
H	0.49715	-0.83465	-3.50316
H	2.10137	-1.58356	-3.60451
H	2.86939	-0.08813	-1.73819
H	2.14060	0.87713	-3.04873
H	-1.09116	4.75191	-1.50180
H	-2.74968	4.59612	-2.12596
H	-1.40275	3.76616	-2.94665
H	-2.65200	1.52016	-2.70845
H	-3.98874	2.37292	-1.90763
H	-3.21123	0.99879	-1.10016
H	-2.66366	2.37981	0.94473
H	-3.49902	3.76007	0.20393
H	-1.82978	3.94202	0.78089
H	3.00839	-2.50675	-1.70093
H	1.99388	-3.95886	-1.74138
H	1.17615	-3.44281	0.55984
H	2.94868	-3.33148	0.60208
H	4.86739	0.13511	3.07918
H	3.63197	1.26998	3.66600
H	5.26252	1.85991	3.27536
H	4.90417	1.46670	-0.46599
H	5.61159	0.23887	0.61183
H	6.02999	1.95612	0.81686
H	2.60750	2.97361	2.09647
H	3.13044	3.06006	0.40031
H	4.22578	3.58586	1.69175
H	0.58703	0.42063	2.11018

^{5}FeAIkBBr
Charge: 0
Energy: -3404901.4780718

C	-3.50869	2.60115	1.79371
H	-4.25555	2.93617	1.06469
H	-3.95011	1.76143	2.33662
N	-1.62377	2.88613	0.12199
H	-1.98225	3.72755	-0.30496
C	-2.25664	2.15401	1.11766
C	-0.55475	2.17634	-0.32091
H	0.09042	2.47396	-1.13394
N	-0.44696	1.04585	0.35251
C	-1.49669	1.02082	1.25164
H	-1.66781	0.16715	1.88742
C	0.17951	-1.46439	4.25033
H	-0.51308	-2.17091	4.71190
H	1.19693	-1.63482	4.61562
C	0.13919	-1.56898	2.73169
O	1.08423	-0.99482	2.09612
O	-0.82774	-2.18171	2.20184
C	5.08703	3.80587	0.24579
H	6.09333	3.57008	0.61571
H	5.15522	3.94706	-0.83621
N	3.80971	2.30925	1.84238
H	4.20573	2.69054	2.68963
C	4.11257	2.71664	0.54868
C	2.89699	1.30420	1.77485
H	2.47286	0.77914	2.61732
N	2.59858	1.04704	0.51497
C	3.34268	1.91728	-0.25735
H	3.25644	1.90067	-1.33427
C	4.98025	-1.13203	0.03345
H	5.39007	-2.04665	0.46817
H	5.76141	-0.62948	-0.54408
N	3.89845	-1.47443	-0.87084
H	3.64873	-0.75403	-1.54254
C	2.77581	-2.18751	-0.41589
N	2.93629	-2.83672	0.83478
H	2.68759	-2.21900	1.60526
H	2.34523	-3.66170	0.87773
N	2.16523	-2.99932	-1.40346
H	2.26104	-2.57716	-2.32401
H	1.17222	-3.09549	-1.19850
Fe	1.14907	-0.46227	-0.06270
O	-0.35590	-2.00819	-0.32540
N	-5.54498	1.42211	-0.79873
C	-1.39968	-2.08258	-1.29222
H	-0.92501	-1.90509	-2.25723
H	-1.85240	-3.07539	-1.24685
H	-0.66612	-2.18547	0.62601
C	-4.45329	-0.34823	-0.07203
N	-5.60427	-0.25898	0.68748
C	-6.23713	0.80611	0.21839
H	-7.18838	1.17879	0.57235
N	-2.44853	-1.10312	-1.10755
C	-2.47021	0.01687	-1.89941
H	-1.62224	0.11389	-2.57248
N	-3.39131	0.94282	-1.90733
C	-4.39704	0.68863	-1.00221
C	-3.39082	-1.28058	-0.02370
N	-3.39234	-2.51134	0.65340
H	-4.33512	-2.74266	0.95605
H	-2.77099	-2.52318	1.46404
H	4.67762	-0.46636	0.85548
H	-3.33315	3.42025	2.50386
H	-5.83953	2.21470	-1.35051
H	4.78464	4.76340	0.68938
H	-0.10789	-0.44544	4.53820
Br	1.31264	0.16680	-2.67806

^{5}FeAIkBCl
Charge: 0
Energy: -2078371.5957800

C	-3.38510	2.65517	1.66946
H	-4.15462	2.95017	0.94655
H	-3.80761	1.84505	2.26931
N	-1.54512	2.86002	-0.06256
H	-1.91367	3.68265	-0.51655
C	-2.15297	2.17390	0.98047
C	-0.49231	2.12531	-0.50461
H	0.13149	2.38235	-1.34739
N	-0.37065	1.02441	0.21292
C	-1.39450	1.04291	1.14104
H	-1.54850	0.21867	1.81897
C	0.44055	-1.35514	4.13082
H	1.47294	-1.52360	4.45234
H	0.17347	-0.32669	4.40418
C	0.32815	-1.50030	2.61895
O	1.24892	-0.95565	1.92526
O	-0.67079	-2.11424	2.15261
C	5.01989	3.90107	-0.27128
H	6.05644	3.70855	0.03473
H	5.01029	4.01488	-1.35864
N	3.90473	2.40911	1.44609
H	4.34167	2.82841	2.25429
C	4.10630	2.78911	0.12468
C	3.02630	1.37092	1.46606
H	2.67501	0.85872	2.34904
N	2.65567	1.06815	0.23702
C	3.31376	1.94067	-0.60626
H	3.15656	1.88669	-1.67389
C	5.07013	-1.03437	-0.38436
H	5.52958	-1.92934	0.04145
H	5.79940	-0.52908	-1.02440
N	3.93832	-1.42136	-1.20598
H	3.61791	-0.71373	-1.86102
C	2.86278	-2.14401	-0.65441
N	3.12215	-2.75680	0.60022
H	2.89319	-2.13144	1.37060
H	2.56607	-3.60151	0.69605
N	2.21510	-3.00236	-1.58036
H	2.22638	-2.58829	-2.50951
H	1.24331	-3.12900	-1.30276
Fe	1.21518	-0.48502	-0.24292
O	-0.27701	-2.05673	-0.39210
N	-5.44401	1.41001	-0.90036
C	-1.34213	-2.15281	-1.33099
H	-0.88631	-2.01621	-2.31169
H	-1.80651	-3.13727	-1.24123
H	-0.56259	-2.19349	0.57378
C	-4.35762	-0.34347	-0.12593
N	-5.49532	-0.21468	0.64782
C	-6.12571	0.83863	0.14944
H	-7.06793	1.23323	0.50380
N	-2.37496	-1.15343	-1.16220
C	-2.39664	-0.06156	-1.99224
H	-1.55390	0.00553	-2.67542
N	-3.31028	0.87140	-2.02132
C	-4.30646	0.65804	-1.09476
C	-3.30215	-1.28156	-0.05980
N	-3.28738	-2.47578	0.67888
H	-4.22198	-2.68879	1.01773
H	-2.64402	-2.44998	1.47210
H	4.80970	-0.35621	0.44211
H	-3.19055	3.51098	2.32968
H	-5.74009	2.18458	-1.47635
H	4.71552	4.86008	0.16782
H	-0.23414	-2.04357	4.64347
Cl	1.25757	0.04384	-2.67224

^{3}FeAIkBF
Charge: 0
Energy: -1852246.1165409

C	-2.68865	3.47645	-1.64236
H	-2.51628	4.06849	-2.55080
H	-3.22192	2.56813	-1.93644
N	-0.36723	4.01564	-0.78952
H	-0.37022	4.98106	-1.08444
C	-1.40256	3.10872	-0.97775
C	0.65665	3.37531	-0.15658
H	1.61181	3.80624	0.10393

N	0.33342	2.11344	0.07328
C	-0.94286	1.93691	-0.42910
H	-1.43934	0.98081	-0.35469
C	2.81607	-3.33453	1.57626
H	3.02754	-4.18585	0.92184
H	3.71087	-3.04289	2.13174
C	2.25735	-2.16112	0.77820
O	2.58911	-0.99811	1.12580
O	1.46222	-2.44920	-0.17953
C	-3.46877	0.59743	3.68649
H	-3.79435	-0.12546	4.44611
H	-3.43318	1.58463	4.15641
N	-1.90570	-0.91054	2.40373
H	-2.62768	-1.52811	2.02819
C	-2.13183	0.25124	3.11931
C	-0.60490	-0.90929	2.00364
H	-0.17615	-1.67096	1.37444
N	0.02506	0.17786	2.43566
C	-0.92319	0.90133	3.14036
H	-0.67300	1.84460	3.60376
C	5.63216	-0.48979	0.18530
H	6.23962	-0.96267	-0.59489
H	6.30734	0.03142	0.86692
N	4.72489	0.48672	-0.38849
H	4.34740	1.24910	0.22786
C	3.83292	0.17483	-1.32884
N	3.85431	-1.01743	-1.98228
H	4.23254	-1.79577	-1.45889
H	2.97087	-1.24321	-2.43603
N	2.93898	1.11574	-1.69221
H	2.85572	1.83153	-0.95115
H	2.04919	0.75376	-2.03206
Fe	1.61305	0.87183	1.24195
O	0.91666	-0.88590	-2.17651
N	-4.94579	-0.28780	-0.61521
C	-0.11054	-1.58072	-2.83283
H	-0.10605	-1.27880	-3.88323
H	0.03167	-2.66356	-2.76414
H	1.09675	-1.34668	-1.28959
C	-3.10755	-1.50307	-0.60873
N	-3.85689	-1.90743	0.48170
C	-4.95519	-1.15640	0.44449
H	-5.77260	-1.20346	1.14944
N	-1.44165	-1.29419	-2.29471
C	-2.17823	-0.28393	-2.83935
H	-1.73233	0.18322	-3.71424
N	-3.33889	0.15857	-2.43262
C	-3.77521	-0.49870	-1.30507
C	-1.83194	-1.93544	-1.05335
N	-1.27765	-3.19077	-0.76693
H	-1.88155	-3.72029	-0.14594
H	-0.31751	-3.15888	-0.40939
H	5.08506	-1.25251	0.75451
H	-3.33948	4.06760	-0.98328
H	-5.66708	0.37049	-0.87306
H	-4.24034	0.62258	2.90514
H	2.05822	-3.65706	2.30155
F	3.15098	2.20628	0.71717

