ELECTRONIC SUPPLEMENTARY INFORMATION

Factors Driving the Ni/Cu Cooperative Asymmetric Propargylation of Aldimine Esters

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1. Computational Details

Theoretical calculations were performed at DFT level of theory using Gaussian16 software.[1] The structures of all the intermediates and transition states were optimized in dichloromethane solvent (DCM, ε= 8.93) with the SMD continuum model[2] using the B3LYP functional[3] combined with the Grimme's D3 correction for dispersion.[4] Basis set BS1 was used for the optimizations. BS1 includes the 6-31G(d,p) basis set for the main group elements,[5] and the scalar relativistic Stuttgart-Dresden SDD pseudopotential and its associated double-ζ basis set,[6] complemented with a set of *f* polarization functions,[7] for the Ni and Cu atoms. Frequency calculations were carried out for all the optimized geometries in order to characterize the stationary points as either minima or transition states. It was confirmed that transition states connect with the corresponding intermediates by usual intrinsic reaction coordinate (IRC) calculations and subsequent optimization to minima.

Gibbs energies in DCM were calculated at 298.15 K adding to the potential energies in DCM, obtained with single point calculations at using an extended basis set (BS2), the thermal and entropic corrections obtained with BS1. BS2 consists in the *def2*-TZVP basis set for the main group elements[7] and the quadruple-ζ *def2*-QZVP basis set for Ni and Cu.[8] The final energies given are relative *qh*-Gibbs (quasi-rigid-rotor-harmonic-oscillator).[9] energies in solution at 298.15 K and 1M[10] obtained with a frequency cut-off of 100 cm^{-1}.[11] A correction of 1.9 kcal mol^{-1} was applied to all Gibbs values to change the standard state from the gas phase (1 atm) to solution (1 M) at 298.15 K.[9]

2. Coodination and conformational landscape

2.1 Coordination modes and conformational analysys

The coordination mode and conformational landscape of $[Ni^0(\mathbf{L_1})(\mathbf{S_1})]$ and $[Cu^I(\mathbf{L_2})(\mathbf{S_2})]^+$ were explored and the results are gathered in Table S1. The preferential coordination mode of a $[Ni^0(\mathbf{L_1})(\mathbf{S_1})]$ square planar complex is that wuth η^2 coordination of S_1. $\mathbf{S_1}$-κO and $\mathbf{S_1}$-κO' coordination shown relative ΔG_{DCM} of 35.0 and 37.6 kcal·mol^{-1}, respectively. $[Cu^I(\mathbf{L_2})(\mathbf{S_2})]^+$ displays two possible coordination isomers, *SS*-15-A and *SS*-15-C with relative ΔG_{DCM} of 1.6 kcal·mol^{-1}. Moroever, *SS*-15-A have an additional low energy isomer with $\mathbf{S_1}$-κN,O' at 1.8 kcal·mol^{-1} (Fig. S1). The same conformational isomer is hindered for the *SS*-15-C isomer due to steric clashes between the benzyl and the $FeCp_2$ groups.

Table S1. DFT (B3LYP-D3 in DCM) evaluation of coordination modes and conformational landscape of the active co-catalyst upon coordination of the respective substrates.[a]

Species	ΔE_{DCM}	qh-ΔG_{DCM}
$[Ni((R)\text{-}\mathbf{L_1})(\eta^2\text{-}\mathbf{S_1})]$	0.0	0.0
$[Ni((R)\text{-}\mathbf{L_1})(\kappa O\text{-}\mathbf{S_1})$	35.0	35.0
$[Ni((R)\text{-}\mathbf{L_1})(\kappa O'\text{-}\mathbf{S_1})]$	38.3	37.6
$[Ni((R)\text{-}\mathbf{L_1})(\eta^2\text{-}\mathbf{S_2})]$	18.1	18.1
SS-15-A-$[Cu((R,S,S_P)\text{-}\mathbf{L_2})(\kappa N,O\text{-}\mathbf{S_2})]^+$	0.0	0.0
SS-15-A-$[Cu((R,S,S_P)\text{-}\mathbf{L_2})(\kappa N,O'\text{-}\mathbf{S_2})]^+$	-0.6	1.8
SS-15-C-$[Cu((R,S,S_P)\text{-}\mathbf{L_2})(\kappa N,O\text{-}\mathbf{S_2})]^+$	0.8	1.6
SS-15-C-$[Cu((R,S,S_P)\text{-}\mathbf{L_2})(\kappa N,O'\text{-}\mathbf{S_2})]^+$	--[b]	--[b]
SS-15-A-$[Cu((R,S,S_P)\text{-}\mathbf{L_2})(\kappa N,O\text{-}\mathbf{S_1})]^+$	6.0	6.3

[a] *Simulations at B3LYP-D3, BS2, smd=DCM. Energies in kcal·mol^{-1}, 298.15 K.* [b] *hindered by steric clashes with FeCp$_2$*

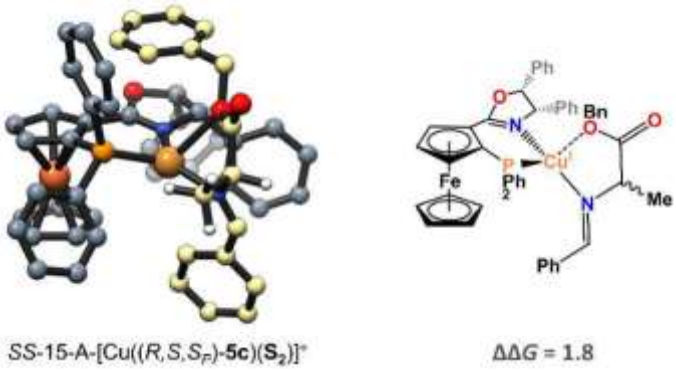


Fig. S1. Optimized geometries for activated co-catalysts *SS*-15-A-[Cu((*R,S,S$_P$*)-**L$_2$**)(κN,O'-**S$_2$**)]$^+$. Hydrogen atoms have been omitted for clarity.

3. Gibbs Energy Profiles

3.1 Nickel cycle

After **TS$_{I\text{-}II}$**, intermediate **II** can evolve toward intermediate **II'**, at 3.8 kcal·mol^{-1}, in which the η^1-**S$_1$** propargylic moiety and $MeOCO_2^-$ coordinate in the equatorial plane. Via **TS$_{II'\text{-}III'}$** (4.6 kcal·mol^{-1}) decarboxylation yields [Ni^{II}(**L$_1$**)(propargyl)(MeO)] at 3.7 kcal·mol^{-1} (see Figure S2).

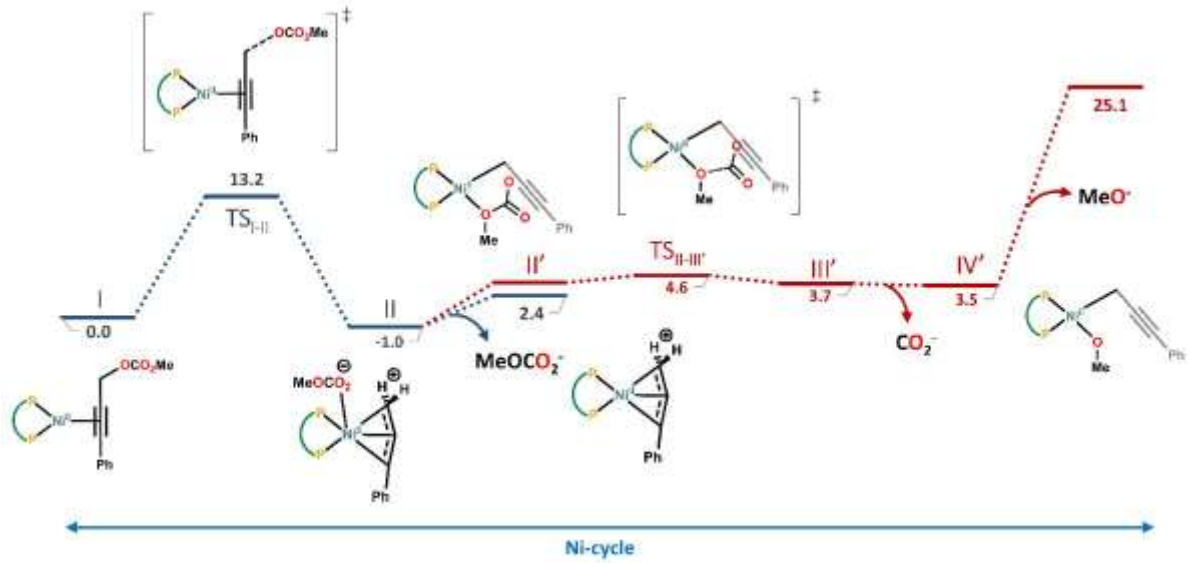


Fig. S2. DFT computed mechanism (B3LYP-D3 in CH_2Cl_2) of the Ni-based activation cycle of propargylic carbonate **S$_1$**. The numbers are relative Gibbs energies in kcal mol^{-1}, taking as zero-energy the separated co-catalyst and substrate **S$_1$**.

3.1 Efficiency of the $MeCO_2^-$ O-groups toward proton abstraction.

We investigated the efficiency of the two possible O-groups of methyl carbonate toward the base-assisted C-H activation. Transition states involving the three groups are depicted in Fig. S4 along with the associated Gibbs energy barriers. As expected the energy follows the basicity order: O-CO_2^- < O-ester. It must be highlighted that the O-ester mediated deprotonation leads to the formation od MeOH and CO_2.

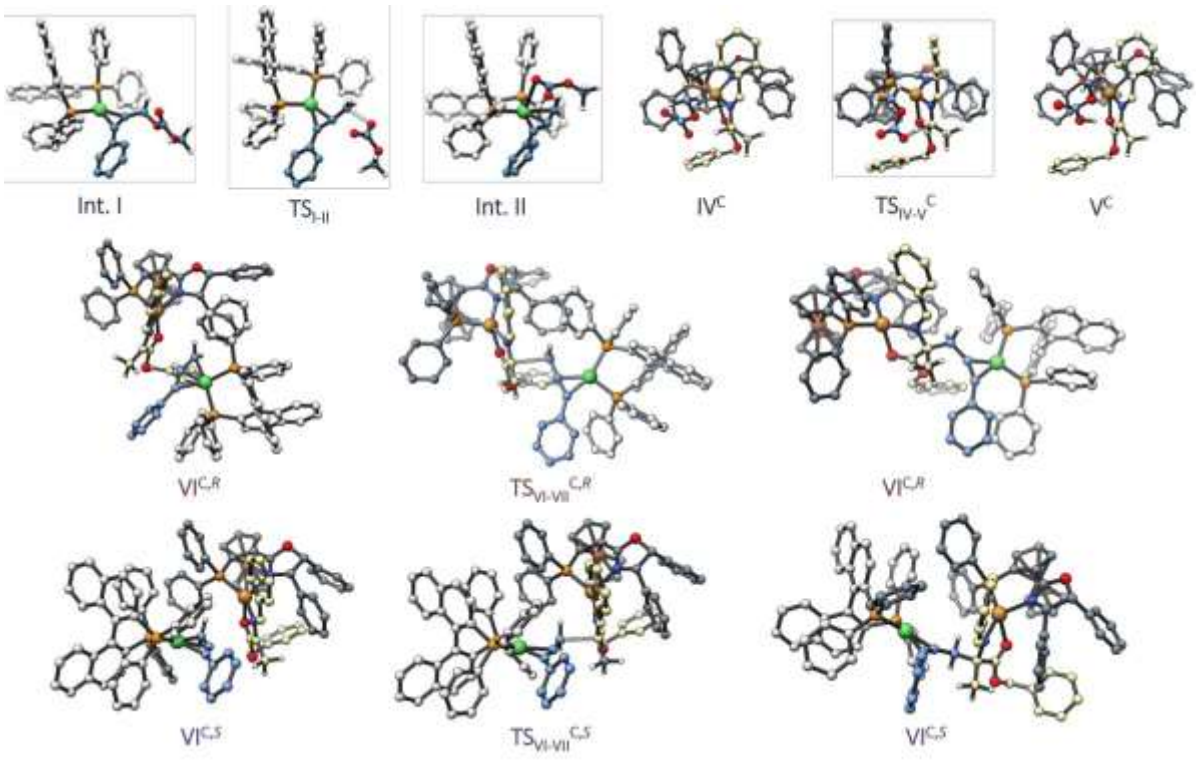


Fig. S3. DFT optimized geometry (B3LYP-D3 in CH_2Cl_2) of the complete interemdiates and transition states shown in Fig. 3 of the main text. Hydrogen atoms have been omitted for clarity.

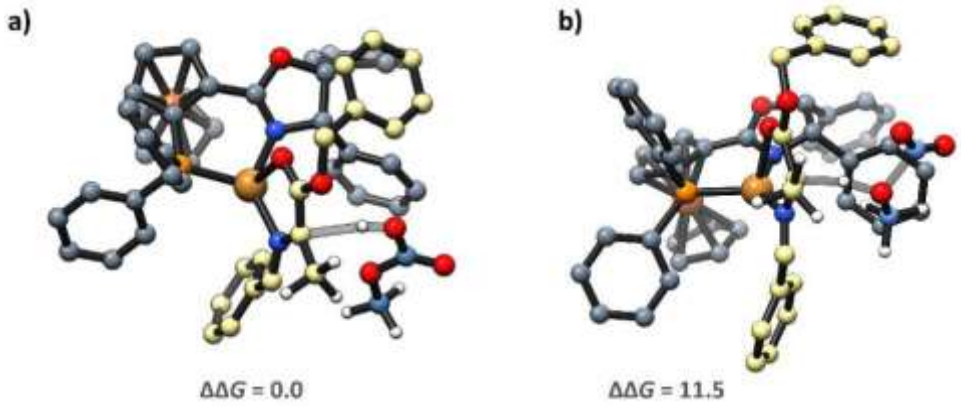


Fig. S4. DFT optimized geometry (B3LYP-D3 in CH_2Cl_2) of the $MeCO_2^-$ mediated C(sp^3) deprotonation: a) O-CO_2^-; b) O-ester. The numbers are relative Gibbs energies in kcal mol^{-1}. Hydrogen atoms have been omitted for clarity.

3.2 Alternative copper cycle (*SS*-15-A-[Cu((*R,S,S*$_P$)-L$_2$)(κN,O'-S$_2$)]$^+$)

TS$_{II\text{-}III}$^{A}, computed considering the *SS*-15-A isomer of the copper co-catalyst, resulted higher by more than 4 kcal·mol^{-1} than the analogous **TS$_{II\text{-}III}$**^{C} (8.0 kcal·mol^{-1}). For sake of completeness, the anticlockwise pathways was computed. The selectivity is reverted giving an ee 81% toward the (*R*) isomer, Fig. S3 and Table S2.

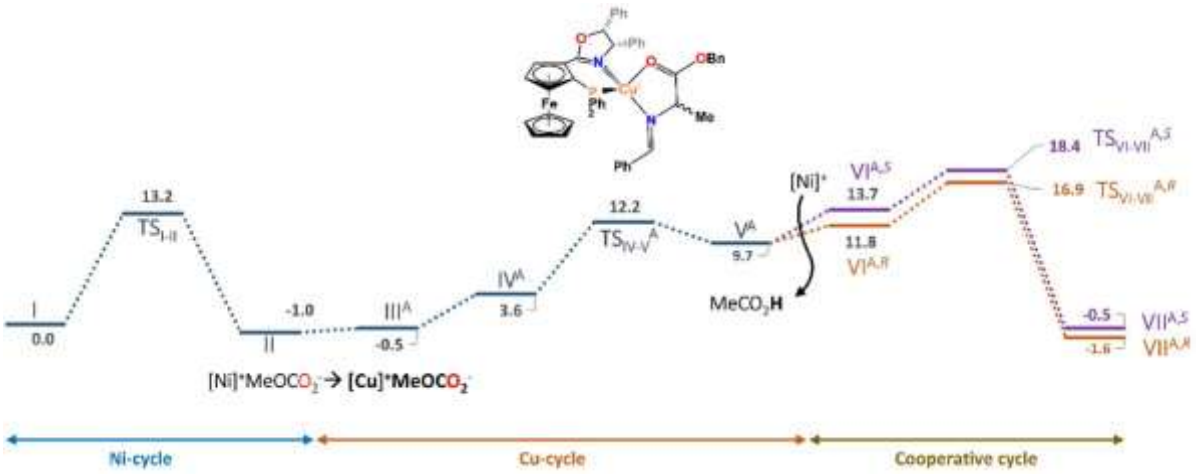
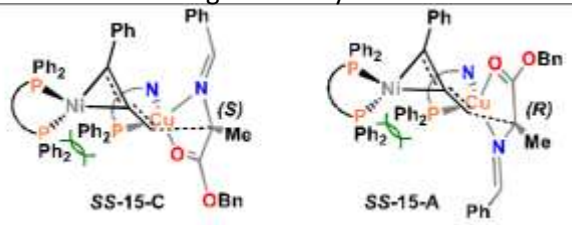


Fig. S5. DFT computed mechanism (B3LYP-D3 in CH_2Cl_2) for the propargylation of aldimine ester **S$_2$** considering the independent activation of the substrates using *SS*-15-A-[Cu((*R,S,S*$_P$)-L$_2$)(κN,O'-S$_2$)]$^+$ isomer. The numbers are relative Gibbs energies in kcal mol^{-1}, taking as zero-energy the separated co-catalysts and substrates **S$_1$** and **S$_2$**.