[5]FeAIkBNCS
Charge: 0
Energy: -2097748.5932032

C	3.74310	-2.71287	-1.57480
H	4.33900	-2.44282	-0.69599
H	3.52143	-3.78255	-1.51462
N	2.41117	-0.60041	-1.99856
H	3.20481	-0.00680	-2.21373
C	2.46993	-1.93633	-1.63542
C	1.11837	-0.18834	-1.90799
H	0.78159	0.81863	-2.09612
N	0.34073	-1.18415	-1.50959
C	1.17464	-2.27773	-1.34308
H	0.78497	-3.22771	-1.00940
C	1.28641	-2.26208	2.20326
H	1.60050	-2.15302	3.24677
H	0.88860	-3.26434	2.03304
C	0.26164	-1.19708	1.84517
O	-0.82286	-1.54021	1.30497
O	0.58225	0.01535	2.11099
C	-7.07488	-2.17001	-0.54252
H	-7.66270	-1.72490	0.27089
H	-7.31262	-1.62656	-1.46092
N	-5.00706	-2.66464	0.83518
H	-5.47799	-3.20248	1.54838
C	-5.60772	-2.09194	-0.27828
C	-3.66880	-2.40960	0.78034
H	-2.94139	-2.73050	1.51116
N	-3.38021	-1.70417	-0.30083
C	-4.57699	-1.50071	-0.96457
H	-4.60754	-0.92213	-1.87607
C	-4.76953	1.32558	1.45138
H	-4.71146	1.07422	2.51521
H	-5.75220	1.75828	1.25326
N	-3.76312	2.32350	1.12201
H	-3.95736	2.91030	0.30591
C	-2.45601	2.14515	1.38070
N	-2.04082	1.08759	2.09819
H	-2.55358	0.22296	1.97068
H	-1.02905	0.89024	2.15039
N	-1.57894	3.09703	1.01182
H	-1.92849	3.76545	0.32842
H	-0.61962	2.78240	0.81922
Fe	-1.51655	-0.81342	-0.66577
O	0.99564	1.99208	0.37479
N	6.42844	-0.43153	-0.88250
C	2.19442	2.55463	0.86625
H	2.26146	3.56752	0.46296
H	2.21462	2.59223	1.95868
H	0.83598	1.14377	0.86998
C	4.89597	-0.00875	0.64409
N	5.66325	-1.04614	1.13504
C	6.57564	-1.26534	0.19796
H	7.35528	-2.01287	0.24410
N	3.37586	1.81141	0.44303
C	3.87646	2.04382	-0.80441
H	3.40590	2.86710	-1.33778
N	4.83734	1.39057	-1.40672
C	5.35805	0.39005	-0.60757
C	3.76906	0.64040	1.21055
N	3.42079	0.60959	2.56843
H	4.05806	0.00065	3.07434
H	2.45135	0.30524	2.70812
H	-4.66054	0.41557	0.84884
H	4.36203	-2.54770	-2.46512
H	7.01174	-0.38384	-1.70539
H	-7.41441	-3.20598	-0.67040
H	2.17246	-2.11018	1.57594
N	-2.12971	0.95774	-1.47288
C	-2.61586	1.99633	-1.75908
S	-3.31237	3.47906	-2.00855

[4]FeAIkBBrOHR1
Charge: 0
Energy: -3405314.6203351

C	-3.63687	2.68392	1.07676
H	-4.14857	3.43813	0.46655
H	-4.36265	1.90724	1.34127
N	-2.48970	1.71734	-0.96280
H	-3.31808	1.66958	-1.54597
C	-2.45805	2.10621	0.36690
C	-1.28383	1.17234	-1.27649
H	-1.01191	0.76149	-2.23660
N	-0.47513	1.21044	-0.23543
C	-1.19169	1.79158	0.79339
H	-0.74516	1.93781	1.76536
C	-0.16589	-0.30044	3.63397
H	-0.19225	-1.10609	4.37400
H	0.45220	0.52548	3.99258
C	0.33479	-0.83031	2.29675
O	1.20291	-0.13892	1.68461
O	-0.16467	-1.92020	1.88683
C	2.28354	6.13084	0.00411
H	2.80664	6.64542	-0.81250
H	1.21534	6.33895	-0.10289
N	3.77413	4.08293	0.08866
H	4.64539	4.58194	0.19672
C	2.51385	4.65645	-0.02570
C	3.64415	2.73394	0.02426
H	4.45795	2.02433	0.07230
N	2.37230	2.40471	-0.12399
C	1.66176	3.59181	-0.15628
H	0.58862	3.59322	-0.26478
C	4.29274	-4.28456	-0.00783
H	4.05893	-5.24996	0.45221
H	5.04512	-4.45475	-0.77970
N	3.10352	-3.73527	-0.65012
H	3.32026	-2.99970	-1.31970
C	1.98585	-3.45459	0.05583
N	1.81048	-3.95805	1.30199
H	2.63707	-4.18500	1.83531
H	1.06232	-3.50098	1.82709
N	0.98999	-2.76910	-0.49701
H	1.17067	-2.07804	-1.26425
H	0.33661	-2.39102	0.20436
Fe	1.60756	0.36916	-0.26043
N	-6.40696	0.51947	-0.25011
C	-1.95457	-2.24626	-1.81680
H	-2.07531	-2.58261	-2.84942
H	-1.83865	-3.11322	-1.16638
H	-1.06261	-1.61544	-1.74791
C	-4.64724	-0.70134	0.25584
N	-5.35145	-0.52895	1.42801
C	-6.40647	0.20001	1.08864
H	-7.18743	0.52984	1.75927
N	-3.15114	-1.51004	-1.40051
C	-3.84291	-0.80232	-2.32244

H	-3.46476	-0.88271	-3.33935
N	-4.89167	-0.02745	-2.12051
C	-5.28980	-0.06378	-0.80007
C	-3.42381	-1.39968	0.01695
N	-2.91898	-2.39459	0.86872
H	-3.57125	-2.55787	1.63236
H	-1.99870	-2.18284	1.26402
H	2.61769	6.57981	0.94865
H	-3.31215	3.16601	2.00376
H	-7.11498	1.02712	-0.76075
H	4.71276	-3.59128	0.73277
H	-1.19647	0.04959	3.49835
O	1.16789	-0.49360	-1.94673
H	1.96228	-0.50038	-2.50575
Br	4.20042	-0.62695	-0.43636

^{4}FeAIkBBrR
Charge: 0
Energy: -3501171.6466149

C	3.99548	2.77402	-0.87201
H	4.71499	1.98782	-1.12530
H	3.75135	3.31080	-1.79339
N	2.68093	1.73263	1.02547
H	3.46852	1.61007	1.65340
C	2.75289	2.20044	-0.27751
C	1.44235	1.20668	1.21982
H	1.10454	0.74854	2.13623
N	0.70956	1.33265	0.13037
C	1.51221	1.95421	-0.80822
H	1.14106	2.15398	-1.80151
C	1.23373	-0.50536	-3.48292
H	2.20413	-0.31754	-3.00540
H	1.34530	-1.38645	-4.12123
C	0.21980	-0.77487	-2.38341
O	-0.58236	0.16977	-2.08955
O	0.26065	-1.89729	-1.80856
C	-2.06419	6.19441	0.62697
H	-2.74308	6.52591	1.42337
H	-1.04006	6.34347	0.97999
N	-3.47712	4.26097	-0.20244
H	-4.31688	4.79790	-0.36535
C	-2.27176	4.75813	0.27795
C	-3.34078	2.92955	-0.42286
H	-4.11754	2.27347	-0.78873
N	-2.11601	2.53984	-0.11237
C	-1.44344	3.66795	0.32351
H	-0.41119	3.61144	0.63097
C	-4.54395	-3.90468	0.19666
H	-4.49585	-4.68551	-0.56861
H	-5.13531	-4.28007	1.03476
N	-3.20412	-3.60987	0.68105
H	-3.10210	-3.22654	1.62037
C	-2.16140	-3.36701	-0.12210
N	-2.27608	-3.48377	-1.47172
H	-3.13836	-3.09007	-1.83704
H	-1.46161	-3.10403	-1.95544
N	-0.96458	-3.10321	0.41379
H	-0.99845	-2.80163	1.39391
H	-0.34459	-2.57170	-0.20454
Fe	-1.34965	0.51361	-0.26400
C	-3.13698	0.13959	2.85693
H	-2.72537	1.12948	3.07702
H	-3.84913	0.25169	2.03004
C	-2.03976	-0.79474	2.38098
O	-2.00473	-1.98027	2.77252
O	-1.17692	-0.30132	1.55333
N	6.46754	0.32833	0.27523
C	1.86412	-2.24500	1.71887
H	1.85313	-2.44936	2.79189
H	1.78340	-3.18577	1.17172
H	1.01344	-1.60157	1.46944
C	4.67760	-0.82973	-0.26921
N	5.39855	-0.65877	-1.43110
C	6.47070	0.03181	-1.06909
H	7.26983	0.34630	-1.72561
N	3.11986	-1.59053	1.35276
C	3.82519	-0.92219	2.29434
H	3.42096	-0.98841	3.30234
N	4.91226	-0.19754	2.11914
C	5.32639	-0.22906	0.80363
C	3.43770	-1.50897	-0.05843
N	2.98954	-2.54992	-0.88843
H	3.64904	-2.69608	-1.64868
H	2.05265	-2.40592	-1.27628
H	-2.21797	6.85296	-0.23774
H	4.48505	3.47992	-0.19012
H	7.18506	0.80661	0.80074
H	-3.64878	-0.26956	3.73065
H	-5.02557	-3.01000	-0.21587
H	0.95481	0.36562	-4.07951
Br	-3.82072	-0.44181	-0.84886