Table S2. DFT (B3LYP-D3 in DCM solvent) energy decomposition in interaction and distortion contributions for the enantiodeterming cooperative C-C coupling TSs. Scheme of the more stable orientations including the main NCIs driving selectivity.



species	E_{int}	E_{dist}^{Ni}	E_{dist}^{Cu}	E_{dist}^{tot}
TS$_{VI\text{-}VII}^{C,S}$	-30.1	4.0	15.3	16.6
TS$_{VI\text{-}VII}^{C,R}$	-23.6	4.9	11.6	19.3
Δ*E*^{a}	-6.5	-0.9	3.7	2.7
TS$_{VI\text{-}VII}^{A,S}$	-23.4	5.2	11.1	16.3
TS$_{VI\text{-}VII}^{A,R}$	-28.0	6.1	11.6	17.7
Δ*E*^{a}	4.6	-0.9	-0.5	-1.4

^{a} Δ*E* in kcal·mol^{-1} computed tacking the pro-(S) TS as energy reference.

3.3 Supramolecular cycle

The cooperativity of the transformation was assessed computing the energy profile involving both co-catalysts in a supramolecular aggregate from the beginning of the reaction. Our results clearly

show the energetic preference for the independent activation of the substrates by the separated co-catalysts both for *SS*-15-A-[Cu((*R,S,S*$_P$)-L$_2$)(κN,O'-S$_2$)]$^+$ (Fig. S4) and *SS*-15-C-[Cu((*R,S,S*$_P$)-L$_2$)(κN,O'-S$_2$)]$^+$ (Fig. S5) Cu-based catalyst.

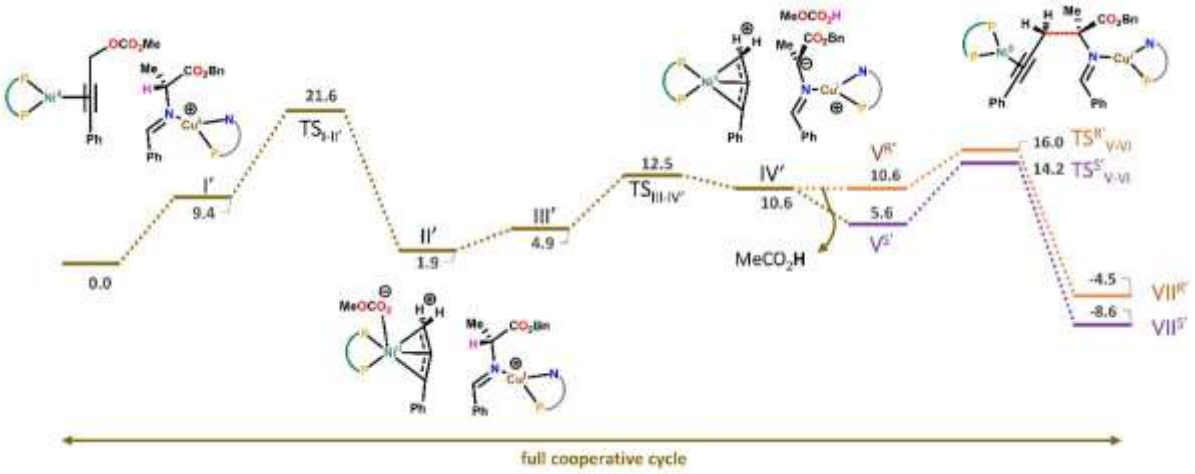


Fig. S6. DFT computed mechanism (B3LYP-D3 in CH_2Cl_2) for the propargylation of aldimine ester **S$_2$** considering the formation of a supramolecular adduct from the beginning of the reaction. Profile related to the *SS*-15-C-[Cu((*R,S,S*$_P$)-L$_2$)(κN,O'-S$_2$)]$^+$ isomer. The numbers are relative Gibbs energies in kcal mol^{-1}, taking as zero-energy the separated co-catalysts and substrates **S$_1$** and **S$_2$**.

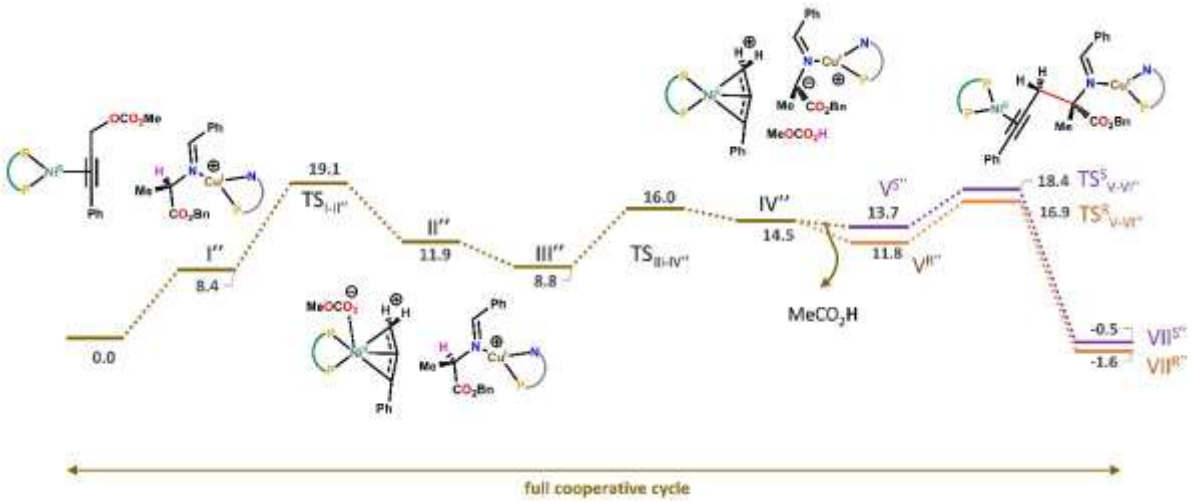


Fig. S7. DFT computed mechanism (B3LYP-D3 in CH_2Cl_2) for the propargylation of aldimine ester **S$_2$** considering the formation of a supramolecular adduct from the beginning of the reaction. Profile related to the *SS*-15-A-[Cu((*R,S,S*$_P$)-L$_2$)(κN,O'-S$_2$)]$^+$ isomer of the copper co-catalyst. The numbers are relative Gibbs energies in kcal mol^{-1}, taking as zero-energy the separated co-catalysts and substrates **S$_1$** and **S$_2$**.

4. Cartesian coordinates and absolute E and G energies of the optimized structures

Int1_Ni

Charge	0
Electronic Energy, BS1 (a.u.)	-3200.754926
Thermal and entropic correction, BS1 (a.u.)	0.721782
Electronic Energy, BS2 (a.u.)	-4539.121275
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Ni	1.127455	0.287622	-0.272967
P	-0.034361	-1.532707	0.151063
C	-0.303354	-2.058060	-2.563633
H	0.485261	-1.315184	-2.655187
C	-1.435904	-1.151177	1.317846
C	0.745619	-4.231465	0.782404
H	0.008233	-4.579446	0.067850
C	0.914778	-2.860156	1.018961
C	-0.798161	-2.377092	-1.289521
C	-1.296427	-1.518268	2.686575
H	-0.463024	-2.140077	2.989866
C	-1.834443	-3.315699	-1.170744
H	-2.243682	-3.550953	-0.193211
C	-3.471642	0.082107	1.911479
C	-2.518652	-0.358318	0.927846
C	1.539684	-5.167229	1.450901
H	1.403695	-6.226314	1.249653
C	-3.297059	-0.285773	3.285045
C	-2.192427	-1.099252	3.638749
H	-2.062566	-1.391453	4.677630
C	1.896441	-2.446559	1.936119
H	2.058296	-1.384559	2.097061
C	-1.858947	-3.611326	-3.572859
H	-2.275688	-4.085776	-4.456840
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H	-0.445677	-2.415185	-4.682800
C	-2.359413	-3.931245	-2.307405
H	-3.169757	-4.647207	-2.206478
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H	-4.071156	-0.116200	5.297012
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C	5.641800	-3.465925	-0.183179
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C	3.653530	-2.420562	-1.088465
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O	6.906184	1.941773	-0.267614
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H	7.637886	0.768487	1.304407

TS12_Ni

Charge	0
Electronic Energy, BS1 (a.u.)	-3200.722440
Thermal and entropic correction, BS1 (a.u.)	0.718048
Electronic Energy, BS2 (a.u.)	-4539.096449
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-194.2i

Molecular Geometry in Cartesian Coordinates

Ni	1.113835	0.278297	-0.288261
P	-0.029777	-1.495952	0.270573
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C	-0.787170	-2.429227	-1.108834
C	-1.230750	-1.220425	2.810616
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H	-0.464739	-2.691846	-4.493117
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H	-5.386775	-1.094506	-4.173536
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C	-4.597015	-1.747031	-0.419946
H	-4.379907	-1.945523	0.622718
C	0.631362	4.902951	-3.713491
H	0.929404	5.628891	-4.464593
H	2.670770	2.931447	-1.056251
C	2.960593	2.297874	-0.227820
H	2.959380	2.731453	0.764351
O	5.467897	1.747806	1.310654
C	3.027814	0.952012	-0.371104
C	2.928431	-0.330441	-0.424796
C	3.803087	-1.494302	-0.455271
C	5.083851	-1.423114	0.128541
C	5.910022	-2.545760	0.138260
H	6.894431	-2.484485	0.595026
C	5.476902	-3.748438	-0.431176
H	6.122416	-4.622451	-0.417131
H	3.864094	-4.755830	-1.453165
C	4.208588	-3.823370	-1.014523
C	3.375316	-2.705338	-1.023740
H	2.383271	-2.763652	-1.460033
H	5.403746	-0.486176	0.579106
C	5.747270	2.413624	0.297556
O	4.988153	3.100609	-0.451935
O	7.071658	2.451481	-0.140950
C	8.000376	1.716118	0.651298
H	8.987048	1.899454	0.215563
H	7.995938	2.044238	1.696636
H	7.791748	0.639748	0.630872

Int2_Ni

Charge	0
Electronic Energy, BS1 (a.u.)	-3200.752941

Thermal and entropic correction, BS1 (a.u.)	0.718399
Electronic Energy, BS2 (a.u.)	-4539.119297
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Ni	1.064231	-0.882892	0.764028
P	0.844549	1.019383	-0.356453
C	0.524782	2.411808	2.024560
H	0.987484	1.531155	2.461704
C	-0.410798	0.656047	-1.673308
C	2.581295	3.058726	-1.350824
H	1.912249	3.788061	-0.910963
C	2.314271	1.684138	-1.253471
C	0.273022	2.442150	0.645044
C	0.085309	0.299803	-2.958683
H	1.138364	0.415213	-3.175969
C	-0.339648	3.571871	0.081897
H	-0.555123	3.598824	-0.981185
C	-2.648725	-0.036021	-2.395170
C	-1.770730	0.508995	-1.394790
C	3.733380	3.508143	-1.999203
H	3.930106	4.574907	-2.060863
C	-2.122674	-0.401838	-3.676003
C	-0.742725	-0.203163	-3.929742
H	-0.341316	-0.467427	-4.904467
C	3.222155	0.769617	-1.812142
H	3.026121	-0.293400	-1.727733
C	-0.432892	4.619917	2.261408
H	-0.711309	5.462998	2.887284
C	0.175120	3.497797	2.829547
H	0.371573	3.463383	3.897341
C	-0.691357	4.654567	0.887926
H	-1.177940	5.518205	0.444724
C	-2.989504	-0.949189	-4.660681
H	-2.570825	-1.222085	-5.625848
C	-4.853587	-0.777168	-3.131881
H	-5.908295	-0.933579	-2.924238
C	4.368959	1.225854	-2.461479
H	5.065346	0.503710	-2.877835
C	-4.327775	-1.133752	-4.397530
H	-4.982312	-1.555400	-5.154990
C	-4.038607	-0.241828	-2.159369
H	-4.456177	0.013731	-1.193065
C	4.631557	2.594387	-2.554219
H	5.532430	2.946668	-3.049045
P	-1.094244	-1.229476	1.161081
C	-1.175131	-3.318651	-0.692539
H	-0.097823	-3.198405	-0.742523
C	-2.212659	0.249666	1.088393
C	-2.116998	-2.853604	3.289004
H	-2.692244	-3.395913	2.546851
C	-1.292853	-1.788176	2.907823
C	-1.942919	-2.477623	0.125839
C	-2.861892	0.699495	2.273083
H	-2.752055	0.139618	3.192548
C	-3.342858	-2.598857	0.137205
H	-3.943241	-1.937772	0.755090

C	-3.173637	2.155193	-0.111857
C	-2.380700	0.956453	-0.100261
C	-2.198108	-3.232963	4.632852
H	-2.836472	-4.065128	4.915820
C	-3.796783	2.602984	1.097086
C	-3.631943	1.835652	2.276513
H	-4.117910	2.162914	3.191842
C	-0.546365	-1.112807	3.890582
H	0.112524	-0.299950	3.597390
C	-3.199846	-4.400911	-1.470179
H	-3.688763	-5.143123	-2.095203
C	-1.809335	-4.276579	-1.487551
H	-1.209416	-4.918443	-2.126727
C	-3.966407	-3.561590	-0.655338
H	-5.049229	-3.647349	-0.647466
C	-4.548281	3.809275	1.096097
H	-5.012125	4.132509	2.024338
C	-4.061350	4.121701	-1.250975
H	-4.161688	4.717140	-2.153853
C	-0.637375	-1.486122	5.229967
H	-0.057385	-0.954377	5.978886
C	-4.678269	4.556837	-0.052280
H	-5.249983	5.480319	-0.043615
C	-3.333559	2.952566	-1.281658
H	-2.861470	2.641127	-2.205704
C	-1.464785	-2.550465	5.604241
H	-1.530500	-2.848543	6.646696
H	1.495110	-3.524231	0.982744
C	1.518650	-2.708305	1.705303
H	1.017186	-2.880687	2.652487
O	2.242699	-4.064090	-1.053825
C	2.592471	-1.845637	1.662147
C	3.106878	-0.756498	1.292190
C	4.283121	0.052349	1.091546
C	5.454875	-0.550756	0.594398
C	6.593029	0.217775	0.361747
H	7.490959	-0.255187	-0.026026
C	6.576600	1.593272	0.612711
H	7.461642	2.192676	0.419277
H	5.394939	3.267211	1.290364
C	5.415482	2.197402	1.104198
C	4.274244	1.434817	1.342439
H	3.364103	1.905076	1.700296
H	5.450333	-1.613638	0.377895
C	2.427671	-2.878015	-1.385118
O	1.610448	-1.914591	-1.400898
O	3.711619	-2.497482	-1.801029
C	4.705982	-3.516010	-1.762551
H	5.635601	-3.051433	-2.104364
H	4.845787	-3.908776	-0.748663
H	4.453895	-4.355316	-2.421080

Int2i_Ni

Charge	0
Electronic Energy, BS1 (a.u.)	-3200.744667
Thermal and entropic correction, BS1 (a.u.)	0.722426
Electronic Energy, BS2 (a.u.)	-4539.114118

Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-2.6i

Molecular Geometry in Cartesian Coordinates

Ni	1.031504	0.417856	-1.024046
P	-0.254202	1.661577	0.420166
C	0.999204	0.412566	2.552833
H	1.692943	0.071003	1.787808
C	-2.019995	1.448793	-0.107635
C	0.434907	4.169269	1.580723
H	0.429060	3.670084	2.542207
C	0.098697	3.471357	0.410030
C	-0.107122	1.190145	2.180819
C	-2.620697	2.447168	-0.925606
H	-2.133592	3.403709	-1.055980
C	-1.015053	1.618462	3.161300
H	-1.878335	2.212897	2.879340
C	-3.944104	-0.004820	-0.557756
C	-2.686972	0.239637	0.095858
C	0.791509	5.519180	1.522804
H	1.048705	6.042526	2.439431
C	-4.508520	1.000503	-1.406933
C	-3.822577	2.231472	-1.552967
H	-4.260949	3.011074	-2.170245
C	0.143969	4.153562	-0.819681
H	-0.074420	3.625862	-1.740290
C	0.288431	0.494118	4.862391
H	0.437386	0.220068	5.902915
C	1.196734	0.066292	3.890795
H	2.052555	-0.541178	4.170742
C	-0.817108	1.268658	4.496699
H	-1.530555	1.591297	5.248995
C	-5.741425	0.751404	-2.068674
H	-6.150552	1.525566	-2.712408
C	-5.853198	-1.439532	-1.054128
H	-6.375612	-2.383212	-0.925977
C	0.495236	5.501302	-0.872584
H	0.530802	6.004894	-1.834039
C	-6.402869	-0.443425	-1.897387
H	-7.344491	-0.626496	-2.406918
C	-4.658595	-1.227249	-0.402475
H	-4.247282	-2.006529	0.227601
C	0.821452	6.189613	0.299300
H	1.104284	7.237573	0.256732
P	-0.098591	-1.452952	-0.752865
C	-1.218941	-0.756699	-3.220063
H	-0.498880	0.058388	-3.221707
C	-1.139527	-1.665054	0.772001
C	0.809348	-4.048713	-1.538342
H	-0.003554	-4.073565	-2.255433
C	0.990584	-2.934602	-0.708505
C	-1.261473	-1.665056	-2.149869
C	-0.796027	-2.680123	1.710663
H	-0.004601	-3.380415	1.482363
C	-2.217384	-2.693683	-2.145461
H	-2.270240	-3.384561	-1.309230
C	-2.875264	-0.893948	2.320696
C	-2.193839	-0.799338	1.057731
C	1.683454	-5.135852	-1.453269

H	1.537075	-5.992116	-2.105369
C	-2.485526	-1.898305	3.263246
C	-1.449902	-2.797608	2.911215
H	-1.167586	-3.579895	3.610621
C	2.065850	-2.918766	0.196772
H	2.225533	-2.053316	0.832237
C	-3.070766	-1.912751	-4.269668
H	-3.778759	-2.004428	-5.088452
C	-2.125758	-0.884231	-4.274274
H	-2.096423	-0.172599	-5.094346
C	-3.113393	-2.819314	-3.206489
H	-3.854958	-3.612625	-3.194152
C	-3.128474	-1.964581	4.528710
H	-2.815700	-2.733503	5.230097
C	-4.508110	-0.070817	3.935743
H	-5.285966	0.637878	4.204793
C	2.923543	-4.013921	0.292597
H	3.744752	-3.991251	1.002438
C	-4.118647	-1.068625	4.862321
H	-4.601484	-1.121571	5.833773
C	-3.907714	0.012063	2.698684
H	-4.213277	0.789722	2.009436
C	2.736032	-5.123927	-0.535961
H	3.410609	-5.972749	-0.469687
H	2.216108	0.123867	-3.165094
C	2.194551	-0.563961	-2.316800
H	1.861929	-1.545447	-2.662590
O	2.649801	3.443170	-3.233917
C	3.432797	-0.643721	-1.603702
C	4.439873	-0.696373	-0.914687
C	5.594148	-0.786747	-0.085340
C	6.204877	0.374371	0.437339
C	7.321823	0.273525	1.264439
H	7.780068	1.176656	1.658306
C	7.853128	-0.979172	1.588299
H	8.723884	-1.052724	2.233503
H	7.668397	-3.112595	1.317233
C	7.258707	-2.136009	1.073672
C	6.142969	-2.046111	0.243841
H	5.683101	-2.942742	-0.159535
H	5.792404	1.347147	0.187692
C	1.825275	2.607061	-2.874789
O	0.795507	2.114149	-3.364567
O	2.073030	2.038190	-1.523939
C	3.164548	2.576766	-0.770034
H	3.134955	2.096948	0.209850
H	4.115030	2.360179	-1.262218
H	3.044764	3.657212	-0.661941

TS23i_Ni

Charge	0
Electronic Energy, BS1 (a.u.)	-3200.737561
Thermal and entropic correction, BS1 (a.u.)	0.717382
Electronic Energy, BS2 (a.u.)	-4539.109017
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-37.9i

Molecular Geometry in Cartesian Coordinates

Ni	1.108100	0.396734	-0.675725
P	-0.504895	1.714003	0.301666
C	0.165711	0.934211	2.877866
H	1.040473	0.509170	2.393122
C	-2.098568	1.301483	-0.557462
C	-0.407800	4.503158	0.948629
H	-0.774018	4.254384	1.938054
C	-0.220093	3.502583	-0.015345
C	-0.804680	1.585280	2.102067
C	-2.520138	2.121570	-1.642336
H	-2.010826	3.056876	-1.837968
C	-1.941909	2.122445	2.725347
H	-2.708136	2.608923	2.129891
C	-3.876301	-0.288618	-1.129902
C	-2.774755	0.108042	-0.296108
C	-0.110539	5.835646	0.648117
H	-0.258519	6.600534	1.405313
C	-4.269476	0.544187	-2.227090
C	-3.568457	1.755509	-2.450168
H	-3.874145	2.398898	-3.271030
C	0.283990	3.858371	-1.278944
H	0.468961	3.088263	-2.016521
C	-1.130475	1.362016	4.874228
H	-1.261634	1.269924	5.948615
C	0.002165	0.822220	4.259631
H	0.754069	0.309284	4.852394
C	-2.100973	2.012700	4.106596
H	-2.988772	2.420305	4.580603
C	-5.349232	0.145138	-3.060861
H	-5.629612	0.788783	-3.890532
C	-5.643491	-1.856433	-1.738334
H	-6.175642	-2.786023	-1.557716
C	0.570240	5.189277	-1.578886
H	0.959971	5.445592	-2.560155
C	-6.025359	-1.029967	-2.823034
H	-6.849853	-1.327343	-3.464547
C	-4.598537	-1.497678	-0.915926
H	-4.312774	-2.148519	-0.098397
C	0.376827	6.181892	-0.613520
H	0.610318	7.218074	-0.842119
P	-0.036843	-1.488849	-0.475824
C	-0.775774	-1.213693	-3.152794
H	-0.104304	-0.360415	-3.142228
C	-1.296799	-1.582592	0.884781
C	1.094608	-4.119622	-0.668610
H	0.356225	-4.349401	-1.428786
C	1.125988	-2.854660	-0.067494
C	-0.945956	-1.977253	-1.987741
C	-1.046014	-2.418162	2.009503
H	-0.182407	-3.070407	2.012930
C	-1.836986	-3.061759	-1.995951
H	-1.998890	-3.640339	-1.091475
C	-3.306391	-0.745553	2.009023
C	-2.426298	-0.764355	0.873751
C	2.025845	-5.094026	-0.298873
H	1.997643	-6.069807	-0.775410
C	-3.015123	-1.569691	3.143462
C	-1.877137	-2.412269	3.102353

H	-1.663381	-3.053148	3.953653
C	2.109135	-2.576197	0.897585
H	2.158264	-1.586680	1.343133
C	-2.358497	-2.624260	-4.317982
H	-2.911876	-2.872016	-5.219256
C	-1.480864	-1.537227	-4.312865
H	-1.350248	-0.935639	-5.207691
C	-2.534115	-3.386434	-3.159711
H	-3.226782	-4.222872	-3.156686
C	-3.860368	-1.518154	4.284968
H	-3.619308	-2.147050	5.137903
C	-5.252319	0.128540	3.192086
H	-6.116261	0.786363	3.219351
C	3.025916	-3.555772	1.276956
H	3.781785	-3.326207	2.021796
C	-4.956427	-0.686085	4.312362
H	-5.595305	-0.650263	5.190042
C	-4.451598	0.099325	2.071813
H	-4.687443	0.738894	1.229899
C	2.986515	-4.817628	0.676490
H	3.706905	-5.578846	0.962226
H	2.392977	0.143142	-2.745068
C	2.374639	-0.569475	-1.915142
H	2.032955	-1.543044	-2.281033
O	4.157434	3.312585	-2.048978
C	3.645807	-0.677272	-1.267583
C	4.702367	-0.768035	-0.662411
C	5.917938	-0.846754	0.073399
C	6.656609	0.321750	0.366623
C	7.839877	0.245560	1.098378
H	8.395115	1.154419	1.314873
C	8.313438	-0.989224	1.555238
H	9.236017	-1.043801	2.126152
H	7.952976	-3.116306	1.620218
C	7.591338	-2.152862	1.270467
C	6.408078	-2.088180	0.536821
H	5.848006	-2.991626	0.315732
H	6.286485	1.279954	0.013740
C	3.222683	2.812935	-2.563801
O	2.426610	2.474469	-3.367822
O	2.306213	1.869172	-0.775722
C	2.918784	2.160105	0.446849
H	2.205058	2.550003	1.197578
H	3.422703	1.284787	0.893226
H	3.688156	2.933180	0.299916

Int3i_Ni

Charge	0
Electronic Energy, BS1 (a.u.)	-3012.144083
Thermal and entropic correction, BS1 (a.u.)	0.710105
Electronic Energy, BS2 (a.u.)	-4350.428289
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-3.0i

Molecular Geometry in Cartesian Coordinates

Ni	1.142407	0.436115	-1.112560
P	-0.554002	1.807127	-0.394992

C	0.450223	1.956479	2.183293
H	1.335263	1.515396	1.732200
C	-2.141612	0.977704	-0.889885
C	-0.878644	4.642713	-0.623759
H	-1.136790	4.662465	0.428768
C	-0.569944	3.431227	-1.259159
C	-0.676955	2.207885	1.386770
C	-2.755869	1.365287	-2.114895
H	-2.393351	2.237553	-2.644256
C	-1.825212	2.764600	1.971197
H	-2.709832	2.940993	1.367492
C	-3.729062	-0.887079	-0.741940
C	-2.627800	-0.136494	-0.202664
C	-0.845091	5.843445	-1.337708
H	-1.084191	6.774322	-0.831094
C	-4.319672	-0.485759	-1.983544
C	-3.807989	0.659057	-2.643717
H	-4.262497	0.977185	-3.578268
C	-0.208635	3.446351	-2.618854
H	0.071278	2.520084	-3.105292
C	-0.713999	2.818451	4.119963
H	-0.732045	3.049700	5.181196
C	0.431028	2.260627	3.545611
H	1.305348	2.055728	4.156739
C	-1.840927	3.070259	3.331928
H	-2.737099	3.489456	3.779336
C	-5.399545	-1.235750	-2.523549
H	-5.831731	-0.916276	-3.468250
C	-5.307694	-2.744254	-0.637469
H	-5.690103	-3.622406	-0.125082
C	-0.190573	4.645175	-3.331691
H	0.083993	4.641052	-4.382800
C	-5.887038	-2.342022	-1.865437
H	-6.712635	-2.909618	-2.284959
C	-4.258042	-2.038953	-0.091827
H	-3.819192	-2.370048	0.841572
C	-0.505793	5.847275	-2.692011
H	-0.481067	6.781909	-3.245505
P	0.274760	-1.413480	-0.230310
C	-0.717647	-2.040950	-2.760793
H	-0.169052	-1.158401	-3.076170
C	-0.844927	-1.218473	1.239808
C	1.737522	-3.850264	0.165725
H	0.994658	-4.358895	-0.438612
C	1.632300	-2.475380	0.413078
C	-0.685423	-2.429974	-1.413046
C	-0.395008	-1.640066	2.522662
H	0.544248	-2.169220	2.615794
C	-1.416784	-3.554992	-1.001187
H	-1.419996	-3.848747	0.044189
C	-2.850525	-0.289608	2.298596
C	-2.070618	-0.563010	1.123329
C	2.809413	-4.577430	0.691103
H	2.884577	-5.642051	0.488402
C	-2.359303	-0.690950	3.582420
C	-1.126134	-1.383936	3.656083
H	-0.759732	-1.708517	4.626359
C	2.624252	-1.838181	1.178809
H	2.568426	-0.766160	1.346006

C	-2.183008	-3.896647	-3.271054
H	-2.769538	-4.462184	-3.989423
C	-1.464864	-2.772163	-3.685275
H	-1.491805	-2.458742	-4.724855
C	-2.156595	-4.287805	-1.929456
H	-2.725393	-5.153187	-1.602324
C	-3.107366	-0.379584	4.750158
H	-2.714794	-0.688157	5.715455
C	-4.794304	0.696656	3.394024
H	-5.734480	1.236719	3.328680
C	3.681164	-2.569544	1.718772
H	4.440675	-2.064019	2.307075
C	-4.300092	0.301507	4.661289
H	-4.863991	0.538904	5.558765
C	-4.091306	0.408257	2.245267
H	-4.479477	0.729615	1.286356
C	3.776276	-3.942593	1.473588
H	4.605607	-4.512135	1.883471
H	2.351050	-0.234603	-3.139697
C	2.442555	-0.708968	-2.156091
H	2.186652	-1.771176	-2.236340
C	3.743478	-0.530833	-1.586639
C	4.823980	-0.377031	-1.038190
C	6.062668	-0.193742	-0.361487
C	6.661436	1.083736	-0.280017
C	7.865953	1.260326	0.397985
H	8.310660	2.250635	0.450226
C	8.500856	0.175062	1.011470
H	9.439078	0.317454	1.540205
H	8.405498	-1.944040	1.410131
C	7.918789	-1.094693	0.937830
C	6.716471	-1.282781	0.258376
H	6.265834	-2.268680	0.202235
H	6.166253	1.928126	-0.750587
O	2.102842	1.893930	-1.828332
C	2.733077	2.663893	-0.851536
H	2.027503	3.197705	-0.180740
H	3.408407	2.077384	-0.198656
H	3.357614	3.441116	-1.327407

Int1-C_Cu

Charge	1
Electronic Energy, BS1 (a.u.)	-3084.089531
Thermal and entropic correction, BS1 (a.u.)	0.786339
Electronic Energy, BS2 (a.u.)	-5668.092190
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	-0.506398	0.703806	0.703977
Fe	0.377923	-1.299381	-2.927959
P	-2.030446	-0.028136	-0.770930
C	-1.167377	-0.068883	-2.376068
C	0.016094	0.707141	-2.707809
C	0.353373	0.434385	-4.076449
H	1.208222	0.839424	-4.598328
C	-0.598150	-0.485357	-4.590010

H	-0.586581	-0.919842	-5.580511
C	-1.530289	-0.790164	-3.557953
H	-2.353218	-1.485553	-3.635586
C	0.876205	-2.501391	-1.316957
H	0.470271	-2.390159	-0.324607
C	2.040011	-1.841627	-1.811480
H	2.651422	-1.141680	-1.260214
C	2.219153	-2.216449	-3.177612
H	2.991234	-1.852847	-3.842711
C	1.163595	-3.115369	-3.526422
H	0.996850	-3.549615	-4.503441
C	0.333442	-3.290418	-2.376663
H	-0.573217	-3.878388	-2.327765
O	1.701815	2.353860	-2.507546
C	0.818077	1.571497	-1.848715
N	0.803708	1.668125	-0.561566
C	1.792238	2.693601	-0.168391
C	2.573790	2.967574	-1.514180
H	2.597344	4.038214	-1.723969
H	1.242741	3.600873	0.107017
C	-3.501085	1.021673	-1.122816
C	-3.520507	1.931676	-2.189762
H	-2.677509	1.992913	-2.871025
C	-4.627561	2.761737	-2.388196
H	-4.632488	3.458759	-3.221616
C	-5.723606	2.689890	-1.526835
H	-6.584444	3.333293	-1.684155
C	-5.706853	1.789544	-0.456795
H	-6.552188	1.734400	0.222923
C	-4.602076	0.964356	-0.251660
H	-4.598509	0.271186	0.585160
C	-2.736110	-1.709268	-0.567630
C	-2.201411	-2.527254	0.438795
H	-1.410300	-2.144904	1.076485
C	-2.676609	-3.828725	0.617071
H	-2.248395	-4.453860	1.393590
C	-3.694821	-4.318117	-0.203893
H	-4.065054	-5.330225	-0.066697
C	-4.247820	-3.500691	-1.195685
H	-5.049772	-3.874603	-1.825964
C	-3.775822	-2.200031	-1.374860
H	-4.222640	-1.564750	-2.133642
C	2.661566	2.279578	0.996327
C	3.147621	3.252634	1.877297
C	3.059237	0.947436	1.164865
C	4.036364	2.904177	2.898203
C	3.940843	0.596120	2.187362
C	4.438825	1.575330	3.052114
H	2.838316	4.288102	1.755949
H	2.661747	0.187833	0.502987
H	4.409757	3.669012	3.573228
H	4.241608	-0.441019	2.306128
H	5.127766	1.302874	3.846450
C	3.962694	2.380799	-1.613961
C	5.040922	3.086893	-1.064919
C	4.189082	1.124658	-2.187723
C	6.321173	2.532967	-1.064816
C	5.472552	0.572775	-2.193188
C	6.540318	1.271103	-1.625705

H	4.873963	4.065025	-0.622266
H	3.366416	0.580051	-2.636717
H	7.147673	3.087266	-0.629376
H	5.634751	-0.403835	-2.641090
H	7.537552	0.840471	-1.626604
H	-0.722337	-7.034285	1.781254
C	-0.301326	-5.509461	3.250541
C	-0.127595	-6.158089	2.023145
C	0.806688	-5.670034	1.106589
H	0.937962	-6.159654	0.145880
C	1.567632	-4.540643	1.417659
H	2.285198	-4.154639	0.699310
H	2.774713	-2.310565	2.116812
C	2.272479	-2.711380	2.999160
H	3.020810	-2.970694	3.751498
C	1.405861	-3.894888	2.648413
H	0.331516	-3.882657	4.517670
C	0.463866	-4.384443	3.563081
H	-1.028551	-5.883525	3.965718
O	1.513141	-1.641947	3.640700
C	0.765218	-0.879592	2.849065
C	1.039824	1.100062	4.383282
H	0.488876	1.803101	5.013274
H	1.647164	1.663166	3.672649
H	1.695618	0.497702	5.014821
C	0.039319	0.203227	3.633064
H	-0.596146	-0.315750	4.363778
N	-0.781996	1.013265	2.718872
C	-1.744480	1.667069	3.273074
H	-1.959189	1.508922	4.335894
C	-2.612650	2.635441	2.600526
C	-2.253953	3.290595	1.407025
H	-1.288365	3.094702	0.952115
H	-2.843624	4.698545	-0.104936
C	-3.125945	4.201220	0.817744
C	-4.365560	4.470605	1.407348
H	-5.046798	5.174438	0.938685
C	-4.724828	3.839376	2.601377
H	-5.683176	4.053057	3.065052
C	-3.849072	2.936314	3.200620
H	-4.122151	2.448641	4.132895
O	0.681803	-1.039179	1.639199