^{4}FeAIkBClR
Charge: 0
Energy: -2174640.0221622

C	-3.65738	3.43780	0.33833
H	-3.75275	4.27009	-0.37122
H	-4.60776	2.89133	0.34612
N	-2.41183	1.86586	-1.20873
H	-3.15928	1.75452	-1.88317
C	-2.51339	2.54169	-0.00005
C	-1.26940	1.12668	-1.18317
H	-0.93477	0.48481	-1.98156
N	-0.62375	1.30950	-0.04884
C	-1.38590	2.18902	0.69676
H	-1.06467	2.48603	1.68305
C	-0.99229	-0.41679	3.84877
H	-2.00753	-0.44282	3.43021
H	-0.81131	-1.37973	4.33697
C	-0.02054	-0.22135	2.70693
O	0.57669	0.87720	2.54502
O	0.12951	-1.17335	1.86320
C	2.70285	5.69487	-1.33955
H	3.47596	5.80517	-2.11128
H	1.73280	5.86505	-1.81493
N	3.82771	3.83704	-0.03384
H	4.70362	4.31780	0.11231
C	2.72538	4.33994	-0.71378
C	3.52731	2.59046	0.41434
H	4.19422	1.94706	0.96955
N	2.29795	2.26297	0.06174
C	1.78946	3.34124	-0.63750
H	0.78331	3.32364	-1.02679
C	4.36941	-3.71728	0.11783
H	4.35613	-4.40252	0.97147
H	5.07937	-4.10341	-0.61720
N	3.05301	-3.68517	-0.50697
H	3.00278	-3.50218	-1.50541
C	1.89909	-3.48824	0.15227
N	1.88777	-3.35225	1.49877
H	2.71975	-2.87899	1.84973
H	1.07458	-2.82607	1.83368
N	0.75840	-3.53701	-0.55245
H	0.88570	-3.26111	-1.53227
H	-0.09763	-3.15023	-0.14007
Fe	1.32476	0.35055	0.55288
C	3.27101	-0.20252	-2.30828
H	2.98103	0.84162	-2.46382
H	3.86437	-0.23444	-1.38620
C	2.03466	-1.05949	-2.09075
O	1.89819	-2.13706	-2.71556
O	1.17747	-0.63398	-1.22754
N	-5.61572	0.43615	0.30305
C	-1.72497	-2.31906	-2.39546
H	-1.89979	-2.25326	-3.47144
H	-1.68230	-3.37022	-2.10180
H	-0.76968	-1.84491	-2.15051
C	-3.83969	-0.86603	0.31501
N	-4.15597	-0.62632	1.63527
C	-5.22540	0.15384	1.59333
H	-5.75917	0.53750	2.45134
N	-2.81776	-1.64479	-1.68936
C	-3.73553	-0.93268	-2.38986
H	-3.62872	-0.98670	-3.47060
N	-4.70998	-0.18924	-1.90775
C	-4.73599	-0.21472	-0.52990
C	-2.78581	-1.62708	-0.25421
N	-1.89057	-2.47439	0.42364
H	-2.38598	-3.17442	0.98175
H	-1.29652	-1.93184	1.06767
H	2.85527	6.49164	-0.59971
H	-3.50871	3.86217	1.33522
H	-6.42280	0.96663	0.00787
H	3.85923	-0.56851	-3.15261
H	4.68432	-2.72355	0.45244
H	-0.91359	0.39418	4.57549
Cl	3.52706	-0.54702	1.37716

^{6}FeAIkBFR
Charge: 0
Energy: -1948509.8559671

C	-3.02329	3.86901	-0.29245
H	-3.03101	4.54438	-1.15789
H	-4.03550	3.46434	-0.17215
N	-2.02318	1.87550	-1.49272
H	-2.77969	1.74451	-2.15395
C	-2.01374	2.78042	-0.43968
C	-0.99660	1.00437	-1.31171
H	-0.76493	0.17472	-1.95882
N	-0.31669	1.31094	-0.22391
C	-0.93712	2.41612	0.32698
H	-0.57000	2.84694	1.24538
C	-1.08986	0.45314	3.82478
H	-2.07764	0.46548	3.34627
H	-1.06238	-0.41630	4.49042

C	-0.04099	0.30613	2.74253
O	0.78920	1.22526	2.51008
O	-0.06539	-0.76155	2.03368
C	4.54645	4.60259	-1.80948
H	5.58883	4.72664	-1.48780
H	4.55929	4.23365	-2.83884
N	3.61459	3.84321	0.42064
H	3.94947	4.63185	0.95478
C	3.80395	3.64282	-0.94027
C	2.90873	2.79038	0.91457
H	2.59421	2.68040	1.94205
N	2.63597	1.92988	-0.04684
C	3.18349	2.44742	-1.20152
H	3.09688	1.92847	-2.14406
C	4.02994	-3.59887	0.62479
H	4.11575	-4.06059	1.61342
H	4.77506	-4.04512	-0.03705
N	2.70954	-3.87926	0.06831
H	2.63082	-3.95499	-0.94395
C	1.56537	-3.54355	0.68632
N	1.61931	-3.00775	1.92709
H	2.32711	-2.25352	1.95250
H	0.74048	-2.58466	2.22202
N	0.40009	-3.83491	0.07812
H	0.49829	-3.88073	-0.93963
H	-0.42305	-3.28113	0.34983
Fe	1.43110	0.16606	0.55889
C	3.22891	-1.20386	-2.13483
H	3.14649	-0.29506	-2.74195
H	3.64895	-0.91648	-1.16536
C	1.83602	-1.79023	-1.90755
O	1.55853	-2.92228	-2.38255
O	1.03211	-1.09192	-1.19964
N	-5.34736	1.12739	0.03852
C	-1.90946	-2.59443	-2.04927
H	-2.05454	-2.66738	-3.12913
H	-2.05528	-3.58067	-1.60150
H	-0.89316	-2.24909	-1.84026
C	-3.81448	-0.42851	0.32338
N	-4.10686	0.06558	1.57704
C	-5.03036	0.99328	1.37219
H	-5.50752	1.58742	2.13865
N	-2.88631	-1.64909	-1.49828
C	-3.65953	-0.91596	-2.33526
H	-3.53664	-1.14646	-3.39050
N	-4.51416	0.03525	-2.01210
C	-4.57636	0.21909	-0.64735
C	-2.89373	-1.42953	-0.08232
N	-2.08096	-2.22380	0.75027
H	-2.64879	-2.75926	1.41169
H	-1.45852	-1.61830	1.30797
H	4.08010	5.59653	-1.81772
H	-2.79544	4.46496	0.59593
H	-6.04831	1.72955	-0.36876
H	3.88151	-1.91450	-2.64808
H	4.19897	-2.52186	0.71526
H	-0.93810	1.36798	4.40148
F	2.94359	-0.80275	1.17112

^{4}FeAIkBN$_2$R
Charge: 0
Energy: -1988902.8299569

C	3.85958	2.70830	-0.97426
H	4.36069	3.43679	-0.32536
H	4.57166	1.90887	-1.20631
N	2.56418	1.74788	0.97769
H	3.35811	1.64407	1.60089
C	2.62180	2.16415	-0.34310
C	1.32675	1.23540	1.20860
H	0.99795	0.81398	2.14575
N	0.58075	1.32066	0.12406
C	1.37348	1.90211	-0.84857
H	0.99062	2.06403	-1.84450
C	0.94668	-0.54647	-3.51622
H	1.04208	-1.43175	-4.15141
H	0.61413	0.31099	-4.10490
C	0.00355	-0.82752	-2.35744
O	-0.81964	0.09124	-2.03982
O	0.11938	-1.93462	-1.76424
C	-2.34064	6.25614	0.23728
H	-2.93897	6.63760	1.07480
H	-1.29349	6.49652	0.44045
N	-3.71428	4.17259	-0.20150
H	-4.59952	4.64595	-0.31284
C	-2.49410	4.78115	0.06766
C	-3.51633	2.83369	-0.30101
H	-4.27995	2.09645	-0.50029
N	-2.24141	2.54653	-0.10994
C	-1.59628	3.74658	0.11984
H	-0.53224	3.77699	0.29818
C	-4.76692	-3.89720	0.17787
H	-4.64200	-4.76806	-0.47354
H	-5.36467	-4.19337	1.04280
N	-3.46497	-3.45466	0.65767
H	-3.38352	-3.04816	1.58879
C	-2.38167	-3.30581	-0.11446
N	-2.44564	-3.52449	-1.45044
H	-3.29578	-3.18267	-1.90471
H	-1.59760	-3.23643	-1.93583
N	-1.20054	-3.02559	0.45216
H	-1.25488	-2.69481	1.42132
H	-0.54685	-2.54019	-0.17109
Fe	-1.47212	0.51635	-0.17034
C	-3.31608	0.27560	2.86884
H	-2.88169	1.24061	3.14705
H	-3.95964	0.43663	1.99569
C	-2.22798	-0.69507	2.44277
O	-2.27993	-1.89162	2.79533
O	-1.28924	-0.21814	1.69176
N	6.35208	0.30721	0.31388
C	1.70016	-2.21909	1.68633
H	1.67739	-2.43329	2.75726
H	1.61456	-3.15436	1.13082
H	0.85863	-1.56414	1.43661
C	4.56486	-0.84197	-0.25748
N	5.31250	-0.68909	-1.40511
C	6.38259	-0.00373	-1.02672
H	7.19832	0.29762	-1.66883
N	2.96746	-1.57612	1.33830
C	3.65852	-0.90466	2.28828
H	3.23338	-0.95981	3.28831
N	4.75406	-0.18891	2.12945
C	5.19556	-0.23631	0.82304
C	3.31261	-1.50486	-0.06682
N	2.86878	-2.54413	-0.90074
H	3.52756	-2.68166	-1.66299
H	1.92833	-2.40559	-1.28223
H	-2.64013	6.80591	-0.66438
H	3.60695	3.21125	-1.91231
H	7.06350	0.78189	0.85083
H	-3.90741	-0.13308	3.69110
H	-5.29081	-3.11456	-0.38052
H	1.93803	-0.33269	-3.09643
N	-3.46600	-0.19158	-0.47130
N	-3.99094	-0.84346	-1.32387
N	-4.53015	-1.49316	-2.13520

^{4}FeAIkBNCSR
Charge: 0
Energy: -2194014.0379868

C	-4.12370	2.67832	1.44384
H	-4.96616	1.97795	1.44635
H	-3.84785	2.87160	2.48397
N	-2.99584	1.76590	-0.63045
H	-3.83543	1.69432	-1.19293
C	-2.95090	2.11937	0.71102
C	-1.78071	1.26558	-0.97847
H	-1.52645	0.88634	-1.95504
N	-0.95588	1.29901	0.05167
C	-1.67012	1.83222	1.10920
H	-1.19963	1.95820	2.07219
C	1.00133	-0.67710	4.02847
H	0.33117	-1.50180	4.28518
H	2.03644	-1.01212	4.17046
C	0.84197	-0.28838	2.57555
O	1.06066	0.91090	2.22407
O	0.54948	-1.17928	1.71529
C	1.94527	6.22824	-0.94051
H	2.51319	6.55361	-1.82183
H	0.88936	6.44175	-1.12816
N	3.35778	4.19871	-0.38881
H	4.23841	4.68971	-0.33066
C	2.12299	4.77174	-0.66669
C	3.17835	2.86829	-0.18202
H	3.96079	2.16598	0.06315
N	1.90409	2.55427	-0.31491
C	1.23794	3.72555	-0.61332
H	0.16777	3.73140	-0.75614
C	4.33395	-3.55938	-0.85689
H	4.47344	-4.35840	-0.12196
H	4.88100	-3.83604	-1.76079
N	2.92670	-3.43465	-1.20767
H	2.69741	-3.11754	-2.14724
C	1.93110	-3.27514	-0.31633
N	2.14385	-3.37520	1.01291
H	3.09607	-3.21839	1.33447
H	1.47752	-2.81151	1.55395
N	0.69013	-3.11834	-0.79237
H	0.64922	-2.75811	-1.75153
H	-0.06487	-2.78996	-0.18537
Fe	1.12549	0.56231	0.11439
C	2.69079	0.26998	-3.05305
H	2.32434	1.29332	-3.17737
H	3.42105	0.28237	-2.23551
C	1.55764	-0.65049	-2.63247
O	1.45431	-1.78985	-3.13916

O	0.75067	-0.20609	-1.72888
N	-6.24269	-0.22553	0.65401
C	-2.02826	-2.02760	-2.34955
H	-2.27859	-1.95061	-3.40982
H	-1.85657	-3.07684	-2.09619
H	-1.11671	-1.45938	-2.15032
C	-4.25105	-1.15704	0.52419
N	-4.58830	-1.14604	1.85981
C	-5.78941	-0.59021	1.90287
H	-6.37697	-0.42909	2.79590
N	-3.14465	-1.50773	-1.55435
C	-4.18135	-0.88488	-2.16928
H	-4.09171	-0.80810	-3.25031
N	-5.25422	-0.37145	-1.60497
C	-5.26282	-0.58441	-0.24264
C	-3.09030	-1.65566	-0.12992
N	-1.85692	-1.99775	0.45938
H	-2.01919	-2.50423	1.32718
H	-1.28182	-1.18753	0.71541
H	2.26413	6.84655	-0.09140
H	-4.46847	3.62340	1.00442
H	-7.13586	0.18277	0.41822
H	3.16526	-0.08645	-3.96987
H	4.74917	-2.63084	-0.45300
H	0.82544	0.18054	4.68163
N	3.13810	-0.21053	0.27081
C	3.85077	-0.66577	1.10228
S	4.80534	-1.36391	2.23656

^{6}FeEgtBBrRe
Charge: 0
Energy: -3920178.0052569

C	-1.03720	-2.75142	2.63989
H	-0.62365	-2.53371	3.62896
H	-1.78857	-1.99127	2.39526
N	-0.24137	-2.84390	0.26086
H	-1.19070	-2.88312	-0.13017
C	0.04093	-2.72502	1.60953
C	0.90495	-2.65313	-0.43024
H	0.96187	-2.65181	-1.50869
N	1.92665	-2.41950	0.39414
C	1.38986	-2.48387	1.67029
H	1.99409	-2.28641	2.54472
C	-4.59611	-2.33275	3.06322
H	-3.99433	-1.41833	3.14437
H	-5.51030	-2.24380	3.65785
N	-4.93098	-2.62220	1.67394
H	-4.16050	-3.00477	1.11818
C	-5.67082	-1.76150	0.95120
N	-6.28656	-0.70292	1.51756
H	-6.55751	0.01537	0.84103
H	-5.84208	-0.32321	2.34297
N	-5.88295	-1.99894	-0.35321
H	-5.26042	-2.67477	-0.78418
H	-6.03304	-1.13986	-0.90048
C	8.05129	0.23457	1.77168
H	8.83576	-0.30994	1.23126
H	8.14145	1.29221	1.51033
N	6.28157	-1.57171	1.61372
H	6.85210	-2.31407	1.99304
C	6.68908	-0.25750	1.41205
C	5.00680	-1.70386	1.17395
H	4.43569	-2.62047	1.16588
N	4.56941	-0.54599	0.71004
C	5.60373	0.35934	0.84713
H	5.49686	1.37551	0.49851
C	-0.43498	2.28501	3.61028
H	-1.05291	1.68300	4.28924
H	0.39756	2.69685	4.18831
N	-0.76318	1.07267	1.44021
H	-1.72890	1.37492	1.30752
C	0.07333	1.48012	2.46066
C	-0.02927	0.43389	0.51434
H	-0.43201	0.01557	-0.38996
N	1.24426	0.38182	0.88061
C	1.31976	1.02527	2.10430
H	2.26116	1.13491	2.62160
Fe	2.78629	-0.37503	-0.36967
C	1.51692	3.45987	-0.32155
C	2.72063	2.83495	-0.09281
N	1.02059	2.86484	-1.46711
C	1.89317	1.90867	-1.85670
N	2.94375	1.84935	-1.03626
H	3.41154	2.99560	0.72320
H	1.74623	1.25618	-2.70522
H	0.02823	2.95398	-1.74440
C	0.75944	4.48692	0.47670
H	1.35572	5.40663	0.54460
H	0.65411	4.11189	1.50283
C	-1.61078	3.64255	-0.05414
O	-2.23137	3.38808	1.00318
O	-1.66691	2.96326	-1.13922
C	-0.64421	4.84579	-0.05983
H	-0.56344	5.24612	-1.07675
O	-2.92976	-2.34963	-0.44791
C	-3.08883	-1.08196	-0.29465
O	-3.09543	-0.47899	0.79304
C	-3.36326	-0.30401	-1.61698
H	-4.21803	-0.79102	-2.09314
C	-2.17356	-0.43522	-2.58798
H	-2.44111	0.06134	-3.52738
H	-1.29233	0.07805	-2.18829
S	-1.82460	-2.18870	-2.95700
N	-3.69755	1.08391	-1.38871
H	-2.92109	1.76625	-1.27028
C	-4.92165	1.46987	-0.99279
O	-5.91255	0.70113	-0.93707
C	-5.04546	2.92746	-0.60639
H	-6.09138	3.15928	-0.39834
H	-4.67403	3.57157	-1.41025
H	-1.54003	-3.72704	2.68859
H	-4.01515	-3.16864	3.45538
H	8.25296	0.13587	2.84602
H	-1.05434	3.10678	3.23231
H	-1.06275	5.62400	0.58538
H	-4.41572	3.12653	0.26875
Br	3.24768	-1.26809	-2.67196