Int4-C_Cu

Charge	0
Electronic Energy, BS1 (a.u.)	-3387.946191
Thermal and entropic correction, BS1 (a.u.)	0.831893
Electronic Energy, BS2 (a.u.)	-5972.086332
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	-0.094362	0.729601	0.351040
Fe	-0.591875	-2.172622	-2.619884
P	-1.693053	0.788728	-1.176864
C	-1.062506	-0.174149	-2.597545
C	0.340331	-0.371167	-2.916081

C	0.418799	-1.147649	-4.120691
H	1.334839	-1.480795	-4.586863
C	-0.905515	-1.429690	-4.548159
H	-1.179797	-2.036284	-5.400853
C	-1.811169	-0.832209	-3.624901
H	-2.888378	-0.900781	-3.662566
C	-1.007862	-2.948624	-0.744566
H	-1.343915	-2.364569	0.096233
C	0.355401	-3.190466	-1.085042
H	1.212920	-2.804669	-0.553099
C	0.384777	-3.966250	-2.284908
H	1.270713	-4.281711	-2.820067
C	-0.967451	-4.204021	-2.685126
H	-1.282491	-4.730044	-3.576852
C	-1.826841	-3.572933	-1.733462
H	-2.907137	-3.534071	-1.775422
O	2.674718	0.034338	-2.868278
C	1.512120	0.073014	-2.170301
N	1.577325	0.479935	-0.950480
C	2.975058	0.885390	-0.689726
C	3.751434	0.268969	-1.914656
H	4.419708	1.010676	-2.354820
H	3.017470	1.978048	-0.761594
C	-2.015498	2.441516	-1.924479
C	-1.481239	2.819143	-3.165185
H	-0.918260	2.106492	-3.759625
C	-1.669068	4.118127	-3.647732
H	-1.253288	4.397959	-4.611919
C	-2.389765	5.048916	-2.896439
H	-2.534912	6.058106	-3.271908
C	-2.922596	4.675509	-1.657726
H	-3.481959	5.395151	-1.065831
C	-2.736609	3.382406	-1.166953
H	-3.142338	3.108808	-0.193155
C	-3.352900	0.078944	-0.873959
C	-3.541930	-0.674702	0.292688
H	-2.745875	-0.742384	1.026497
C	-4.773088	-1.287254	0.536032
H	-4.908830	-1.868681	1.441984
C	-5.822805	-1.138182	-0.372811
H	-6.781262	-1.612272	-0.179099
C	-5.648667	-0.360589	-1.522966
H	-6.470171	-0.225964	-2.221255
C	-4.418992	0.249369	-1.772112
H	-4.290614	0.863351	-2.658946
C	3.490186	0.476282	0.669723
C	4.418656	1.287296	1.330812
C	3.084072	-0.720887	1.268968
C	4.929365	0.912823	2.576338
C	3.586173	-1.095417	2.515393
C	4.511538	-0.279169	3.173872
H	4.733221	2.221212	0.873657
H	2.351178	-1.340054	0.768257
H	5.647029	1.554076	3.080588
H	3.252045	-2.021322	2.974983
H	4.902222	-0.570064	4.144943
C	4.493656	-1.018842	-1.644235
C	5.805077	-0.959008	-1.156387
C	3.878124	-2.266467	-1.800119

C	6.484393	-2.127247	-0.809289
C	4.559833	-3.436407	-1.457080
C	5.861807	-3.370353	-0.955685
H	6.288872	0.006404	-1.034313
H	2.869266	-2.326079	-2.192176
H	7.499681	-2.067219	-0.427556
H	4.071079	-4.398998	-1.580511
H	6.390584	-4.280313	-0.686500
H	-4.838233	-4.658513	2.443957
C	-3.579131	-3.264573	3.506886
C	-3.819899	-4.337858	2.644513
C	-2.744906	-4.989825	2.034629
H	-2.922555	-5.817967	1.354232
C	-1.437453	-4.567856	2.284988
H	-0.604076	-5.066215	1.796439
H	0.882824	-3.302459	2.589122
C	0.233599	-3.089037	3.441939
H	0.623718	-3.609029	4.320883
C	-1.192121	-3.496469	3.151894
H	-2.089854	-2.006480	4.425003
C	-2.271254	-2.847056	3.762572
H	-4.409205	-2.746650	3.978737
O	0.354984	-1.687158	3.799024
C	0.210095	-0.802840	2.808687
C	0.945897	0.873351	4.598742
H	0.739147	1.877072	4.978876
H	2.027697	0.747323	4.488212
H	0.589253	0.161445	5.344553
C	0.208846	0.638424	3.282214
N	0.561669	1.493762	2.140267
C	1.246637	2.559930	2.333137
H	1.661155	2.790937	3.315298
C	1.555537	3.541277	1.281917
C	0.701251	3.769034	0.190748
H	-0.245565	3.246490	0.134422
H	0.370748	4.854831	-1.631463
C	1.048827	4.685164	-0.800490
C	2.254738	5.388529	-0.712052
H	2.527847	6.100126	-1.486236
C	3.097512	5.192930	0.387242
H	4.026461	5.750095	0.468099
C	2.742574	4.286505	1.386286
H	3.395452	4.133402	2.241239
O	0.016954	-1.143280	1.648017
H	-0.881921	0.823714	3.419076
O	-2.738848	0.959092	2.969039
C	-2.912065	2.116602	2.516456
O	-1.944211	3.032254	3.000215
O	-3.786677	2.560334	1.745437
H	-1.919737	4.457100	1.459974
C	-2.071515	4.371908	2.541906
H	-3.055983	4.792712	2.779935
H	-1.296851	4.951368	3.054763

TS45-C_Cu

Charge	0
Electronic Energy, BS1 (a.u.)	-3387.934493
Thermal and entropic correction, BS1 (a.u.)	0.825707

Electronic Energy, BS2 (a.u.)	-5972.071956
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-1422.6i

Molecular Geometry in Cartesian Coordinates

Cu	-0.019774	0.712091	0.283435
Fe	-0.311462	-2.242186	-2.666082
P	-1.469310	0.759307	-1.382257
C	-0.721272	-0.229640	-2.725806
C	0.701233	-0.473355	-2.894041
C	0.878984	-1.275657	-4.070328
H	1.827483	-1.645228	-4.432720
C	-0.402352	-1.527909	-4.628231
H	-0.605869	-2.143280	-5.494345
C	-1.379624	-0.886594	-3.814137
H	-2.448818	-0.925749	-3.962484
C	-0.855444	-2.970474	-0.800280
H	-1.180068	-2.355278	0.023664
C	0.501548	-3.307481	-1.082613
H	1.361613	-2.979098	-0.515562
C	0.527742	-4.093428	-2.276091
H	1.411899	-4.473361	-2.771594
C	-0.820737	-4.243349	-2.730661
H	-1.134302	-4.754839	-3.631727
C	-1.673937	-3.547168	-1.818900
H	-2.746671	-3.434394	-1.906040
O	3.034310	-0.148713	-2.590901
C	1.801348	-0.056114	-2.032356
N	1.742805	0.373004	-0.820801
C	3.112958	0.733227	-0.404030
C	4.002542	0.069182	-1.522031
H	4.739902	0.782036	-1.894514
H	3.203697	1.822389	-0.485647
C	-1.757296	2.393812	-2.177231
C	-1.077883	2.791698	-3.337563
H	-0.416614	2.098735	-3.848753
C	-1.245922	4.083911	-3.845282
H	-0.716981	4.378865	-4.747500
C	-2.090971	4.988585	-3.199118
H	-2.220564	5.992194	-3.594263
C	-2.769885	4.596306	-2.040255
H	-3.429004	5.294021	-1.530902
C	-2.603654	3.309818	-1.527109
H	-3.127381	3.023782	-0.618085
C	-3.149425	0.053573	-1.194765
C	-3.427895	-0.667504	-0.024915
H	-2.675281	-0.740372	0.753567
C	-4.678424	-1.265829	0.146067
H	-4.883970	-1.821484	1.054369
C	-5.657588	-1.138116	-0.841276
H	-6.630705	-1.601903	-0.704245
C	-5.393718	-0.397818	-1.998885
H	-6.160198	-0.282070	-2.760257
C	-4.145860	0.200400	-2.173935
H	-3.949234	0.787798	-3.066139
C	3.433256	0.334416	1.017279
C	4.331537	1.103205	1.765745
C	2.854112	-0.798149	1.599664
C	4.642541	0.750213	3.080927

C	3.155201	-1.147797	2.916448
C	4.050996	-0.375195	3.661633
H	4.774989	1.990535	1.322263
H	2.131367	-1.374896	1.035610
H	5.337189	1.358562	3.653717
H	2.682638	-2.017747	3.363773
H	4.283147	-0.645983	4.687914
C	4.668613	-1.235349	-1.150494
C	5.892272	-1.204449	-0.468749
C	4.065627	-2.470047	-1.416395
C	6.492440	-2.388264	-0.039346
C	4.668463	-3.655964	-0.989189
C	5.879609	-3.618768	-0.295106
H	6.367234	-0.249304	-0.261278
H	3.129646	-2.507385	-1.962134
H	7.438541	-2.350392	0.493207
H	4.188636	-4.607996	-1.199427
H	6.346743	-4.540778	0.039202
H	-5.576642	-4.290953	2.459906
C	-4.299468	-2.931982	3.547541
C	-4.553903	-3.990932	2.670349
C	-3.487191	-4.650722	2.054172
H	-3.676048	-5.463644	1.358453
C	-2.173533	-4.260292	2.323793
H	-1.345487	-4.770120	1.837923
H	0.194160	-3.154938	2.759633
C	-0.485686	-2.859083	3.562321
H	-0.180341	-3.365020	4.483301
C	-1.913077	-3.211935	3.214558
H	-2.788223	-1.719090	4.496149
C	-2.985597	-2.544769	3.819134
H	-5.124327	-2.405758	4.019845
O	-0.307008	-1.459286	3.867234
C	-0.226680	-0.616353	2.811608
C	0.185406	1.158477	4.603750
H	-0.129510	2.183770	4.826221
H	1.262176	1.079698	4.811230
H	-0.339559	0.495751	5.293739
C	-0.161896	0.794858	3.172788
N	0.393438	1.567664	2.104753
C	1.064803	2.643558	2.336724
H	1.316122	2.936050	3.356953
C	1.568131	3.532031	1.280353
C	0.881447	3.728272	0.069143
H	-0.080611	3.252613	-0.079094
H	0.865365	4.687449	-1.852381
C	1.415351	4.545857	-0.926562
C	2.640380	5.190143	-0.725009
H	3.056967	5.826500	-1.500896
C	3.315264	5.031616	0.490405
H	4.259492	5.541918	0.659836
C	2.777259	4.220140	1.489409
H	3.304956	4.092909	2.430968
O	-0.285806	-1.049630	1.649580
H	-1.524584	1.075048	2.972906
O	-2.705454	1.255283	2.677171
C	-2.960763	2.435761	2.210434
O	-1.982581	3.342876	2.536548
O	-3.952518	2.770140	1.565172

H	-2.079254	4.678001	0.926870
C	-2.157071	4.665503	2.017800
H	-3.126567	5.080484	2.309860
H	-1.351165	5.264069	2.447072

Int5-C_Cu

Charge	0
Electronic Energy, BS1 (a.u.)	-3387.942359
Thermal and entropic correction, BS1 (a.u.)	0.830284
Electronic Energy, BS2 (a.u.)	-5972.080030
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	-0.016148	0.649421	0.343101
Fe	-0.250436	-2.142315	-2.756998
P	-1.416260	0.831227	-1.360272
C	-0.655935	-0.125857	-2.720412
C	0.767101	-0.366534	-2.880041
C	0.959934	-1.108712	-4.092624
H	1.912322	-1.463322	-4.459798
C	-0.314434	-1.328387	-4.680193
H	-0.507256	-1.899027	-5.578812
C	-1.301362	-0.725410	-3.848477
H	-2.368710	-0.751072	-4.013303
C	-0.866197	-2.982410	-0.959426
H	-1.247772	-2.420242	-0.121801
C	0.513103	-3.263483	-1.188238
H	1.332002	-2.937388	-0.562520
C	0.624466	-3.985106	-2.416455
H	1.543708	-4.312083	-2.884335
C	-0.693216	-4.150753	-2.947414
H	-0.944109	-4.624090	-3.887726
C	-1.612882	-3.528803	-2.047179
H	-2.682571	-3.444625	-2.185621
O	3.092842	-0.046242	-2.528248
C	1.852428	0.006663	-1.980910
N	1.773334	0.364948	-0.747865
C	3.133848	0.714790	-0.294592
C	4.045524	0.124511	-1.437413
H	4.778734	0.864811	-1.761126
H	3.213665	1.807846	-0.312010
C	-1.646994	2.492666	-2.121564
C	-0.890852	2.918208	-3.223425
H	-0.199404	2.235740	-3.707638
C	-1.020179	4.223388	-3.708033
H	-0.431326	4.537794	-4.565367
C	-1.901678	5.116899	-3.096137
H	-2.001332	6.130722	-3.473326
C	-2.657476	4.698795	-1.995379
H	-3.347829	5.386143	-1.514151
C	-2.530652	3.397917	-1.507717
H	-3.121660	3.088885	-0.650118
C	-3.116476	0.153039	-1.258581
C	-3.432639	-0.652856	-0.155237
H	-2.694889	-0.805334	0.626250
C	-4.696954	-1.238486	-0.056654

H	-4.931462	-1.860689	0.800047
C	-5.653709	-1.012406	-1.048612
H	-6.638123	-1.465375	-0.967203
C	-5.351615	-0.189811	-2.139149
H	-6.099183	-0.000407	-2.904570
C	-4.088715	0.393595	-2.243592
H	-3.861523	1.040596	-3.085803
C	3.458457	0.235806	1.100067
C	4.417353	0.922960	1.854454
C	2.844564	-0.896958	1.643548
C	4.760926	0.482741	3.133744
C	3.179298	-1.333252	2.926345
C	4.140221	-0.647718	3.674536
H	4.885698	1.812878	1.441735
H	2.068126	-1.403232	1.081620
H	5.504001	1.026166	3.711060
H	2.675043	-2.198388	3.347631
H	4.398486	-0.986806	4.673949
C	4.721251	-1.190918	-1.127706
C	5.961115	-1.184499	-0.475613
C	4.107377	-2.415543	-1.415625
C	6.567398	-2.382719	-0.097016
C	4.716187	-3.615486	-1.040140
C	5.944125	-3.602848	-0.374840
H	6.444901	-0.237613	-0.251707
H	3.158046	-2.433490	-1.938600
H	7.526373	-2.363770	0.413061
H	4.227936	-4.559462	-1.266531
H	6.415757	-4.536024	-0.080085
H	-6.071581	-3.891014	2.583955
C	-4.559562	-2.664555	3.517931
C	-5.007093	-3.713816	2.709756
C	-4.076674	-4.523557	2.050518
H	-4.415419	-5.331043	1.406785
C	-2.709211	-4.292548	2.211748
H	-1.987993	-4.921645	1.694819
H	-0.207559	-3.354794	2.376991
C	-0.770562	-3.088370	3.275524
H	-0.448293	-3.744797	4.091003
C	-2.255462	-3.256322	3.038836
H	-2.842424	-1.624569	4.311583
C	-3.190766	-2.438806	3.683690
H	-5.275977	-2.020468	4.020839
O	-0.406905	-1.774132	3.718807
C	-0.258381	-0.820077	2.745349
C	0.430959	0.713678	4.669984
H	0.084622	1.704064	4.993796
H	1.515903	0.674097	4.857065
H	-0.042418	-0.033608	5.308294
C	0.095608	0.466077	3.224583
N	0.474327	1.363715	2.234386
C	1.170630	2.430237	2.510003
H	1.545232	2.596744	3.520459
C	1.562970	3.429055	1.518473
C	0.803753	3.706100	0.364141
H	-0.142154	3.198498	0.219721
H	0.630662	4.837867	-1.450795
C	1.239777	4.640892	-0.573314
C	2.439798	5.333088	-0.375581

H	2.778912	6.062506	-1.105926
C	3.188598	5.093777	0.782264
H	4.115529	5.635291	0.952582
C	2.751058	4.161264	1.722431
H	3.340634	3.973942	2.616567
O	-0.435967	-1.135722	1.539912
H	-1.789549	1.009142	2.839651
O	-2.729163	1.136348	2.532316
C	-2.961133	2.383683	2.135995
O	-1.945005	3.206985	2.453265
O	-3.985962	2.726878	1.578995
H	-2.114210	4.690531	0.986820
C	-2.112412	4.586880	2.073883
H	-3.043247	4.986819	2.484035
H	-1.254752	5.110080	2.495527

Int6-C_S_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.406895
Thermal and entropic correction, BS1 (a.u.)	1.480112
Electronic Energy, BS2 (a.u.)	-9902.761123
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	2.631344	0.229022	-0.306642
Fe	4.965865	-3.216190	-0.710127
P	1.951304	-1.626787	-1.320977
C	3.457837	-2.476177	-1.893292
C	4.720196	-1.822893	-2.187632
C	5.645581	-2.824785	-2.632705
H	6.675443	-2.638106	-2.898716
C	4.982296	-4.079469	-2.609626
H	5.429680	-5.035722	-2.842596
C	3.646525	-3.872082	-2.159065
H	2.907260	-4.641374	-1.990426
C	4.522849	-2.817461	1.278959
H	3.706156	-2.200699	1.615234
C	5.814075	-2.316677	0.958970
H	6.110618	-1.281380	1.028949
C	6.619145	-3.407819	0.516575
H	7.641830	-3.348377	0.169176
C	5.818407	-4.591561	0.565538
H	6.128109	-5.580898	0.256888
C	4.519324	-4.223561	1.034368
H	3.667071	-4.881426	1.137900
O	6.198566	-0.045031	-2.697929
C	5.067919	-0.416486	-2.041782
N	4.444669	0.504020	-1.388387
C	5.119782	1.781710	-1.723988
C	6.524824	1.290386	-2.218784
H	6.854975	1.871162	-3.082377
H	4.583999	2.194151	-2.588833
C	0.941509	-1.431228	-2.852257
C	-0.010891	-0.399507	-2.855666
H	-0.093001	0.241702	-1.982248
C	-0.818044	-0.174123	-3.970217

H	-1.543341	0.632823	-3.956782
C	-0.672689	-0.974624	-5.106450
H	-1.291095	-0.795809	-5.981175
C	0.282225	-1.994958	-5.121141
H	0.406297	-2.610812	-6.007163
C	1.086908	-2.222385	-4.001561
H	1.836442	-3.007266	-4.027857
C	1.085676	-2.954065	-0.382322
C	1.085180	-2.871208	1.019160
H	1.539663	-2.011772	1.502238
C	0.503082	-3.884398	1.781282
H	0.497498	-3.808171	2.864190
C	-0.092607	-4.981169	1.154013
H	-0.549078	-5.766646	1.749451
C	-0.118098	-5.057370	-0.239986
H	-0.606245	-5.892180	-0.733318
C	0.467017	-4.047675	-1.004686
H	0.422770	-4.105142	-2.087232
C	5.137559	2.831650	-0.647223
C	5.053828	4.177240	-1.024663
C	5.312044	2.506211	0.701199
C	5.150438	5.189985	-0.071155
C	5.412426	3.519260	1.654344
C	5.332589	4.860859	1.273703
H	4.890397	4.431600	-2.068811
H	5.364462	1.464424	0.997506
H	5.077716	6.229896	-0.375925
H	5.556113	3.267826	2.700014
H	5.412385	5.644099	2.021942
C	7.613947	1.222474	-1.168958
C	8.259090	2.402322	-0.775916
C	7.955541	0.019340	-0.543384
C	9.207688	2.383036	0.245016
C	8.905363	-0.000128	0.480123
C	9.530335	1.181059	0.881252
H	7.995748	3.343662	-1.249622
H	7.483654	-0.903832	-0.857099
H	9.693311	3.306637	0.545203
H	9.151161	-0.940319	0.964821
H	10.268881	1.166137	1.677385
H	8.450652	-0.961974	3.583570
C	6.633670	-1.903370	4.270006
C	7.383852	-0.845874	3.749662
C	6.752852	0.359441	3.436093
H	7.323860	1.180240	3.011998
C	5.381244	0.504592	3.651119
H	4.884965	1.437372	3.415993
H	2.899526	-0.326003	5.433171
C	3.124911	-0.417754	4.365789
H	2.612492	-1.307098	3.981614
C	4.620297	-0.555320	4.149251
H	4.677399	-2.599120	4.838060
C	5.258294	-1.760999	4.459426
H	7.115452	-2.846476	4.510811
O	2.563015	0.765604	3.789287
C	2.502134	0.805746	2.418211
C	1.945208	3.279706	2.690597
H	2.019551	3.041505	3.751109
H	0.954589	3.720361	2.507348

H	2.690376	4.055765	2.463149
C	2.165587	2.051674	1.857048
N	2.086728	2.083867	0.484923
C	1.865845	3.216725	-0.140551
H	1.776227	4.131939	0.442079
C	1.775318	3.416307	-1.576677
C	1.853429	2.395496	-2.547708
H	1.994778	1.370869	-2.226819
H	1.828568	1.864238	-4.623976
C	1.771699	2.679972	-3.908128
C	1.606754	3.997286	-4.353197
H	1.545259	4.217835	-5.414450
C	1.523363	5.025059	-3.407144
H	1.399258	6.054405	-3.732671
C	1.604199	4.739659	-2.046819
H	1.548905	5.549920	-1.323551
Ni	-2.546602	0.590303	0.946694
P	-4.192129	1.493704	-0.235040
C	-5.553148	2.199997	2.079675
H	-4.669341	1.815683	2.579554
C	-4.888764	0.236459	-1.407459
C	-4.149683	4.026623	-1.572277
H	-5.087043	4.269947	-1.085703
C	-3.519032	2.802034	-1.328634
C	-5.610166	2.181477	0.679262
C	-4.501250	0.269826	-2.775279
H	-3.922990	1.104513	-3.148905
C	-6.770008	2.627671	0.028101
H	-6.841260	2.576122	-1.054194
C	-6.057625	-1.875219	-1.828009
C	-5.661654	-0.824864	-0.934460
C	-3.552276	4.959777	-2.424604
H	-4.041206	5.913992	-2.596148
C	-5.623700	-1.841084	-3.192453
C	-4.849156	-0.741977	-3.635642
H	-4.531795	-0.704472	-4.674175
C	-2.277243	2.537445	-1.932651
H	-1.759904	1.610663	-1.704338
C	-7.782260	3.125645	2.167208
H	-8.629826	3.483565	2.743381
C	-6.635056	2.671105	2.821002
H	-6.588639	2.669687	3.905713
C	-7.848175	3.104205	0.772049
H	-8.747750	3.437013	0.264286
C	-5.983226	-2.900248	-4.067647
H	-5.641959	-2.861899	-5.098525
C	-7.194962	-3.982914	-2.278947
H	-7.805257	-4.812380	-1.934540
C	-1.692461	3.458696	-2.796541
H	-0.732319	3.242321	-3.249624
C	-6.753463	-3.950006	-3.623493
H	-7.027875	-4.752487	-4.301402
C	-6.854211	-2.976461	-1.404170
H	-7.191333	-3.020965	-0.375609
C	-2.335227	4.674985	-3.043847
H	-1.870319	5.403058	-3.701384
P	-3.419671	-1.416310	1.228965
C	-2.438051	-2.240846	-1.225120
H	-1.910546	-1.294229	-1.205809

C	-5.243652	-1.240340	1.528563
C	-2.640821	-3.584245	2.924166
H	-2.833750	-4.252854	2.094849
C	-2.803235	-2.202557	2.772764
C	-3.237716	-2.609766	-0.136636
C	-5.728667	-1.301989	2.864622
H	-5.060258	-1.585809	3.667545
C	-3.939570	-3.825466	-0.174257
H	-4.607661	-4.097300	0.637191
C	-7.488525	-0.597711	0.783843
C	-6.114429	-0.893678	0.493535
C	-2.189264	-4.110139	4.137035
H	-2.062592	-5.183826	4.240319
C	-7.949274	-0.641480	2.139135
C	-7.037446	-1.007569	3.158731
H	-7.387439	-1.058117	4.186265
C	-2.499327	-1.356786	3.854891
H	-2.609997	-0.280522	3.743228
C	-3.033686	-4.279656	-2.370021
H	-2.968803	-4.922386	-3.242750
C	-2.343172	-3.067557	-2.343107
H	-1.734642	-2.758844	-3.185496
C	-3.823918	-4.661816	-1.282662
H	-4.380333	-5.593070	-1.313608
C	-9.301755	-0.319930	2.429895
H	-9.634667	-0.355547	3.463569
C	-9.726053	0.066024	0.082417
H	-10.419263	0.340072	-0.707135
C	-2.048652	-1.883087	5.063922
H	-1.814865	-1.217046	5.888835
C	-10.174610	0.025773	1.424409
H	-11.207755	0.266450	1.655600
C	-8.419737	-0.234064	-0.230023
H	-8.089726	-0.189572	-1.260794
C	-1.893271	-3.265202	5.206904
H	-1.539501	-3.678464	6.146535
H	-0.546478	-0.518817	2.425978
C	-0.631600	0.047333	1.503956
H	-0.023672	-0.336390	0.686458
C	-0.838133	1.411857	1.559539
C	-1.593553	2.403734	1.391297
C	-1.902725	3.811789	1.343975
C	-2.864643	4.360608	2.209733
C	-3.177331	5.716228	2.140997
H	-3.919563	6.131377	2.815946
C	-2.540882	6.536824	1.206179
H	-2.790214	7.592282	1.151097
H	-1.091724	6.624387	-0.392821
C	-1.584633	5.995929	0.342659
C	-1.262483	4.644008	0.408733
H	-0.537372	4.218010	-0.270191
H	-3.359709	3.722312	2.931912
O	2.751651	-0.251409	1.770340

TS56-C_S_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.396718
Thermal and entropic correction, BS1 (a.u.)	1.479765

Electronic Energy, BS2 (a.u.)	-9902.748579
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-262.7i

Molecular Geometry in Cartesian Coordinates

Cu	2.769011	0.309510	-0.387044
Fe	5.119672	-3.108473	-0.944915
P	2.074761	-1.515100	-1.441824
C	3.590797	-2.312556	-2.069213
C	4.844798	-1.624562	-2.332176
C	5.779998	-2.585962	-2.842108
H	6.805757	-2.370183	-3.101924
C	5.132023	-3.847297	-2.894866
H	5.589292	-4.781153	-3.190866
C	3.796855	-3.685703	-2.423435
H	3.069479	-4.474483	-2.298819
C	4.605382	-3.004978	1.062380
H	3.701981	-2.556375	1.436378
C	5.819263	-2.299903	0.836142
H	5.971085	-1.248533	1.029376
C	6.769839	-3.218374	0.298399
H	7.781330	-2.987912	-0.007108
C	6.137105	-4.495697	0.192526
H	6.582536	-5.392888	-0.215442
C	4.795147	-4.361496	0.663691
H	4.040615	-5.136276	0.671187
O	6.337848	0.190252	-2.678849
C	5.178670	-0.224829	-2.108283
N	4.512965	0.661157	-1.448465
C	5.192297	1.959030	-1.663092
C	6.622161	1.508192	-2.122001
H	6.978986	2.131729	-2.944062
H	4.695192	2.431610	-2.520385
C	1.037436	-1.266509	-2.944127
C	0.044660	-0.274407	-2.880446
H	-0.055408	0.319488	-1.975544
C	-0.798210	-0.039978	-3.966975
H	-1.562545	0.727118	-3.902801
C	-0.649323	-0.788171	-5.137883
H	-1.299837	-0.602923	-5.987517
C	0.344020	-1.767181	-5.217162
H	0.468392	-2.344074	-6.128944
C	1.184631	-2.005723	-4.127004
H	1.960500	-2.761110	-4.202185
C	1.209806	-2.857345	-0.532039
C	1.122903	-2.749249	0.864314
H	1.563325	-1.890756	1.357638
C	0.486713	-3.739752	1.611391
H	0.408277	-3.638504	2.689054
C	-0.074352	-4.845353	0.969140
H	-0.581142	-5.610403	1.549479
C	-0.004809	-4.954318	-0.421084
H	-0.468591	-5.795582	-0.926022
C	0.628491	-3.962139	-1.169788
H	0.638855	-4.034583	-2.252638
C	5.116226	2.916297	-0.502512
C	4.908950	4.275053	-0.762013
C	5.263530	2.486272	0.822032
C	4.848730	5.199189	0.281711

C	5.208688	3.410596	1.864228
C	4.999184	4.766795	1.599892
H	4.765656	4.609379	-1.786285
H	5.405384	1.431663	1.033348
H	4.678087	6.249575	0.065153
H	5.334077	3.080401	2.889912
H	4.956353	5.480424	2.417542
C	7.667853	1.407050	-1.033967
C	8.298917	2.573225	-0.583036
C	7.980881	0.184657	-0.432219
C	9.214108	2.519286	0.466998
C	8.898541	0.130209	0.618271
C	9.514969	1.296421	1.073326
H	8.055779	3.528911	-1.039234
H	7.514104	-0.724358	-0.790118
H	9.693395	3.430932	0.810682
H	9.123601	-0.824401	1.083604
H	10.230133	1.254080	1.889601
H	8.657154	-1.077795	3.648762
C	6.850870	-2.154689	4.130149
C	7.580553	-1.017600	3.776426
C	6.918659	0.196986	3.585348
H	7.474925	1.081671	3.291184
C	5.535806	0.270838	3.755209
H	5.017323	1.211107	3.616827
H	3.015204	-0.843311	5.308307
C	3.291774	-0.815516	4.250170
H	2.832936	-1.675836	3.750237
C	4.797053	-0.866855	4.085805
H	4.900720	-2.977555	4.520801
C	5.464829	-2.080801	4.275264
H	7.357114	-3.104281	4.275620
O	2.686620	0.399133	3.772085
C	2.648977	0.567712	2.423291
C	1.615114	2.849759	2.937830
H	1.601466	2.475173	3.960693
H	0.627611	3.273160	2.716047
H	2.349535	3.664896	2.879887
C	1.961496	1.747289	1.978575
N	2.059787	1.986591	0.606675
C	1.719688	3.147103	0.123084
H	1.440900	3.950743	0.802440
C	1.692519	3.518648	-1.288983
C	1.841706	2.613699	-2.356216
H	1.997145	1.562287	-2.146671
H	1.901335	2.322551	-4.480534
C	1.793696	3.047439	-3.678571
C	1.591049	4.400261	-3.973107
H	1.551370	4.737232	-5.004547
C	1.435042	5.313395	-2.925292
H	1.276724	6.366304	-3.139706
C	1.484335	4.878047	-1.603633
H	1.365388	5.594773	-0.795269
Ni	-2.768884	0.736607	0.994260
P	-4.406368	1.450654	-0.265919
C	-5.897488	2.165298	1.964002
H	-5.016096	1.838697	2.507703
C	-5.037040	0.115315	-1.386834
C	-4.415509	3.950539	-1.683841

H	-5.372811	4.176290	-1.228137
C	-3.766919	2.742541	-1.407943
C	-5.893198	2.110569	0.563402
C	-4.697383	0.139476	-2.767589
H	-4.184836	1.000594	-3.177175
C	-7.046660	2.476295	-0.146233
H	-7.067754	2.396570	-1.229251
C	-6.079132	-2.075853	-1.720077
C	-5.719097	-0.984070	-0.860843
C	-3.813845	4.891103	-2.525730
H	-4.319120	5.832364	-2.720171
C	-5.694680	-2.046732	-3.099459
C	-5.006136	-0.912514	-3.593541
H	-4.727169	-0.880743	-4.643444
C	-2.501401	2.503369	-1.973586
H	-1.969812	1.593532	-1.710582
C	-8.175965	2.966859	1.935545
H	-9.066444	3.288657	2.466727
C	-7.035003	2.591372	2.647461
H	-7.036108	2.615152	3.732981
C	-8.180038	2.910487	0.539687
H	-9.073451	3.183448	-0.013295
C	-6.014516	-3.146950	-3.938647
H	-5.710129	-3.111189	-4.981241
C	-7.096603	-4.260786	-2.087963
H	-7.643091	-5.117608	-1.705189
C	-1.909669	3.432429	-2.824785
H	-0.925983	3.238144	-3.239817
C	-6.701718	-4.232576	-3.446976
H	-6.946566	-5.066322	-4.098089
C	-6.791321	-3.214566	-1.247294
H	-7.092209	-3.255122	-0.207466
C	-2.570989	4.632280	-3.103121
H	-2.103577	5.369157	-3.749338
P	-3.363783	-1.391374	1.253527
C	-2.372395	-2.156646	-1.216527
H	-1.898406	-1.181336	-1.187666
C	-5.190848	-1.351214	1.594879
C	-2.572431	-3.562029	2.966907
H	-2.905468	-4.247803	2.198063
C	-2.653390	-2.177871	2.764245
C	-3.144388	-2.576146	-0.125347
C	-5.625433	-1.418947	2.947915
H	-4.909052	-1.646723	3.728381
C	-3.784127	-3.824681	-0.178840
H	-4.442350	-4.135675	0.626344
C	-7.493151	-0.844013	0.923553
C	-6.113443	-1.059538	0.586848
C	-2.029504	-4.073325	4.147021
H	-1.969569	-5.148655	4.288445
C	-7.906561	-0.909935	2.293346
C	-6.938907	-1.202127	3.285537
H	-7.250318	-1.260254	4.325193
C	-2.185232	-1.317808	3.771817
H	-2.250123	-0.242430	3.625207
C	-2.873521	-4.208207	-2.385589
H	-2.784479	-4.835090	-3.267880
C	-2.242642	-2.964214	-2.345607
H	-1.655958	-2.615955	-3.188369

C	-3.637122	-4.640895	-1.298914
H	-4.153681	-5.594482	-1.340611
C	-9.268832	-0.684367	2.626199
H	-9.564593	-0.736764	3.670559
C	-9.794249	-0.342964	0.293311
H	-10.529254	-0.121279	-0.474694
C	-1.640811	-1.828255	4.950772
H	-1.282709	-1.148728	5.718570
C	-10.196550	-0.409003	1.648619
H	-11.236573	-0.242263	1.912223
C	-8.480240	-0.550064	-0.059570
H	-8.186521	-0.485303	-1.100208
C	-1.559394	-3.210270	5.139340
H	-1.135296	-3.611799	6.054870
H	-0.046608	0.022941	2.700883
C	-0.063919	0.570708	1.763901
H	0.382466	0.080626	0.906118
C	-0.991166	1.552119	1.566149
C	-1.902151	2.418886	1.327912
C	-2.181478	3.846590	1.247004
C	-3.192878	4.420426	2.034663
C	-3.486366	5.778977	1.926796
H	-4.267713	6.210112	2.545779
C	-2.787004	6.580753	1.021350
H	-3.024668	7.636582	0.931440
H	-1.249034	6.622094	-0.494720
C	-1.786903	6.014150	0.227290
C	-1.481947	4.660719	0.342397
H	-0.734135	4.213887	-0.296625
H	-3.746750	3.796091	2.726147
O	3.139219	-0.301378	1.672452