^{6}FeEgtBClRe
Charge: 0
Energy: -2593649.7257309

C	0.83953	-3.02963	-2.24737
H	0.37312	-2.92083	-3.23095
H	1.57393	-2.22664	-2.11349
N	0.15642	-2.91499	0.16605
H	1.12288	-2.88210	0.51207
C	-0.19056	-2.93904	-1.17243
C	-0.96600	-2.70050	0.89012
H	-0.97346	-2.58841	1.96409
N	-2.03235	-2.58844	0.09836
C	-1.55002	-2.75551	-1.18987
H	-2.20022	-2.66957	-2.04948
C	4.35104	-2.56117	-2.89982
H	3.71814	-1.67512	-3.03858
H	5.23154	-2.50846	-3.54725
N	4.76302	-2.70218	-1.50823
H	4.03306	-3.04715	-0.87820
C	5.51100	-1.75497	-0.91339
N	6.06622	-0.74362	-1.61294
H	6.34887	0.04546	-1.02595
H	5.57065	-0.45971	-2.44768
N	5.79402	-1.85470	0.39541
H	5.21315	-2.49838	0.92300
H	5.94468	-0.94113	0.84586
C	-8.23344	-0.15765	-1.32371
H	-8.99954	-0.67330	-0.73105
H	-8.34339	0.91544	-1.14638
N	-6.42266	-1.90827	-1.04741
H	-6.98075	-2.68996	-1.36037
C	-6.85638	-0.59094	-0.94526
C	-5.13892	-1.97752	-0.61786
H	-4.54488	-2.87700	-0.54969
N	-4.72153	-0.77757	-0.25392
C	-5.77747	0.09177	-0.44734
H	-5.68715	1.13492	-0.18402
C	0.01469	1.84763	-3.67281
H	0.60817	1.19195	-4.32335
H	-0.85813	2.18436	-4.24001
N	0.49035	0.86309	-1.41591
H	1.45564	1.19048	-1.36951
C	-0.41035	1.15267	-2.42213
C	-0.17648	0.30557	-0.39197
H	0.28455	-0.01667	0.52382
N	-1.46682	0.19553	-0.67791
C	-1.62434	0.71370	-1.95205
H	-2.59538	0.75587	-2.42223
Fe	-2.90097	-0.46502	0.73568
C	-1.76793	3.38271	0.20544
C	-2.97114	2.72168	0.11742
N	-1.19361	2.91861	1.37449
C	-2.02437	1.99838	1.91460
N	-3.12078	1.83992	1.17155
H	-3.71265	2.78844	-0.66687
H	-1.81157	1.43736	2.81295
H	-0.18956	3.05340	1.58247
C	-1.07933	4.32992	-0.74030
H	-1.70286	5.22359	-0.87681
H	-1.01595	3.84604	-1.72343
C	1.33959	3.60222	-0.25389
O	1.91405	3.25251	-1.30986
O	1.47095	3.04396	0.89214
C	0.33954	4.77601	-0.32246
H	0.30026	5.28081	0.64944
O	2.86178	-2.27048	0.68114
C	2.97443	-1.02154	0.39391
O	2.90965	-0.53208	-0.74774

C	3.29029	-0.10625	1.61514
H	4.18267	-0.51982	2.09183
C	2.15523	-0.16851	2.65589
H	2.45449	0.42702	3.52562
H	1.23995	0.27925	2.25413
S	1.87938	-1.88413	3.21579
N	3.56922	1.25910	1.23085
H	2.76604	1.90387	1.08151
C	4.75936	1.63386	0.73390
O	5.77060	0.89033	0.70646
C	4.81705	3.04546	0.19244
H	5.84354	3.28240	-0.09248
H	4.46427	3.76042	0.94304
H	1.37430	-3.98931	-2.22904
H	3.77725	-3.44652	-3.17713
H	-8.44611	-0.34598	-2.38388
H	0.63420	2.71414	-3.41378
H	0.70169	5.49011	-1.06815
H	4.13927	3.13360	-0.66488
Cl	-3.07509	-1.06093	2.95337

^{6}FeEgtBFRe
Charge: 0
Energy: -2367506.8276699

C	-0.52206	5.59335	2.33858
H	-0.37669	5.03998	3.27047
H	0.44256	6.04235	2.06728
N	-1.28033	5.07441	-0.02356
H	-1.14809	6.00598	-0.38930
C	-1.02185	4.66766	1.27991
C	-1.69607	3.99174	-0.73613
H	-1.93452	3.97134	-1.78921
N	-1.72813	2.92463	0.03730
C	-1.30973	3.32588	1.28802
H	-1.21483	2.61226	2.09272
C	7.39302	3.40585	-0.85081
H	6.44505	3.89958	-1.09785
H	7.84835	3.90735	0.01278
N	7.19945	1.98651	-0.60555
H	7.70488	1.31924	-1.16951
C	6.35094	1.47545	0.31173
N	5.70699	2.27697	1.17330
H	4.87734	1.85838	1.62993
H	5.78192	3.27938	1.10617
N	6.18691	0.15325	0.40388
H	6.21498	-0.40795	-0.45902
H	5.36069	-0.10035	0.97948
C	-7.78516	-0.02345	-0.90984
H	-8.43935	0.77812	-1.27701
H	-7.74018	-0.79475	-1.68353
N	-6.14243	1.45353	0.33085
H	-6.82998	1.92851	0.89767
C	-6.40779	0.47047	-0.61475
C	-4.79888	1.67667	0.34798
H	-4.30296	2.39313	0.98592
N	-4.19464	0.89308	-0.51983
C	-5.17779	0.14222	-1.12786
H	-4.92034	-0.57264	-1.89515
C	-2.42265	-2.77440	3.47395
H	-2.36536	-2.48982	4.53316
H	-3.45539	-3.06903	3.26160
N	-0.65055	-1.42552	2.32244
H	0.08600	-2.13669	2.47281
C	-1.99026	-1.66520	2.57082
C	-0.56610	-0.40213	1.44636
H	0.35950	0.03370	1.11248
N	-1.77084	0.04894	1.11309
C	-2.66829	-0.72972	1.82882
H	-3.73371	-0.58665	1.72923
Fe	-2.02522	0.94239	-0.96284
C	-1.79077	-3.31985	-0.75462
C	-2.70907	-2.30411	-0.84378
N	-0.78913	-2.97542	-1.65249
C	-1.11935	-1.77398	-2.19298
N	-2.27603	-1.32761	-1.72581
H	-3.63433	-2.19011	-0.30111
H	-0.49572	-1.24125	-2.89286
H	0.16476	-3.33483	-1.55074
C	-1.75305	-4.55683	0.09913
H	-2.38724	-5.33908	-0.34291
H	-2.20131	-4.30476	1.06585
C	0.63611	-4.08908	0.88350
O	0.57006	-3.81745	2.10583
O	1.38814	-3.53741	0.01216
C	-0.34360	-5.14832	0.33744
H	0.04994	-5.56395	-0.59712
O	1.94648	1.39262	0.81165
C	2.87411	0.54916	0.74787
O	3.78950	0.40605	1.61509
C	2.94934	-0.32145	-0.54250
H	3.67613	0.17494	-1.19612
C	1.59135	-0.43140	-1.25328
H	1.76729	-0.84816	-2.25231
H	0.97132	-1.14524	-0.70729
S	0.69637	1.14364	-1.45316
N	3.43371	-1.67287	-0.30334
H	2.73653	-2.33175	0.08268
C	4.50533	-2.20834	-0.92483
O	5.34253	-1.54364	-1.56910
C	4.66918	-3.70795	-0.74964
H	5.08278	-4.12056	-1.67359
H	3.72465	-4.19876	-0.49993
H	-1.22494	6.41281	2.54121
H	8.06555	3.52092	-1.70215
H	-8.26316	-0.46517	-0.02554
H	-1.76634	-3.64023	3.32867
H	-0.43522	-5.96310	1.06283
H	5.39196	-3.89865	0.05288
F	-2.20539	1.84899	-2.54161

^{6}FeEgtBN$_3$Re
Charge: 0
Energy: -2407897.4816441

C	-1.47193	-4.91480	0.92105
H	-1.60259	-4.58831	1.95847
H	-2.44489	-4.84996	0.41396
N	-0.00402	-4.28971	-1.04000
H	-0.33055	-5.01506	-1.66134
C	-0.45109	-4.05769	0.25168
C	0.87956	-3.31224	-1.36620
H	1.36767	-3.21723	-2.32441
N	1.03737	-2.47751	-0.35824
C	0.21308	-2.92756	0.65236
H	0.11895	-2.38086	1.57871
C	-5.74102	-4.46629	1.75663
H	-4.92827	-4.99285	1.24477
H	-5.44530	-4.27568	2.79819
N	-6.08333	-3.24995	1.03722
H	-7.05582	-2.97796	1.03069
C	-5.18429	-2.25476	0.78874
N	-3.90986	-2.38158	1.12728
H	-3.24127	-1.59991	0.81402
H	-3.59918	-3.15784	1.68821
N	-5.61575	-1.13969	0.19091
H	-6.49378	-1.14130	-0.30732
H	-4.96804	-0.39788	-0.11239
C	7.29918	-0.76243	1.32774
H	7.88631	-1.46737	0.72536
H	7.56130	0.24842	1.00370
N	5.20219	-2.16942	1.49074
H	5.66577	-3.01779	1.78158
C	5.83390	-0.98149	1.15222
C	3.89086	-2.06554	1.15122
H	3.17299	-2.86597	1.24427
N	3.63396	-0.86831	0.65827
C	4.83690	-0.18706	0.64887
H	4.89946	0.80893	0.23838
C	0.07328	1.30106	4.41886
H	-0.93167	1.07414	4.79720
H	0.79011	0.68977	4.97530
N	-0.55649	1.69473	2.00484
H	-1.18207	2.50953	2.09495
C	0.19082	1.02600	2.95628
C	-0.20620	1.22555	0.79317
H	-0.60580	1.63510	-0.11328
N	0.71977	0.28461	0.88897
C	0.97652	0.15069	2.24379
H	1.72849	-0.53671	2.60048
Fe	1.95311	-0.43730	-0.75631
C	1.82151	3.65793	0.23626
C	2.63070	2.56005	0.39533
N	1.44188	3.63194	-1.09859
C	1.98134	2.52046	-1.65903
N	2.70874	1.83760	-0.78506
H	3.10028	2.19802	1.29832
H	1.80930	2.22251	-2.68215
H	0.58440	4.09649	-1.42048
C	1.31601	4.68457	1.21420
H	2.10175	5.42272	1.42829
H	1.10482	4.17223	2.16057
C	-1.11376	4.47009	0.43299
O	-1.80733	4.04307	1.39082
O	-1.22958	4.13447	-0.79085
C	0.04195	5.43866	0.76380
H	0.26554	6.05755	-0.11260
O	-1.66208	-1.39702	-1.33357
C	-2.26558	-0.37308	-0.93397
O	-2.83379	-0.24128	0.19226
C	-2.39915	0.78988	-1.95705
H	-3.07550	0.37902	-2.71617
C	-1.04965	1.15264	-2.62269
H	-1.23895	1.51294	-3.63831
H	-0.58967	1.97691	-2.07310
S	0.13904	-0.23825	-2.71908
N	-2.99682	1.99100	-1.41216
H	-2.38525	2.77817	-1.14144