Int6-C_S_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.438605
Thermal and entropic correction, BS1 (a.u.)	1.483070
Electronic Energy, BS2 (a.u.)	-9902.789011
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	2.580402	-0.016897	-0.415514
Fe	5.028790	-3.490698	-0.297086
P	1.908751	-2.064286	-0.944024
C	3.401704	-2.985010	-1.445198
C	4.616929	-2.389727	-1.971755
C	5.519955	-3.452869	-2.311449
H	6.517823	-3.316084	-2.701373
C	4.886665	-4.685018	-2.000298
H	5.330395	-5.665927	-2.099011
C	3.594048	-4.403560	-1.469948
H	2.883978	-5.129189	-1.099179
C	4.806293	-2.665149	1.582667
H	4.037018	-1.955350	1.838183
C	6.083465	-2.327385	1.044418
H	6.431716	-1.329103	0.823109
C	6.790799	-3.539415	0.785774

H	7.773313	-3.622076	0.341434
C	5.947276	-4.628590	1.165134
H	6.180436	-5.678819	1.055072
C	4.720254	-4.088291	1.656100
H	3.854467	-4.651180	1.976795
O	6.069426	-0.698067	-2.798007
C	4.948435	-0.975657	-2.087112
N	4.309555	0.034694	-1.602664
C	4.977272	1.255703	-2.110537
C	6.377021	0.708826	-2.562821
H	6.654811	1.134190	-3.529752
H	4.432595	1.557369	-3.013861
C	0.826055	-2.200747	-2.426897
C	-0.158666	-1.216483	-2.610863
H	-0.250901	-0.411290	-1.885853
C	-1.020365	-1.273359	-3.707172
H	-1.785004	-0.515734	-3.833553
C	-0.897920	-2.305880	-4.639806
H	-1.566347	-2.346396	-5.494684
C	0.087048	-3.281842	-4.473455
H	0.190015	-4.083065	-5.199328
C	0.945433	-3.230511	-3.373484
H	1.711931	-3.989649	-3.260126
C	1.143221	-3.145341	0.321881
C	1.305878	-2.779407	1.667105
H	1.826828	-1.859249	1.910533
C	0.796476	-3.586949	2.682685
H	0.912160	-3.289621	3.719654
C	0.100065	-4.754793	2.361204
H	-0.311043	-5.376158	3.151481
C	-0.093503	-5.108063	1.024313
H	-0.669042	-5.992263	0.770344
C	0.428077	-4.308288	0.006559
H	0.252239	-4.576115	-1.029712
C	4.936630	2.407596	-1.140847
C	4.627208	3.690465	-1.604007
C	5.187805	2.214316	0.222040
C	4.572691	4.769442	-0.719158
C	5.132996	3.287810	1.108932
C	4.826524	4.568612	0.639096
H	4.402142	3.843063	-2.656339
H	5.409438	1.220423	0.591099
H	4.326131	5.760058	-1.089667
H	5.333194	3.125373	2.161128
H	4.786042	5.405553	1.330431
C	7.531580	0.836467	-1.588826
C	8.063304	2.105141	-1.318886
C	8.096503	-0.282860	-0.969498
C	9.123356	2.252619	-0.426509
C	9.162368	-0.135135	-0.077428
C	9.676569	1.132094	0.199264
H	7.635506	2.982116	-1.795129
H	7.713594	-1.270805	-1.196067
H	9.520212	3.242402	-0.223051
H	9.594293	-1.013742	0.393162
H	10.507805	1.246260	0.888723
H	8.649415	2.724861	3.484264
C	7.298714	1.097650	3.071687
C	7.670931	2.297279	3.681639

C	6.784057	2.947454	4.544944
H	7.075189	3.875568	5.027664
C	5.520653	2.405176	4.784930
H	4.826601	2.914793	5.448407
H	3.395295	0.807379	5.388499
C	3.750420	0.661938	4.367368
H	3.683863	-0.394528	4.099651
C	5.137139	1.207632	4.166270
H	5.739003	-0.371087	2.841160
C	6.037342	0.554984	3.316806
H	7.980917	0.597039	2.392778
O	2.773701	1.411659	3.567322
C	2.641608	1.090432	2.285238
C	1.451250	3.318142	2.131067
H	1.394580	3.285843	3.218774
H	0.560190	3.830951	1.772323
H	2.339088	3.888423	1.845374
C	1.533899	1.887001	1.583335
N	1.768864	1.774098	0.124222
C	1.378783	2.744718	-0.624811
H	0.970852	3.648466	-0.177629
C	1.435595	2.795770	-2.090674
C	1.682744	1.686611	-2.914783
H	1.816409	0.706604	-2.474317
H	1.944006	0.959966	-4.918159
C	1.759957	1.832121	-4.297747
C	1.586599	3.091173	-4.882740
H	1.648186	3.204168	-5.961059
C	1.313049	4.199225	-4.075635
H	1.158938	5.175807	-4.523953
C	1.230626	4.050735	-2.693058
H	1.003295	4.909323	-2.068384
Ni	-2.652562	0.944895	0.577237
P	-4.344955	1.333524	-0.775541
C	-5.472946	3.124855	1.007285
H	-4.486534	3.090324	1.461321
C	-5.119265	-0.233635	-1.405066
C	-4.493286	3.167482	-2.990251
H	-5.469517	3.474054	-2.630029
C	-3.772615	2.178470	-2.311494
C	-5.721103	2.360571	-0.142922
C	-4.871763	-0.650300	-2.742543
H	-4.378148	0.027769	-3.428430
C	-6.992455	2.392252	-0.732970
H	-7.199266	1.781988	-1.607173
C	-6.201314	-2.391729	-0.980834
C	-5.773383	-1.099640	-0.525990
C	-3.948318	3.783733	-4.121036
H	-4.510444	4.561226	-4.630155
C	-5.911207	-2.802027	-2.321914
C	-5.243483	-1.897042	-3.182590
H	-5.036307	-2.198819	-4.206191
C	-2.499098	1.822298	-2.785191
H	-1.913484	1.107579	-2.215356
C	-7.752573	3.929495	0.971542
H	-8.545467	4.528701	1.409393
C	-6.485887	3.908320	1.559686
H	-6.289055	4.494343	2.452715
C	-8.003939	3.173852	-0.176085

H	-8.992545	3.176101	-0.624586
C	-6.305679	-4.094739	-2.758729
H	-6.072664	-4.392619	-3.777710
C	-7.279365	-4.544298	-0.593931
H	-7.813435	-5.220836	0.066838
C	-1.964626	2.415952	-3.926608
H	-0.976727	2.130325	-4.271473
C	-6.976860	-4.950158	-1.915780
H	-7.280084	-5.933838	-2.261790
C	-6.898908	-3.302669	-0.137790
H	-7.128251	-3.008120	0.879306
C	-2.690632	3.406743	-4.594688
H	-2.271297	3.888650	-5.473195
P	-3.305543	-0.946933	1.499999
C	-2.562459	-2.542555	-0.627955
H	-2.099590	-1.622966	-0.964887
C	-5.113740	-0.703245	1.897881
C	-2.269053	-2.543459	3.672724
H	-2.484830	-3.429352	3.088822
C	-2.538529	-1.271461	3.153424
C	-3.238769	-2.544413	0.597576
C	-5.479698	-0.308471	3.215023
H	-4.736377	-0.318300	4.002484
C	-3.883110	-3.717859	1.019420
H	-4.461963	-3.721196	1.938175
C	-7.433209	-0.319489	1.194464
C	-6.082254	-0.701837	0.889564
C	-1.689249	-2.686128	4.936339
H	-1.488347	-3.681436	5.322868
C	-7.766942	0.107274	2.519656
C	-6.757997	0.094658	3.512984
H	-7.010095	0.401406	4.524827
C	-2.201122	-0.145070	3.926191
H	-2.385396	0.845082	3.518398
C	-3.153658	-4.853599	-0.989749
H	-3.139193	-5.744876	-1.610348
C	-2.522459	-3.686639	-1.423544
H	-2.010014	-3.656511	-2.379696
C	-3.828930	-4.868867	0.233858
H	-4.347265	-5.766146	0.557730
C	-9.094271	0.521659	2.810396
H	-9.326835	0.849238	3.820175
C	-9.748313	0.066825	0.530781
H	-10.520228	0.049151	-0.233032
C	-1.627946	-0.287415	5.188858
H	-1.382829	0.595216	5.773149
C	-10.067659	0.503315	1.838795
H	-11.080398	0.818344	2.071651
C	-8.468529	-0.329832	0.216355
H	-8.239513	-0.651168	-0.792352
C	-1.370053	-1.562952	5.699437
H	-0.924740	-1.678373	6.683386
H	0.095532	1.070934	2.996142
C	0.228801	1.065833	1.908352
H	0.406602	0.024329	1.620584
C	-0.996838	1.555740	1.233506
C	-1.606135	2.543102	0.667460
C	-1.721526	3.969858	0.422834
C	-1.937573	4.839467	1.513074

C	-2.074931	6.212478	1.317019
H	-2.242519	6.862183	2.171628
C	-2.000964	6.753492	0.030536
H	-2.112545	7.822799	-0.121459
H	-1.740270	6.305890	-2.064967
C	-1.790441	5.902475	-1.057022
C	-1.656542	4.527562	-0.867762
H	-1.504121	3.878251	-1.718649
H	-2.001537	4.419008	2.512800
O	3.262731	0.173643	1.756623

Int5-C_R_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.393881
Thermal and entropic correction, BS1 (a.u.)	1.477239
Electronic Energy, BS2 (a.u.)	-9902.752778
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	-3.535411	-0.507227	0.607174
Fe	-6.687171	1.036239	-1.717262
P	-5.692021	-0.972036	0.927925
C	-6.622573	0.438926	0.250584
C	-6.085654	1.778963	0.097630
C	-7.124676	2.614337	-0.433577
H	-7.011389	3.658942	-0.683434
C	-8.282380	1.813766	-0.617159
H	-9.216100	2.143719	-1.051149
C	-7.980621	0.486254	-0.196073
H	-8.642771	-0.366245	-0.247033
C	-5.276972	0.003029	-2.830601
H	-4.459775	-0.557950	-2.395923
C	-5.255402	1.390024	-3.174452
H	-4.415978	2.059157	-3.049497
C	-6.547627	1.750230	-3.658593
H	-6.860048	2.740518	-3.960809
C	-7.372573	0.585695	-3.617903
H	-8.420356	0.540011	-3.881874
C	-6.589015	-0.491779	-3.106617
H	-6.938623	-1.494646	-2.906072
O	-4.590111	3.596499	0.377550
C	-4.730828	2.249941	0.360052
N	-3.658191	1.556651	0.563760
C	-2.522224	2.499245	0.622690
C	-3.257970	3.855318	0.908957
H	-3.373802	3.948584	1.996759
H	-1.889101	2.250619	1.479839
C	-6.238440	-1.069407	2.677420
C	-7.391772	-0.449584	3.179533
H	-8.036737	0.120874	2.518359
C	-7.708438	-0.552804	4.535942
H	-8.601880	-0.067768	4.918678
C	-6.879449	-1.273794	5.397994
H	-7.126028	-1.347073	6.453201
C	-5.727546	-1.891071	4.903982
H	-5.068469	-2.435908	5.573276

C	-5.405471	-1.786133	3.552189
H	-4.492268	-2.236597	3.173866
C	-6.468843	-2.421916	0.114989
C	-5.752637	-3.034270	-0.924412
H	-4.771421	-2.650352	-1.183941
C	-6.303384	-4.115418	-1.614511
H	-5.743854	-4.584901	-2.418875
C	-7.566751	-4.598385	-1.264293
H	-7.994335	-5.441961	-1.798250
C	-8.274548	-4.005870	-0.214323
H	-9.249745	-4.390829	0.069435
C	-7.726979	-2.924523	0.477532
H	-8.270361	-2.479976	1.306667
C	-1.688374	2.446061	-0.649740
C	-0.537505	3.238507	-0.758006
C	-2.042938	1.625684	-1.723289
C	0.224018	3.231330	-1.923881
C	-1.272390	1.601336	-2.887996
C	-0.140967	2.408971	-2.994258
H	-0.250531	3.881422	0.063860
H	-2.896138	0.970872	-1.636507
H	1.104001	3.862059	-1.994970
H	-1.553767	0.938568	-3.697864
H	0.460242	2.388472	-3.898011
C	-2.698816	5.126935	0.346145
C	-1.942124	5.965949	1.170714
C	-2.865190	5.456979	-1.003829
C	-1.335284	7.109818	0.649230
C	-2.270550	6.605572	-1.522231
C	-1.497857	7.430291	-0.699848
H	-1.825735	5.720378	2.223357
H	-3.452817	4.804820	-1.641132
H	-0.751197	7.756680	1.297550
H	-2.405060	6.855562	-2.570346
H	-1.033981	8.323907	-1.106750
H	0.717623	0.263636	-6.072797
C	0.723482	-0.943974	-4.282694
C	0.151128	-0.413656	-5.440317
C	-1.163362	-0.751367	-5.770904
H	-1.626677	-0.335157	-6.660575
C	-1.890110	-1.616470	-4.950638
H	-2.917100	-1.864498	-5.208171
H	-1.988325	-4.177127	-3.462424
C	-2.103248	-3.188776	-3.003423
H	-3.165101	-2.924554	-3.021815
C	-1.312903	-2.169120	-3.800564
H	0.450714	-2.227754	-2.571886
C	0.001809	-1.822426	-3.470859
H	1.738589	-0.665883	-4.012579
O	-1.659967	-3.375739	-1.657123
C	-2.115689	-2.457259	-0.733641
C	-1.281265	-4.077640	1.068580
H	-1.194276	-4.772308	0.234619
H	-1.945727	-4.523863	1.823010
H	-0.289293	-3.994734	1.531243
C	-1.828421	-2.757285	0.613248
N	-2.122181	-1.755512	1.510310
C	-1.762116	-1.841970	2.770274
H	-1.214956	-2.721314	3.112906

C	-1.987531	-0.829979	3.793662
C	-2.770757	0.331010	3.618740
H	-3.271651	0.497056	2.673843
H	-3.558854	2.127634	4.481801
C	-2.937027	1.251409	4.648478
C	-2.330132	1.050481	5.892943
H	-2.466816	1.767079	6.697111
C	-1.556830	-0.098577	6.090565
H	-1.083762	-0.276532	7.052377
C	-1.390148	-1.021938	5.060146
H	-0.788475	-1.912059	5.230435
Ni	2.583138	-0.757492	0.068868
P	4.598948	-1.569175	-0.373957
C	5.001608	-2.151572	2.314343
H	3.986556	-1.783002	2.432642
C	5.667391	-0.301146	-1.205677
C	5.089462	-4.144240	-1.535531
H	5.747542	-4.366630	-0.703598
C	4.442134	-2.907589	-1.617918
C	5.576396	-2.186410	1.035637
C	5.886305	-0.380773	-2.608766
H	5.548901	-1.249790	-3.158203
C	6.903961	-2.613523	0.884849
H	7.371337	-2.604041	-0.095350
C	6.815094	1.863053	-1.186571
C	6.138706	0.803478	-0.495662
C	4.859062	-5.116311	-2.512645
H	5.352517	-6.079954	-2.432780
C	6.982746	1.784772	-2.606424
C	6.518846	0.632532	-3.285876
H	6.670040	0.556304	-4.359271
C	3.551642	-2.668496	-2.678253
H	3.011565	-1.728035	-2.716336
C	7.056455	-2.988320	3.269421
H	7.635474	-3.290698	4.136409
C	5.738951	-2.552492	3.426845
H	5.291479	-2.509983	4.414992
C	7.636703	-3.019774	1.999197
H	8.666626	-3.340372	1.879025
C	7.607471	2.856799	-3.297477
H	7.723951	2.783811	-4.375296
C	7.906697	4.041626	-1.212297
H	8.269667	4.915956	-0.680401
C	3.334275	-3.630877	-3.658958
H	2.634657	-3.426242	-4.463513
C	8.059475	3.964173	-2.617635
H	8.537681	4.778007	-3.154100
C	7.301810	3.020401	-0.515248
H	7.186178	3.097388	0.559184
C	3.993372	-4.860704	-3.576312
H	3.817901	-5.623300	-4.328948
P	3.186482	1.298215	0.578725
C	3.168649	1.890282	-2.129208
H	2.704754	0.913295	-2.221398
C	4.750837	1.245780	1.575605
C	1.779215	3.521256	1.706820
H	2.287812	4.162507	0.997105
C	1.993495	2.137468	1.697083
C	3.500476	2.379013	-0.857628