C	-4.29595	2.04426	-1.04960
O	-5.09872	1.11849	-1.25967
C	-4.70582	3.34100	-0.37298
H	-4.68085	4.16820	-1.09228
H	-4.00285	3.58908	0.43117
H	-1.18055	-5.97304	0.94731
H	-6.61276	-5.12320	1.75982
H	7.61183	-0.87150	2.37454
H	0.27819	2.35433	4.64938
H	-0.26883	6.09912	1.57899
H	-5.72050	3.23431	0.01555
N	3.10003	-1.25008	-2.22440
N	3.96071	-2.06837	-2.01539
N	4.78698	-2.86187	-1.82461

^{6}FeEgtBNCSRe
Charge: 0
Energy: -2613008.3644987

C	-0.58734	4.78201	2.52576
H	0.29783	4.38210	3.02955
H	-0.29827	5.72339	2.03866
N	-2.23802	4.00925	0.76205
H	-2.79510	4.85139	0.74563
C	-1.11734	3.77861	1.55343
C	-2.46777	2.89656	0.01166
H	-3.29475	2.80079	-0.67727
N	-1.56408	1.97042	0.27387
C	-0.71532	2.50737	1.22507
H	0.14148	1.95272	1.57539
C	1.45093	5.45120	-0.78319
H	0.73789	4.61892	-0.82990
H	1.32686	6.00384	0.15361
N	2.82747	4.96965	-0.90337
H	3.19299	4.94851	-1.84531
C	3.31149	4.00755	-0.08223
N	2.71072	3.76875	1.10065
H	2.82969	2.77968	1.39968
H	1.71575	3.96366	1.08342
N	4.44537	3.37634	-0.39880
H	4.86020	3.56293	-1.30158
H	4.67554	2.42305	-0.05085
C	-6.75306	-2.08154	0.86898
H	-7.52674	-1.41542	0.46672
H	-6.67636	-2.94135	0.19816
N	-5.20464	-0.29077	1.76419
H	-5.89425	0.16493	2.34384
C	-5.43255	-1.39274	0.95247
C	-3.92903	0.13307	1.55942
H	-3.49580	0.99799	2.03816
N	-3.31988	-0.64363	0.68492
C	-4.24421	-1.59576	0.30046
H	-3.99184	-2.32811	-0.45072
C	1.03730	-1.40370	4.40531
H	2.00262	-0.94101	4.64586
H	0.27267	-0.93619	5.03294
N	1.45447	-1.76818	1.94208
H	2.27705	-2.38911	1.96506
C	0.69402	-1.23162	2.96333
C	0.89212	-1.42020	0.77371
H	1.27808	-1.75224	-0.17075
N	-0.19777	-0.69038	0.96140
C	-0.33363	-0.57050	2.33459
H	-1.15595	-0.02425	2.77002
Fe	-1.55279	-0.14565	-0.61138
C	-0.19185	-4.17675	-0.46730
C	-1.26256	-3.37473	-0.15753
N	0.20664	-3.76575	-1.73248
C	-0.58501	-2.72560	-2.09901
N	-1.48961	-2.45427	-1.16931
H	-1.84374	-3.34672	0.75267
H	-0.46492	-2.17741	-3.02110
H	1.16638	-3.89661	-2.05762
C	0.54361	-5.22545	0.32162
H	0.04460	-6.19949	0.21942
H	0.48199	-4.95073	1.38095
C	2.79278	-4.05044	0.03175
O	3.21809	-3.70420	1.16309
O	2.85971	-3.36929	-1.04346
C	2.03604	-5.39134	-0.05967
H	2.12113	-5.79681	-1.07455
O	1.42204	2.03839	-0.71457
C	2.24213	1.17545	-0.26645
O	2.63260	1.08230	0.92112
C	2.90414	0.30940	-1.37187
H	3.48622	1.04946	-1.93595
C	1.86802	-0.32296	-2.33022
H	2.28595	-0.36427	-3.34016
H	1.67116	-1.35237	-2.02703
S	0.27930	0.60121	-2.40536
N	3.81738	-0.68824	-0.86328
H	3.52521	-1.67953	-0.85341
C	4.97877	-0.34306	-0.26987
O	5.40613	0.82569	-0.21685
C	5.77663	-1.50220	0.29741
H	6.46756	-1.11639	1.04981
H	6.36249	-1.97232	-0.50214
H	-1.32115	5.03107	3.30350
H	1.25939	6.14101	-1.60675
H	-7.09275	-2.44655	1.84695
H	1.10153	-2.46317	4.68333
H	2.48654	-6.10804	0.63321
H	5.12018	-2.26526	0.73014
N	-2.94659	0.41104	-2.02281
C	-4.04251	0.86823	-2.05790
S	-5.52794	1.53860	-2.04419

^{6}FeEgtBOHRe
Charge: 0
Energy: -2352425.8598642

C	0.74144	-3.08891	-2.20657
H	0.14111	-3.05336	-3.12053
H	1.43179	-2.23660	-2.20495
N	0.35371	-2.88883	0.27581
H	1.34308	-2.69892	0.49402
C	-0.14574	-3.01844	-1.00861
C	-0.69121	-2.75451	1.12468
H	-0.59585	-2.56579	2.18493
N	-1.84990	-2.80338	0.46373
C	-1.50878	-2.97736	-0.86697
H	-2.26263	-3.00431	-1.64105
C	4.55099	-3.82057	-1.39281
H	3.51988	-3.47871	-1.25615
H	4.86932	-3.67347	-2.42805
N	5.45395	-3.09677	-0.49842
H	5.39045	-3.37999	0.47164
C	5.69227	-1.77923	-0.66066
N	5.27934	-1.13152	-1.76540
H	5.40776	-0.11675	-1.70091
H	4.33771	-1.35622	-2.07895
N	6.43546	-1.10909	0.22941
H	6.76764	-1.57550	1.06087
H	6.28179	-0.08880	0.24709
C	-7.73365	-0.56117	-1.88582
H	-8.64643	-0.97180	-1.43572
H	-7.81070	0.52903	-1.85695
N	-6.13839	-2.32979	-1.02353
H	-6.64568	-3.12264	-1.38976
C	-6.50798	-0.99850	-1.15490
C	-4.98553	-2.38820	-0.30597
H	-4.45987	-3.29568	-0.04660
N	-4.59332	-1.17234	0.02606
C	-5.52944	-0.30084	-0.49295
H	-5.43550	0.76470	-0.35047
C	-0.95780	2.09276	-3.48488
H	-0.42326	1.54520	-4.27234
H	-1.94226	2.36826	-3.87562
N	-0.02283	0.95090	-1.44728
H	0.92873	1.28917	-1.55985
C	-1.10479	1.27625	-2.24396
C	-0.47219	0.25769	-0.38324
H	0.16348	-0.12814	0.39408
N	-1.78686	0.09971	-0.43994
C	-2.19100	0.72532	-1.60597
H	-3.23103	0.74925	-1.89557
Fe	-2.81023	-0.87820	1.23154
C	-2.16777	3.17697	0.78588
C	-3.32752	2.46526	0.99614
N	-1.26061	2.64520	1.68040
C	-1.87089	1.63907	2.34835
N	-3.13622	1.48958	1.95536
H	-4.27925	2.58592	0.49655
H	-1.37459	0.99981	3.06346
H	-0.25143	2.87485	1.65047
C	-1.80846	4.21784	-0.23981
H	-2.55975	5.01819	-0.21622
H	-1.87834	3.75861	-1.23460
C	0.73855	3.83127	-0.32193
O	1.11758	3.61036	-1.49136
O	1.19811	3.26219	0.73299
C	-0.40465	4.84516	-0.09541
H	-0.29826	5.29681	0.89730
O	2.93743	-1.87983	0.53360
C	2.89957	-0.69547	0.05070
O	2.58384	-0.38814	-1.11650
C	3.34181	0.40226	1.06078
H	4.32721	0.10051	1.42519
C	2.37883	0.41113	2.26336
H	2.73676	1.14492	2.99427
H	1.38089	0.72739	1.94322
S	2.34024	-1.22712	3.07156
N	3.43829	1.71595	0.46710
H	2.58876	2.32346	0.49435
C	4.47625	2.08839	-0.28982
O	5.50626	1.38388	-0.45909
C	4.36024	3.45181	-0.93617
H	5.16887	3.57361	-1.65903

H	4.44522	4.23266	-0.17089
H	1.33292	-4.01451	-2.22905
H	4.62035	-4.88478	-1.15917
H	-7.71306	-0.86707	-2.93967
H	-0.38860	3.00216	-3.26144
H	-0.30848	5.63386	-0.84794
H	3.38101	3.56813	-1.41434
O	-2.50385	-1.23743	3.02820
H	-2.99626	-0.68998	3.65684

^{5}FeEgtBBrP
Charge: 0
Energy: -3967013.2587179

C	4.19592	-5.92751	-1.12337
H	4.03482	-6.23876	-0.08735
H	3.58654	-6.57739	-1.76516
N	3.92772	-3.80893	-2.48773
H	4.25764	-4.19492	-3.36061
C	3.83357	-4.48792	-1.27939
C	3.52860	-2.52501	-2.29413
H	3.52325	-1.75292	-3.04898
N	3.18375	-2.33993	-1.03469
C	3.36732	-3.54929	-0.39450
H	3.14169	-3.65998	0.65549
C	-8.45559	-4.07848	0.84401
H	-7.74079	-4.88563	0.63048
H	-8.42475	-3.84609	1.91275
N	-8.18976	-2.87465	0.07174
H	-8.64287	-2.78500	-0.82600
C	-7.13497	-2.04987	0.30850
N	-6.26969	-2.32334	1.28534
H	-5.42053	-1.68424	1.34385
H	-6.11921	-3.29368	1.52369
N	-7.02016	-0.93319	-0.40880
H	-7.76992	-0.62764	-1.01100
H	-6.17564	-0.34209	-0.42755
C	6.41075	1.54953	3.50963
H	7.29888	0.94840	3.74467
H	6.72794	2.37016	2.86069
N	4.75860	-0.36818	3.39117
H	4.95992	-0.74455	4.30621
C	5.35949	0.74589	2.81913
C	3.85778	-0.86975	2.50245
H	3.23050	-1.72743	2.68946
N	3.84578	-0.14454	1.40108
C	4.77531	0.86212	1.58354
H	4.96462	1.57403	0.79367
C	-1.88844	-1.24601	3.29341
H	-2.11454	-2.09126	3.95656
H	-1.60822	-0.39311	3.91853
N	-0.85856	-2.57403	1.39916
H	-1.75500	-2.91632	1.03967
C	-0.77246	-1.56761	2.35398
C	0.29790	-2.56022	0.68347
H	0.47818	-3.18764	-0.17653
N	1.13393	-1.63747	1.13080
C	0.47373	-1.01796	2.18021
H	0.92629	-0.19178	2.70818
Fe	2.53200	-0.36197	-0.38454
O	0.97024	-0.59218	-1.94167
C	0.23146	3.19638	0.72045
C	1.30153	2.36015	0.99128
N	-0.44916	2.69444	-0.37392
C	0.25144	1.60261	-0.69973
N	1.29907	1.32870	0.08227
H	2.07685	2.43791	1.74164
H	-1.29140	4.02192	-1.04078
C	-0.18199	4.48331	1.36969
H	0.52238	4.69564	2.18200
H	-1.17094	4.38217	1.83953
C	-1.46829	5.88060	-0.42564
O	-2.10616	6.91162	-0.42116
O	-1.84691	4.84328	-1.19381
C	-0.19900	5.70709	0.41349
H	0.66319	5.64195	-0.26320
O	-3.34538	-2.35121	-0.01328
C	-3.59672	-1.12695	0.09174
O	-4.33253	-0.57826	0.96834
C	-2.92787	-0.17491	-0.96326
H	-3.33850	-0.45734	-1.93930
C	-1.44398	-0.50460	-0.89530
H	-1.06919	-0.38359	0.12134
H	-1.31680	-1.54153	-1.20224
S	-0.22084	0.40354	-1.94385
N	-3.20281	1.23207	-0.74182
H	-2.46674	1.83143	-0.37426
C	-4.45225	1.72788	-0.90416
O	-5.38246	1.03188	-1.34168
C	-4.65295	3.17598	-0.51068
H	-5.58666	3.53191	-0.94978
H	-3.82530	3.81907	-0.82435
H	5.25000	-6.11457	-1.36657
H	-9.45914	-4.43308	0.60059
H	6.04577	1.98708	4.44819
H	-2.80474	-0.98506	2.75059
H	-0.10230	6.63102	0.98857
H	-4.73671	3.23783	0.58185
Br	4.22645	0.89684	-1.91657

^{3}FeEgtBClP
Charge: 0
Energy: -2640465.7121098

C	-4.45084	5.48546	1.24578
H	-4.65411	5.10814	2.25185
H	-3.75441	6.32894	1.34068
N	-3.52863	4.56761	-0.92852
H	-3.61794	5.42223	-1.45814
C	-3.89087	4.39040	0.40041
C	-3.06433	3.38749	-1.41509
H	-2.74457	3.20487	-2.42884
N	-3.10351	2.46691	-0.46958
C	-3.61391	3.07335	0.66168
H	-3.74255	2.51493	1.57536
C	8.38422	3.60355	-0.42292
H	7.56857	4.27383	-0.12943
H	9.13786	3.58108	0.37604
N	7.86883	2.28035	-0.73169
H	8.20668	1.80634	-1.55627
C	7.07219	1.55873	0.08830
N	6.75605	2.00461	1.30786
H	5.97834	1.51010	1.79052
H	7.19298	2.81757	1.71067
N	6.61003	0.36947	-0.31006
H	6.34387	0.22639	-1.28820
H	5.89151	-0.01335	0.33676
C	-7.62164	-1.94556	0.26033
H	-8.42298	-1.41026	0.78650
H	-7.86942	-1.95218	-0.80448
N	-5.69916	-1.15090	1.70637
H	-6.08464	-1.46424	2.58560
C	-6.29136	-1.29791	0.45877
C	-4.50089	-0.52546	1.53769
H	-3.81657	-0.29965	2.34135
N	-4.29438	-0.26480	0.26157
C	-5.39887	-0.73748	-0.42076
H	-5.45091	-0.63093	-1.49462
C	0.91037	-0.99916	3.58711
H	0.59496	-1.02771	4.63849
H	0.97001	-2.02570	3.20550
N	0.13215	1.18136	2.57552
H	1.03200	1.63983	2.72719
C	-0.02297	-0.18738	2.74884
C	-0.78417	1.59648	1.66376
H	-0.84057	2.60272	1.27823
N	-1.54796	0.59157	1.26263
C	-1.08650	-0.52707	1.94794
H	-1.50140	-1.50736	1.77008
Fe	-2.49808	0.60004	-0.74603
O	-0.49724	1.30140	-1.56258
C	-1.00458	-3.30407	-0.69210
C	-2.08501	-2.44954	-0.67729
N	0.06758	-2.54239	-1.13006
C	-0.38187	-1.27763	-1.28986
N	-1.67718	-1.18351	-1.03275
H	-3.11384	-2.63918	-0.41393
H	1.05240	-2.82173	-0.91249
C	-0.86134	-4.72922	-0.22700
H	-1.30156	-5.41621	-0.96272
H	-1.44812	-4.82924	0.69292
C	1.31015	-4.08952	0.94409
O	0.95825	-3.96820	2.12393
O	2.15209	-3.36012	0.29220
C	0.59426	-5.15470	0.07357
H	1.14800	-5.29973	-0.86008
O	2.89079	1.55020	1.90666
C	3.58072	0.72813	1.27072
O	4.72372	0.28211	1.60382
C	3.03158	0.23666	-0.12961
H	3.44059	0.92339	-0.88024
C	1.51518	0.31981	-0.08349
H	1.11136	-0.42875	0.59850
H	1.22417	1.30870	0.26017
S	0.57381	0.19549	-1.67931
N	3.46912	-1.09471	-0.49972
H	3.07971	-1.88885	0.03236
C	4.29355	-1.34688	-1.54052
O	4.81767	-0.45369	-2.23328
C	4.57821	-2.81424	-1.80575
H	4.50058	-2.99092	-2.88273
H	3.90394	-3.47757	-1.25877
H	-5.39320	5.87599	0.84012
H	8.85006	4.01323	-1.32078
H	-7.62953	-2.98577	0.61153
H	1.91522	-0.56271	3.55102
H	0.56623	-6.10942	0.60864
H	5.61310	-3.02881	-1.51348