C	4.657792	1.363011	2.990923
H	3.712977	1.629209	3.447744
C	4.102010	3.641385	-0.740305
H	4.419725	4.006869	0.231101
C	7.128055	0.698921	1.815791
C	5.974697	0.918939	0.989801
C	0.872497	4.085662	2.607838
H	0.700741	5.157282	2.588245
C	7.007035	0.801797	3.238999
C	5.750108	1.145031	3.794095
H	5.657646	1.239155	4.872750
C	1.291255	1.331629	2.610937
H	1.440537	0.254455	2.608966
C	4.008418	3.916529	-3.141270
H	4.212588	4.511366	-4.026123
C	3.429109	2.652354	-3.266278
H	3.176803	2.260132	-4.246668
C	4.341369	4.411134	-1.877576
H	4.816959	5.381535	-1.780232
C	8.141901	0.559616	4.057764
H	8.032811	0.640179	5.135834
C	9.482135	0.133091	2.092657
H	10.442406	-0.126218	1.657158
C	0.394090	1.895388	3.516602
H	-0.139415	1.261659	4.213965
C	9.355840	0.233016	3.498925
H	10.218976	0.052968	4.132461
C	8.399225	0.357111	1.273239
H	8.510219	0.268323	0.199347
C	0.179867	3.276710	3.510027
H	-0.530003	3.711298	4.207486
H	0.080553	0.235496	0.645282
C	0.558458	-0.270728	-0.186922
H	0.337555	0.161422	-1.161719
C	0.799100	-1.624394	-0.093099
C	1.634523	-2.567867	0.024436
C	1.927481	-3.983137	0.021528
C	1.377644	-4.810417	-0.974463
C	1.659786	-6.173491	-0.981095
H	1.230031	-6.804926	-1.752945
C	2.484495	-6.730304	0.000272
H	2.699114	-7.794729	-0.009088
H	3.663058	-6.341302	1.765757
C	3.026342	-5.914921	0.996385
C	2.754254	-4.549162	1.005827
H	3.179000	-3.915396	1.774134
H	0.712105	-4.380245	-1.712871
O	-2.726054	-1.434016	-1.155263

TS56-C_R_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.383860
Thermal and entropic correction, BS1 (a.u.)	1.4742901
Electronic Energy, BS2 (a.u.)	-9902.742598
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-140.5i

Molecular Geometry in Cartesian Coordinates

Cu	-3.864590	-0.475995	0.563802
Fe	-7.213643	0.984307	-1.397683
P	-5.912197	-1.322699	0.807849
C	-7.062683	0.031898	0.415659
C	-6.748144	1.442135	0.547201
C	-7.905033	2.193532	0.149699
H	-7.960962	3.271455	0.114395
C	-8.919019	1.273404	-0.224410
H	-9.893063	1.531469	-0.616236
C	-8.410143	-0.046934	-0.058190
H	-8.928034	-0.964574	-0.296999
C	-5.711227	0.298602	-2.654318
H	-4.860305	-0.276160	-2.318097
C	-5.769578	1.722639	-2.699092
H	-4.973414	2.394896	-2.415154
C	-7.072595	2.103897	-3.137818
H	-7.440744	3.115872	-3.238625
C	-7.822450	0.910492	-3.370962
H	-8.858985	0.861502	-3.675509
C	-6.982383	-0.204302	-3.070260
H	-7.269579	-1.246361	-3.095733
O	-5.554209	3.378198	1.198987
C	-5.477301	2.059587	0.904423
N	-4.303262	1.523956	0.933987
C	-3.331827	2.571142	1.301014
C	-4.196818	3.896558	1.238108
H	-4.096851	4.459193	2.169363
H	-3.018414	2.400561	2.338846
C	-6.393925	-1.833051	2.503376
C	-7.479007	-1.283809	3.199717
H	-8.122899	-0.553983	2.719184
C	-7.731387	-1.667120	4.519598
H	-8.572852	-1.234732	5.053305
C	-6.907102	-2.599953	5.150063
H	-7.101914	-2.890764	6.178108
C	-5.825693	-3.153855	4.459247
H	-5.169673	-3.865308	4.950891
C	-5.567632	-2.769774	3.145941
H	-4.705925	-3.174682	2.623221
C	-6.479835	-2.694858	-0.268218
C	-5.698716	-3.006783	-1.391021
H	-4.777369	-2.459195	-1.564073
C	-6.107551	-4.007623	-2.274342
H	-5.499863	-4.243201	-3.143405
C	-7.290694	-4.710773	-2.034812
H	-7.607321	-5.491829	-2.719742
C	-8.059802	-4.420823	-0.903689
H	-8.971031	-4.978479	-0.708086
C	-7.655039	-3.419761	-0.020047
H	-8.243947	-3.207746	0.868078
C	-2.111981	2.571728	0.413966
C	-0.900262	3.074399	0.897034
C	-2.202807	2.167734	-0.921375
C	0.195799	3.215509	0.045290
C	-1.107616	2.295371	-1.771975
C	0.088527	2.832687	-1.293502
H	-0.816709	3.366836	1.940507
H	-3.123272	1.730125	-1.285020

H	1.127197	3.624386	0.420100
H	-1.190218	1.978910	-2.803440
H	0.935335	2.942797	-1.961285
C	-3.956588	4.801656	0.050779
C	-2.857364	5.668636	0.060858
C	-4.785641	4.765224	-1.074664
C	-2.571082	6.459799	-1.050030
C	-4.501204	5.560968	-2.186374
C	-3.389773	6.404135	-2.180789
H	-2.211055	5.709904	0.932822
H	-5.659007	4.123696	-1.077265
H	-1.710591	7.121916	-1.031839
H	-5.152521	5.522637	-3.054949
H	-3.167952	7.021857	-3.045822
H	0.884503	2.375217	-5.423016
C	0.946439	0.619842	-4.166952
C	0.330070	1.527227	-5.032054
C	-1.009427	1.342407	-5.382784
H	-1.502508	2.048830	-6.043871
C	-1.723785	0.257177	-4.869981
H	-2.771054	0.128619	-5.132346
H	-1.662401	-2.732011	-4.216046
C	-1.876623	-1.884067	-3.557109
H	-2.951339	-1.686196	-3.580296
C	-1.106008	-0.664286	-4.016420
H	0.725559	-1.171731	-2.997456
C	0.237104	-0.474088	-3.667508
H	1.984312	0.765821	-3.880265
O	-1.490208	-2.354368	-2.255727
C	-2.083513	-1.761838	-1.176583
C	-0.903349	-3.559902	0.216533
H	-0.583769	-3.925827	-0.756479
H	-1.542546	-4.326342	0.677370
H	-0.003908	-3.467967	0.838264
C	-1.649330	-2.260894	0.088905
N	-2.246883	-1.667173	1.188113
C	-1.977256	-2.091418	2.396201
H	-1.305668	-2.940560	2.530590
C	-2.491502	-1.528901	3.637073
C	-3.243386	-0.341064	3.719574
H	-3.484575	0.197938	2.813279
H	-4.285720	1.047469	4.979082
C	-3.695967	0.135443	4.945119
C	-3.403656	-0.552042	6.127805
H	-3.760394	-0.178585	7.082747
C	-2.651398	-1.728789	6.066391
H	-2.418194	-2.274246	6.976281
C	-2.203396	-2.209511	4.838266
H	-1.626604	-3.131146	4.800130
Ni	3.215939	-0.891121	-0.202845
P	5.252256	-1.095597	-0.968805
C	5.793211	-2.934598	1.051956
H	4.721555	-2.886752	1.225384
C	6.101634	0.547520	-1.055691
C	6.267609	-2.563598	-3.213657
H	7.101322	-2.876611	-2.595667
C	5.273139	-1.725505	-2.694808
C	6.356101	-2.167060	0.021037
C	6.225370	1.180623	-2.323567

H	5.955728	0.636179	-3.220616
C	7.744058	-2.199024	-0.182263
H	8.197200	-1.569902	-0.942330
C	6.948188	2.586214	0.005327
C	6.460190	1.239588	0.103780
C	6.172246	-3.032836	-4.525454
H	6.941319	-3.693168	-4.914924
C	7.045844	3.211803	-1.279509
C	6.680976	2.471415	-2.430569
H	6.768952	2.938521	-3.407901
C	4.187003	-1.368638	-3.510151
H	3.389915	-0.761210	-3.093271
C	7.983925	-3.765520	1.644208
H	8.617913	-4.377272	2.278571
C	6.604673	-3.731030	1.859145
H	6.161932	-4.314211	2.660829
C	8.551539	-3.001019	0.622454
H	9.625888	-3.007857	0.469503
C	7.501808	4.553726	-1.371862
H	7.568097	5.014125	-2.353938
C	7.766441	4.642176	1.028162
H	8.047546	5.201151	1.915696
C	4.097276	-1.828434	-4.820912
H	3.241962	-1.550039	-5.429225
C	7.856311	5.256763	-0.243683
H	8.207229	6.281066	-0.324953
C	7.322989	3.344928	1.150370
H	7.251618	2.891027	2.131377
C	5.092165	-2.666870	-5.330351
H	5.019684	-3.042585	-6.346500
P	3.552456	0.748536	1.261110
C	3.429147	2.652656	-0.749709
H	3.163171	1.801809	-1.369842
C	5.160716	0.446944	2.136163
C	1.632395	1.870643	3.083918
H	1.924497	2.857067	2.743909
C	2.266661	0.730590	2.575904
C	3.663988	2.454160	0.617801
C	5.144225	-0.135993	3.432807
H	4.203653	-0.249292	3.957763
C	4.030434	3.544967	1.420228
H	4.259701	3.394539	2.471005
C	7.598384	0.203212	2.097368
C	6.375407	0.615649	1.467660
C	0.597548	1.744166	4.015924
H	0.108924	2.637265	4.395160
C	7.554379	-0.417015	3.387455
C	6.302673	-0.563255	4.033648
H	6.268925	-1.013860	5.022016
C	1.843674	-0.536586	3.020763
H	2.303686	-1.429746	2.603226
C	3.896022	5.009867	-0.499635
H	3.994764	6.000116	-0.933313
C	3.548674	3.924477	-1.306748
H	3.377214	4.067107	-2.369333
C	4.134875	4.819303	0.863637
H	4.427974	5.657837	1.487298
C	8.759976	-0.862957	3.991970
H	8.707703	-1.336646	4.968526

C	10.021253	-0.068555	2.091040
H	10.979009	0.066808	1.597430
C	0.822568	-0.656755	3.959066
H	0.498726	-1.637826	4.288070
C	9.970026	-0.693626	3.359916
H	10.886671	-1.033774	3.832068
C	8.868965	0.364529	1.475272
H	8.924957	0.831827	0.499665
C	0.187938	0.485909	4.456338
H	-0.629519	0.384344	5.162980
H	0.229841	-0.673301	0.985826
C	0.408084	-0.771451	-0.078901
H	-0.034387	-0.014628	-0.721541
C	1.346996	-1.622752	-0.551471
C	2.299857	-2.364387	-1.004093
C	2.469459	-3.602352	-1.751987
C	1.471269	-4.030923	-2.648887
C	1.647829	-5.190265	-3.399756
H	0.870478	-5.507955	-4.088914
C	2.817976	-5.943329	-3.269027
H	2.955508	-6.844871	-3.858635
H	4.720256	-6.112271	-2.265891
C	3.808716	-5.532068	-2.374621
C	3.637454	-4.371315	-1.624011
H	4.411126	-4.052479	-0.936285
H	0.561092	-3.450209	-2.742144
O	-2.927956	-0.851676	-1.353482

Int6-C_R_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.420425
Thermal and entropic correction, BS1 (a.u.)	1.478893
Electronic Energy, BS2 (a.u.)	-9902.779492
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	-4.004014	-0.662998	0.320666
Fe	-7.496847	1.167094	-1.122791
P	-5.975084	-1.644662	0.160597
C	-7.217867	-0.316729	0.261850
C	-7.000445	0.993408	0.854296
C	-8.222735	1.737431	0.743143
H	-8.357017	2.758466	1.068683
C	-9.181179	0.916105	0.094592
H	-10.184750	1.211182	-0.178388
C	-8.573957	-0.338831	-0.196237
H	-9.035588	-1.160949	-0.723545
C	-5.943875	1.131280	-2.490241
H	-5.016235	0.599280	-2.331847
C	-6.208597	2.475326	-2.089509
H	-5.519497	3.137310	-1.585483
C	-7.560784	2.782655	-2.423860
H	-8.072932	3.711434	-2.212802
C	-8.133872	1.628350	-3.038076
H	-9.157954	1.528690	-3.370737
C	-7.136702	0.608601	-3.079399

H	-7.271340	-0.401235	-3.440114
O	-5.903121	2.699485	2.087623
C	-5.762758	1.560521	1.375077
N	-4.560152	1.122016	1.212383
C	-3.633572	2.035928	1.907654
C	-4.570543	3.247580	2.307712
H	-4.487352	3.449834	3.378145
H	-3.290457	1.537121	2.822613
C	-6.407836	-2.776964	1.538606
C	-7.514564	-2.589678	2.376308
H	-8.200899	-1.767739	2.199251
C	-7.735935	-3.458079	3.449192
H	-8.595278	-3.305213	4.095580
C	-6.861098	-4.518234	3.686953
H	-7.034932	-5.190080	4.522149
C	-5.756380	-4.711789	2.851850
H	-5.065863	-5.527828	3.040888
C	-5.526738	-3.842300	1.789338
H	-4.651244	-3.975848	1.159160
C	-6.414093	-2.571293	-1.356246
C	-5.575298	-2.432107	-2.472145
H	-4.684044	-1.815352	-2.396605
C	-5.888104	-3.079446	-3.669101
H	-5.237715	-2.966151	-4.531477
C	-7.031607	-3.877327	-3.753803
H	-7.273412	-4.383103	-4.683767
C	-7.856560	-4.039894	-2.636463
H	-8.735413	-4.674875	-2.697026
C	-7.547621	-3.394091	-1.439239
H	-8.177081	-3.540186	-0.565796
C	-2.428380	2.376946	1.065703
C	-1.159388	2.453883	1.645563
C	-2.577783	2.674490	-0.294632
C	-0.054894	2.844624	0.883240
C	-1.480343	3.068400	-1.053821
C	-0.214648	3.153430	-0.467870
H	-1.027368	2.196787	2.693373
H	-3.556804	2.589412	-0.750203
H	0.928972	2.898421	1.334157
H	-1.602889	3.313854	-2.103206
H	0.642276	3.442426	-1.064658
C	-4.395737	4.524956	1.518922
C	-3.286676	5.338369	1.782516
C	-5.288030	4.891946	0.507310
C	-3.056105	6.483925	1.023944
C	-5.058561	6.042952	-0.250427
C	-3.939549	6.837208	0.000328
H	-2.587069	5.060240	2.565818
H	-6.165846	4.284171	0.319997
H	-2.187367	7.101137	1.231659
H	-5.759001	6.319409	-1.033298
H	-3.760410	7.730598	-0.590077
H	3.052377	3.949524	-4.483340
C	2.451876	2.137911	-3.478374
C	2.230967	3.276566	-4.255304
C	0.947885	3.545467	-4.738518
H	0.764363	4.430492	-5.340313
C	-0.104188	2.677883	-4.443323
H	-1.102306	2.895506	-4.817575

H	-1.242122	-0.061476	-4.226206
C	-1.055618	0.620260	-3.387530
H	-1.972107	1.180236	-3.192366
C	0.113828	1.535248	-3.663283
H	1.576320	0.402256	-2.548893
C	1.399516	1.267897	-3.178544
H	3.446500	1.928891	-3.095250
O	-0.748232	-0.204626	-2.237738
C	-1.713865	-0.572357	-1.410708
C	-1.085534	-2.888347	-0.836386
H	-0.495587	-2.917543	-1.751389
H	-2.092386	-3.266133	-1.038638
H	-0.599267	-3.543077	-0.109259
C	-1.174956	-1.451256	-0.274015
N	-2.179422	-1.425729	0.829605
C	-1.873593	-2.090486	1.890149
H	-0.924124	-2.630688	1.930647
C	-2.676664	-2.241686	3.105229
C	-3.788611	-1.443417	3.424617
H	-4.096031	-0.654745	2.750684
H	-5.372437	-1.056188	4.820142
C	-4.505931	-1.669736	4.594604
C	-4.127698	-2.694442	5.466844
H	-4.696444	-2.873481	6.374117
C	-3.016490	-3.487090	5.169473
H	-2.715029	-4.281183	5.845518
C	-2.293261	-3.256283	4.001837
H	-1.428570	-3.873145	3.771463
Ni	3.289277	-0.989098	-0.323123
P	5.345933	-1.129606	-1.097296
C	5.916895	-3.256214	0.590673
H	4.835840	-3.280156	0.706040
C	6.122040	0.556984	-0.936093
C	6.510212	-2.353764	-3.428917
H	7.282585	-2.767507	-2.790848
C	5.505230	-1.539455	-2.889957
C	6.487155	-2.287033	-0.247415
C	6.153182	1.393589	-2.087780
H	5.910834	0.972537	-3.056430
C	7.882517	-2.231144	-0.380027
H	8.336728	-1.462585	-0.997966
C	6.837787	2.477936	0.412263
C	6.457010	1.095141	0.309643
C	6.512824	-2.661526	-4.791520
H	7.292879	-3.301424	-5.194059
C	6.834405	3.304579	-0.757057
C	6.486658	2.722778	-2.000794
H	6.500817	3.340855	-2.895071
C	4.501990	-1.050858	-3.743424
H	3.689045	-0.468549	-3.324873
C	8.116007	-4.092786	1.144775
H	8.749500	-4.784560	1.691972
C	6.727999	-4.155700	1.283313
H	6.278442	-4.897031	1.937657
C	8.691929	-3.131056	0.311371
H	9.771394	-3.064538	0.220411
C	7.186275	4.676164	-0.648426
H	7.174906	5.288058	-1.546673
C	7.557691	4.406058	1.721935