Cl	-3.48042	0.56265	-2.92433

^{5}FeEgtBFP
Charge: 0
Energy: -2414353.9124392

C	-4.54654	5.72548	1.37582
H	-4.34143	5.50719	2.42771
H	-4.02078	6.65520	1.12080
N	-4.24283	4.55854	-0.85303
H	-4.65614	5.28634	-1.41758
C	-4.10261	4.58008	0.52773
C	-3.74476	3.38044	-1.31775
H	-3.75529	3.04421	-2.34389
N	-3.28623	2.65063	-0.31910
C	-3.50812	3.38058	0.83085
H	-3.23737	2.99147	1.80133
C	8.06032	3.95580	-0.70830
H	7.22005	4.57747	-0.37983
H	8.85938	4.00284	0.04419
N	7.61698	2.59452	-0.95778
H	7.94142	2.12043	-1.78765
C	6.90230	1.84992	-0.08449
N	6.61637	2.31173	1.13732
H	5.91126	1.77452	1.67910
H	7.05555	3.13519	1.51568
N	6.48843	0.62843	-0.43148
H	6.18770	0.44094	-1.39199
H	5.83167	0.21874	0.26533
C	-7.74123	-1.92220	-0.53194
H	-8.57148	-1.45075	0.01049
H	-7.90667	-1.75847	-1.60027
N	-5.92496	-1.41719	1.15973
H	-6.39011	-1.84160	1.94907
C	-6.41864	-1.35302	-0.13771
C	-4.70542	-0.80783	1.18258
H	-4.08732	-0.71468	2.06323
N	-4.39520	-0.36500	-0.01738
C	-5.44796	-0.69278	-0.84831
H	-5.39834	-0.41045	-1.88975
C	0.75975	-1.24381	3.56503
H	0.40895	-1.30509	4.60384
H	0.85229	-2.26023	3.16520
N	0.02609	0.96462	2.59959
H	0.93219	1.40732	2.76927
C	-0.14914	-0.40624	2.72414
C	-0.87695	1.42128	1.69376
H	-0.90311	2.43897	1.33464
N	-1.65561	0.44507	1.25342
C	-1.21306	-0.70113	1.90200
H	-1.65034	-1.66588	1.69127
Fe	-2.61252	0.60033	-0.92193
O	-0.52445	1.23738	-1.61559
C	-0.86155	-3.37825	-0.67147
C	-1.98982	-2.61153	-0.87340
N	0.20434	-2.55300	-0.99248
C	-0.31031	-1.34714	-1.31262
N	-1.63024	-1.34128	-1.26746
H	-3.03032	-2.87037	-0.74148
H	1.18730	-2.78813	-0.69804
C	-0.67856	-4.76918	-0.11885
H	-1.19046	-5.49197	-0.76830
H	-1.17506	-4.81454	0.85850
C	1.52288	-4.19637	1.01907
O	1.25393	-4.23149	2.22466
O	2.28811	-3.35439	0.40682
C	0.79113	-5.19390	0.08267
H	1.30603	-5.25591	-0.88250
O	2.77581	1.45268	2.04253
C	3.53295	0.76244	1.33267
O	4.73720	0.44724	1.59495
C	2.99977	0.28137	-0.07562
H	3.40569	0.97908	-0.81744
C	1.48033	0.33905	-0.05815
H	1.07460	-0.40790	0.62447
H	1.16108	1.32682	0.26490
S	0.58991	0.17410	-1.67848
N	3.47465	-1.03782	-0.44946
H	3.15251	-1.83884	0.11348
C	4.24755	-1.27249	-1.53452
O	4.69047	-0.36925	-2.26914
C	4.58176	-2.72987	-1.79452
H	4.46736	-2.92321	-2.86523
H	3.95818	-3.41197	-1.21170
H	-5.62357	5.91653	1.27972
H	8.44426	4.37296	-1.64086
H	-7.79584	-3.00337	-0.34837
H	1.76218	-0.80061	3.57838
H	0.79621	-6.18663	0.54378
H	5.63567	-2.89792	-1.54248
F	-3.51628	0.85244	-2.51892

^{5}FeEgtBN$_3$P
Charge: 0
Energy: -2454745.3412182

C	5.61662	-5.06902	-0.64878
H	6.17006	-4.89665	0.27864
H	5.19634	-6.08241	-0.60486
N	3.68974	-3.99316	-1.88746
H	3.75658	-4.56849	-2.71453
C	4.55898	-4.02813	-0.80595
C	2.88667	-2.90695	-1.75670
H	2.14791	-2.59234	-2.47806
N	3.16224	-2.26252	-0.63628
C	4.20178	-2.94984	-0.03888
H	4.63025	-2.60510	0.89045
C	-7.57737	-4.79794	1.51258
H	-6.67554	-5.42005	1.60018
H	-7.75924	-4.29381	2.46649
N	-7.47768	-3.81227	0.44720
H	-7.79849	-4.08292	-0.47103
C	-6.67848	-2.71420	0.51523
N	-5.92869	-2.48947	1.59352
H	-5.24707	-1.67190	1.52831
H	-5.61039	-3.29275	2.11761
N	-6.71387	-1.83491	-0.48614
H	-7.41084	-1.90808	-1.21197
H	-6.02493	-1.08176	-0.61823
C	7.40641	1.73744	2.33334
H	8.09970	1.02183	2.79467
H	7.86016	2.08605	1.40173
N	5.25952	0.58475	3.02750
H	5.46520	0.55518	4.01561
C	6.07777	1.12235	2.04206
C	4.12964	0.11007	2.43183
H	3.31274	-0.35874	2.95890
N	4.17848	0.31223	1.12988
C	5.38269	0.93866	0.87348
H	5.64517	1.19703	-0.14194
C	-1.76407	-0.07223	3.37955
H	-1.91205	-0.68451	4.27866
H	-1.58736	0.95866	3.69984
N	-0.59559	-1.79741	1.94770
H	-1.45163	-2.30934	1.71699
C	-0.60764	-0.55407	2.56522
C	0.55358	-1.88603	1.22438
H	0.80132	-2.71970	0.58504
N	1.29375	-0.79925	1.35806
C	0.57958	0.03567	2.20318
H	0.94516	1.02282	2.44663
Fe	2.68098	-0.11283	-0.47760
O	0.97605	-0.57321	-1.89190
C	0.49236	3.63300	0.14135
C	1.64768	2.90141	0.37618
N	-0.27754	2.93497	-0.76358
C	0.43662	1.83844	-1.01689
N	1.59770	1.74094	-0.36062
H	2.50339	3.12529	0.99914
H	-1.69769	3.62784	-0.99389
C	0.01463	4.93038	0.73607
H	0.88902	5.53889	0.99649
H	-0.51383	4.74560	1.68360
C	-2.36646	5.31111	-0.25415
O	-3.28739	5.99071	0.14763
O	-2.58126	4.10946	-0.81515
C	-0.90594	5.77539	-0.18124
H	-0.48701	5.78973	-1.19558
O	-2.98875	-2.21796	0.45326
C	-3.44859	-1.06624	0.27355
O	-4.34774	-0.49114	0.96131
C	-2.85270	-0.23956	-0.92585
H	-3.06021	-0.82124	-1.82967
C	-1.35961	-0.17699	-0.66094
H	-1.14332	0.38134	0.25122
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S	-0.18786	0.45051	-1.95987
N	-3.46849	1.06582	-1.08299
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C	-4.77229	1.15450	-1.44943
O	-5.40868	0.16098	-1.83642
C	-5.41883	2.51938	-1.36002
H	-6.06224	2.65788	-2.23316
H	-4.70136	3.33793	-1.27822
H	6.33731	-5.04111	-1.47613
H	-8.42769	-5.45024	1.30391
H	7.32187	2.60067	3.00654
H	-2.69636	-0.09413	2.80099
H	-0.94094	6.80305	0.18729
H	-6.06072	2.52759	-0.47052
N	4.06412	0.33558	-1.91179
N	4.48975	-0.46929	-2.70188
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^{5}FeEgtBNCSP
Charge: 0
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C	2.96714	-2.70109	-1.59565
H	2.19046	-2.45679	-2.30436
N	2.91298	-2.43540	-0.29719
C	4.15195	-2.79919	0.20885
H	4.38908	-2.65837	1.25277
C	-7.74788	-4.93090	1.17030
H	-6.83112	-5.51393	1.33593
H	-8.02810	-4.43014	2.10192
N	-7.60223	-3.94741	0.10795
H	-7.84152	-4.23389	-0.83011
C	-6.85710	-2.81727	0.23022
N	-6.20719	-2.55580	1.36421
H	-5.55173	-1.71690	1.34486
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C	7.26266	1.13237	2.76030
H	7.82070	0.32536	3.25279
H	7.79808	1.39563	1.84421
N	4.94404	0.31450	3.37593
H	5.10686	0.25768	4.37087
C	5.86798	0.72166	2.42248
C	3.77920	0.01076	2.73967
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H	0.57685	1.05781	2.52229
Fe	2.40347	-0.19193	-0.17003
O	0.83359	-0.60870	-1.70525
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C	1.45992	2.90033	0.51082
N	-0.40577	2.94241	-0.72320
C	0.29802	1.82900	-0.91901
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H	-1.86715	3.55366	-0.93197
C	-0.16264	4.95675	0.76058
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C	-3.68225	-1.07516	0.21411
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C	-4.93475	1.10010	-1.63198
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H	-4.91175	3.28134	-1.42418
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H	-8.55030	-5.61947	0.89835
H	7.28504	2.00677	3.42373
H	-3.05777	-0.09256	2.76327
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H	3.31331	-2.78631	1.15933
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H	-3.93451	-3.53125	0.58816
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H	5.38289	0.41263	2.77764
C	6.19927	-0.58542	1.06413
C	4.05703	0.05251	1.17393
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H	-2.62073	2.07735	3.92748
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N	1.13165	0.88646	2.23071
C	0.21091	1.91067	2.36914
H	0.48292	2.95248	2.28843
Fe	2.85369	-0.92440	-1.67933
O	0.72217	-0.91921	-2.69465
C	1.72421	3.28552	-0.82247
C	2.71730	2.32665	-0.90612
N	0.63480	2.75494	-1.48031
C	0.98639	1.52220	-1.87358
N	2.23090	1.20564	-1.55228
H	3.73071	2.34964	-0.53561
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H	-2.75628	-0.57491	-1.59620
C	-0.88340	0.02816	-0.67889
H	-0.57992	0.86949	-0.05129
H	-0.35853	-0.85558	-0.32558
S	-0.18300	0.29051	-2.39238
N	-3.01995	1.13910	-0.43703
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C	-4.32222	1.39664	-0.63587
O	-5.14126	0.55667	-1.07247
C	-4.77265	2.79668	-0.27679
H	-5.52457	3.12294	-0.99970
H	-3.93782	3.50145	-0.23956
H	0.88196	-5.27455	2.72277
H	-4.79749	-2.95720	-3.04296
H	8.11269	0.19157	1.69385
H	-3.15904	1.48137	2.34653
H	0.25865	6.25473	0.23111
H	-5.24582	2.76788	0.71240
O	4.13469	-1.46072	-2.90007
H	3.83998	-1.71309	-3.78699

[5]FeEgtBOHP
Charge: 0
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C	1.13283	-4.20785	2.77768
H	2.07600	-4.11220	3.32286

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