H	7.841018	4.836975	2.677772
C	4.513463	-1.344435	-5.104208
H	3.720204	-0.966234	-5.741363
C	7.543205	5.219349	0.564192
H	7.817104	6.267725	0.635812
C	7.211006	3.075755	1.649508
H	7.216932	2.469677	2.547269
C	5.520281	-2.155830	-5.631909
H	5.523406	-2.403148	-6.689439
P	3.643349	0.237485	1.460055
C	3.254178	2.521389	-0.055412
H	2.979862	1.799787	-0.816668
C	5.296925	-0.071050	2.247986
C	1.682319	0.850645	3.488368
H	1.888814	1.902995	3.329992
C	2.414959	-0.121574	2.796093
C	3.598369	2.056846	1.221386
C	5.378533	-0.825944	3.450272
H	4.472229	-1.075533	3.988633
C	3.964810	2.980288	2.211540
H	4.272588	2.630289	3.192827
C	7.741033	-0.140009	2.089675
C	6.468542	0.272690	1.568596
C	0.669853	0.478164	4.379405
H	0.108892	1.246810	4.904193
C	7.795272	-0.939084	3.276609
C	6.586200	-1.255359	3.942409
H	6.625613	-1.841716	4.856787
C	2.116976	-1.477948	3.027324
H	2.651093	-2.238499	2.462955
C	3.639403	4.799095	0.648071
H	3.672489	5.861100	0.424620
C	3.282304	3.884569	-0.344989
H	3.036290	4.224062	-1.347027
C	3.973832	4.345921	1.927026
H	4.272065	5.054436	2.693613
C	9.052044	-1.390799	3.760461
H	9.073747	-2.003102	4.658090
C	10.172934	-0.254063	1.947771
H	11.096389	0.010797	1.441228
C	1.124398	-1.848301	3.932455
H	0.916285	-2.900562	4.104780
C	10.218678	-1.058576	3.111666
H	11.174704	-1.407120	3.490687
C	8.969474	0.191555	1.450196
H	8.950356	0.797693	0.552538
C	0.385709	-0.868655	4.604822
H	-0.405249	-1.157922	5.289904
H	0.331302	-1.195669	1.258627
C	0.199238	-0.888286	0.220008
H	0.126488	0.203510	0.263247
C	1.428130	-1.274035	-0.511253
C	2.053776	-1.942099	-1.418231
C	2.081037	-2.782291	-2.599892
C	1.235508	-2.538042	-3.699317
C	1.334815	-3.306218	-4.859353
H	0.682024	-3.095030	-5.702391
C	2.272192	-4.337377	-4.943397
H	2.353089	-4.930849	-5.849183

H	3.855700	-5.384569	-3.918263
C	3.113545	-4.594104	-3.856231
C	3.024722	-3.822026	-2.702314
H	3.702843	-3.989118	-1.871160
H	0.521208	-1.725526	-3.640456
O	-2.893930	-0.276238	-1.570297

Int4-A_Cu

Charge	0
Electronic Energy, BS1 (a.u.)	-3387.941107
Thermal and entropic correction, BS1 (a.u.)	0.831300
Electronic Energy, BS2 (a.u.)	-5972.084308
Number of Imaginary Frequencies	2
Imaginary frequencies (cm-1)	-13.7i, -7.7i

Molecular Geometry in Cartesian Coordinates

Cu	0.377490	-1.001874	-0.177502
Fe	3.101490	2.552010	-0.108504
P	2.505940	-0.817247	-0.768621
C	2.800766	0.904288	-1.295138
C	1.770958	1.904982	-1.521026
C	2.412358	3.099139	-1.989914
H	1.909493	4.030382	-2.208059
C	3.810418	2.854280	-2.054453
H	4.566971	3.577571	-2.327564
C	4.050808	1.515720	-1.634404
H	5.018837	1.042928	-1.550363
C	2.573940	2.131836	1.843131
H	1.976411	1.277575	2.129727
C	2.079170	3.418627	1.467328
H	1.040770	3.715232	1.413948
C	3.193761	4.232588	1.103079
H	3.143878	5.247799	0.731981
C	4.379347	3.450548	1.255985
H	5.385983	3.770008	1.020366
C	3.997580	2.153573	1.713458
H	4.659925	1.315888	1.881661
O	-0.405696	2.825007	-1.744348
C	0.339348	1.817481	-1.239666
N	-0.278251	0.917504	-0.559328
C	-1.716401	1.251056	-0.525129
C	-1.786141	2.619093	-1.314287
H	-2.377197	2.471797	-2.220254
H	-2.244036	0.488292	-1.100949
C	2.963823	-1.808020	-2.246559
C	2.927597	-1.267704	-3.540554
H	2.716529	-0.212621	-3.686374
C	3.161775	-2.083802	-4.650669
H	3.135040	-1.653051	-5.647906
C	3.432826	-3.443360	-4.480873
H	3.616701	-4.074948	-5.345214
C	3.466050	-3.989087	-3.193365
H	3.675366	-5.046092	-3.053264
C	3.227487	-3.179571	-2.082943
H	3.251009	-3.613384	-1.086525
C	3.822601	-1.170015	0.457856
C	3.435291	-1.302941	1.799078

H	2.384319	-1.237448	2.061526
C	4.393639	-1.506171	2.794535
H	4.080433	-1.601609	3.830040
C	5.745654	-1.588446	2.453059
H	6.493420	-1.747089	3.224908
C	6.136843	-1.479246	1.113597
H	7.186667	-1.557058	0.845218
C	5.180604	-1.275137	0.117925
H	5.489671	-1.206865	-0.920737
C	-2.234181	1.225224	0.896984
C	-3.268674	0.353528	1.249762
C	-1.651943	2.027541	1.889766
C	-3.734334	0.300905	2.568829
C	-2.113939	1.980255	3.203481
C	-3.160822	1.116643	3.545113
H	-3.699630	-0.309183	0.505380
H	-0.833049	2.686891	1.628283
H	-4.532993	-0.393225	2.810277
H	-1.656069	2.612142	3.959765
H	-3.519865	1.075382	4.569971
C	-2.285622	3.833047	-0.569286
C	-3.658680	3.943111	-0.311876
C	-1.418872	4.825252	-0.098468
C	-4.155146	5.020676	0.420996
C	-1.917820	5.906991	0.632295
C	-3.285082	6.006340	0.897668
H	-4.333684	3.172197	-0.672311
H	-0.355674	4.748216	-0.299132
H	-5.220704	5.090463	0.620877
H	-1.234997	6.670318	0.995574
H	-3.671567	6.845518	1.469108
H	-5.533659	2.356442	-2.725783
C	-5.143660	0.350334	-2.026075
C	-5.008618	1.423681	-2.911691
C	-4.185179	1.293451	-4.034276
H	-4.064376	2.125283	-4.722901
C	-3.505347	0.095260	-4.266391
H	-2.854695	0.000899	-5.132647
H	-2.059441	-2.124965	-4.301515
C	-2.956475	-2.291994	-3.699082
H	-3.619358	-2.975707	-4.235927
C	-3.655092	-0.986864	-3.389770
H	-4.574806	-1.672612	-1.549379
C	-4.478325	-0.856275	-2.262946
H	-5.768121	0.447766	-1.142218
O	-2.604122	-3.034488	-2.502591
C	-1.610122	-2.540900	-1.765334
C	-0.427437	-4.559645	-0.950711
H	-0.256447	-5.215102	-0.092248
H	0.537570	-4.180394	-1.303271
H	-0.891679	-5.145145	-1.749378
C	-1.345573	-3.394298	-0.538436
N	-0.704125	-2.566988	0.502651
C	-0.759111	-3.046177	1.695278
H	-1.237362	-4.010014	1.872546
C	-0.188700	-2.382801	2.873184
C	-0.094719	-0.984277	2.969520
H	-0.505434	-0.365501	2.180355
H	0.536348	0.686562	4.161393

C	0.484164	-0.395517	4.091898
C	0.979869	-1.194327	5.128107
H	1.434929	-0.733252	6.000106
C	0.867927	-2.586266	5.050601
H	1.237227	-3.208696	5.860362
C	0.271633	-3.177508	3.936583
H	0.174845	-4.258564	3.877851
O	-0.962370	-1.552074	-2.078897
H	-2.318865	-3.743002	-0.178014
O	-4.286014	-2.867965	0.223949
C	-4.586724	-2.808456	1.439334
O	-3.605133	-3.433375	2.258486
O	-5.575321	-2.309548	2.009797
H	-3.726541	-2.335985	4.039387
C	-3.821732	-3.361330	3.660470
H	-4.811748	-3.737964	3.941936
H	-3.050139	-3.981224	4.129483

TS45-A_Cu

Charge	0
Electronic Energy, BS1 (a.u.)	-3387.925948
Thermal and entropic correction, BS1 (a.u.)	0.825241
Electronic Energy, BS2 (a.u.)	-5972.064893
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-1415.1i

Molecular Geometry in Cartesian Coordinates

Cu	0.284668	-0.912469	0.138777
Fe	2.978618	2.538905	-0.514027
P	2.350521	-0.879144	-0.683638
C	2.627473	0.748482	-1.463738
C	1.583800	1.712136	-1.769131
C	2.194253	2.836067	-2.418406
H	1.674070	3.729133	-2.734186
C	3.589873	2.587740	-2.511861
H	4.328646	3.270219	-2.910255
C	3.857746	1.314911	-1.930957
H	4.831947	0.859994	-1.823000
C	2.676213	2.302614	1.514866
H	2.189004	1.441459	1.948706
C	2.029477	3.492527	1.062354
H	0.967908	3.692940	1.096036
C	3.021554	4.349908	0.498011
H	2.840949	5.309328	0.031301
C	4.285218	3.691748	0.606319
H	5.230063	4.065379	0.234071
C	4.072591	2.427184	1.234640
H	4.823282	1.671316	1.419690
O	-0.627503	2.512599	-2.108307
C	0.164738	1.655619	-1.423202
N	-0.405573	0.911374	-0.543048
C	-1.854081	1.176129	-0.575720
C	-1.967874	2.425687	-1.536275
H	-2.649433	2.194112	-2.355935
H	-2.330947	0.317510	-1.056697
C	2.493713	-2.080775	-2.071719
C	3.065341	-1.790570	-3.318295

H	3.478509	-0.806724	-3.515406
C	3.098564	-2.764343	-4.320990
H	3.540948	-2.528038	-5.284877
C	2.565900	-4.033885	-4.086943
H	2.590691	-4.787426	-4.869212
C	1.992476	-4.330295	-2.846029
H	1.566026	-5.312369	-2.661351
C	1.949296	-3.357347	-1.848337
H	1.473056	-3.575397	-0.896141
C	3.874492	-1.153370	0.306908
C	3.770706	-1.064085	1.703043
H	2.805360	-0.873398	2.160005
C	4.902929	-1.220094	2.506094
H	4.807294	-1.147377	3.585349
C	6.145169	-1.476824	1.920749
H	7.026036	-1.600974	2.544406
C	6.251503	-1.590351	0.530252
H	7.213314	-1.805876	0.073161
C	5.121516	-1.434561	-0.274086
H	5.208391	-1.540817	-1.351463
C	-2.427726	1.340263	0.813176
C	-3.666367	0.776326	1.130353
C	-1.736906	2.064182	1.794862
C	-4.216253	0.944037	2.405066
C	-2.282879	2.235652	3.066259
C	-3.528518	1.678057	3.373466
H	-4.187533	0.177115	0.390873
H	-0.764818	2.481842	1.558811
H	-5.161715	0.467856	2.641875
H	-1.736492	2.799960	3.817167
H	-3.953827	1.805992	4.365167
C	-2.344708	3.737277	-0.893274
C	-3.698290	4.004854	-0.650508
C	-1.379157	4.661754	-0.479760
C	-4.079409	5.170382	0.014398
C	-1.761463	5.832003	0.180922
C	-3.110863	6.087103	0.434955
H	-4.451448	3.289517	-0.970269
H	-0.330349	4.467887	-0.676648
H	-5.131689	5.363913	0.202769
H	-1.002833	6.542258	0.498507
H	-3.407415	6.995060	0.952456
H	-5.234099	1.610570	-3.547348
C	-4.959384	-0.242681	-2.471253
C	-4.681663	0.676850	-3.487553
C	-3.683542	0.388924	-4.423533
H	-3.452821	1.100799	-5.211403
C	-2.970247	-0.809481	-4.340649
H	-2.182451	-1.021452	-5.059721
H	-1.513262	-2.942910	-3.753688
C	-2.490832	-3.044899	-3.274045
H	-3.045794	-3.840542	-3.780052
C	-3.252809	-1.737476	-3.330985
H	-4.459159	-2.140471	-1.587132
C	-4.254734	-1.446984	-2.395940
H	-5.727047	-0.024804	-1.733654
O	-2.327155	-3.545085	-1.930039
C	-1.524919	-2.803929	-1.122395
C	-1.828645	-4.661552	0.614443

H	-2.322155	-4.769749	1.585734
H	-0.888063	-5.230413	0.645220
H	-2.479184	-5.112755	-0.135716
C	-1.595817	-3.193327	0.283781
N	-0.688644	-2.448065	1.094779
C	-0.367631	-2.850847	2.280206
H	-0.685397	-3.825488	2.651334
C	0.414501	-2.028578	3.211913
C	0.296003	-0.625716	3.231794
H	-0.415145	-0.141815	2.571058
H	0.941556	1.215870	4.133216
C	1.053406	0.135463	4.121697
C	1.942514	-0.488120	5.003769
H	2.535051	0.106673	5.693063
C	2.049499	-1.882924	5.007760
H	2.729908	-2.374340	5.697551
C	1.281283	-2.647782	4.129388
H	1.364012	-3.731833	4.136637
O	-0.907034	-1.833220	-1.575613
H	-2.873421	-2.701720	0.565073
O	-4.067876	-2.459617	0.749251
C	-4.405073	-2.309944	1.991327
O	-3.330644	-2.458127	2.834999
O	-5.530123	-2.069590	2.417438
H	-3.938103	-1.240032	4.420586
C	-3.601633	-2.262663	4.225826
H	-4.362221	-2.962994	4.585256
H	-2.656214	-2.441466	4.741813

TS5-A_Cu

Charge	0
Electronic Energy, BS1 (a.u.)	-3387.934203
Thermal and entropic correction, BS1 (a.u.)	0.830005
Electronic Energy, BS2 (a.u.)	-5972.073187
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	0.312022	-0.930179	0.116290
Fe	2.972002	2.535007	-0.569858
P	2.380979	-0.893520	-0.699933
C	2.661248	0.725418	-1.496488
C	1.612448	1.670142	-1.838058
C	2.221308	2.791241	-2.493930
H	1.696294	3.672020	-2.835255
C	3.621706	2.559479	-2.555344
H	4.359769	3.244753	-2.950281
C	3.893530	1.299357	-1.948574
H	4.870772	0.858285	-1.813615
C	2.682364	2.300865	1.460898
H	2.239711	1.420832	1.902924
C	1.975161	3.451839	0.999382
H	0.904450	3.596222	1.032497
C	2.921995	4.354047	0.426714
H	2.692624	5.299298	-0.047478
C	4.217948	3.761895	0.538960
H	5.142210	4.180423	0.162788

C	4.070230	2.493085	1.177976
H	4.857781	1.776844	1.368370
O	-0.604233	2.399372	-2.277831
C	0.186735	1.597863	-1.523801
N	-0.392250	0.890150	-0.619230
C	-1.844876	1.113210	-0.723521
C	-1.947142	2.341486	-1.710803
H	-2.630930	2.103693	-2.526600
H	-2.270961	0.230280	-1.209432
C	2.540486	-2.105108	-2.078465
C	3.190739	-1.846529	-3.293689
H	3.653073	-0.881120	-3.472254
C	3.240425	-2.827657	-4.288036
H	3.744897	-2.616417	-5.226966
C	2.643722	-4.073079	-4.077824
H	2.681468	-4.832520	-4.853905
C	1.989365	-4.336667	-2.870372
H	1.511898	-5.298608	-2.705497
C	1.931260	-3.356190	-1.880176
H	1.392403	-3.546933	-0.956190
C	3.901075	-1.147908	0.304642
C	3.786721	-1.039150	1.698785
H	2.816527	-0.850433	2.146286
C	4.913414	-1.176684	2.513042
H	4.808098	-1.088801	3.590317
C	6.161651	-1.434951	1.941441
H	7.038329	-1.544845	2.573661
C	6.279069	-1.568585	0.553689
H	7.245477	-1.785714	0.107089
C	5.154559	-1.430838	-0.261710
H	5.251893	-1.553056	-1.336403
C	-2.504093	1.305641	0.621711
C	-3.823386	0.883006	0.814141
C	-1.836715	1.953353	1.668955
C	-4.474485	1.121419	2.026974
C	-2.481248	2.186006	2.884269
C	-3.805829	1.776641	3.064008
H	-4.337246	0.359656	0.014181
H	-0.807742	2.265030	1.528064
H	-5.491602	0.770577	2.168728
H	-1.950700	2.686943	3.689375
H	-4.310622	1.959751	4.008515
C	-2.304405	3.669403	-1.088326
C	-3.654378	3.977296	-0.874558
C	-1.321997	4.569634	-0.660473
C	-4.015676	5.156944	-0.223492
C	-1.683985	5.753909	-0.013532
C	-3.030403	6.048289	0.212257
H	-4.421053	3.282238	-1.206084
H	-0.275105	4.347645	-0.836431
H	-5.065700	5.381235	-0.057964
H	-0.911792	6.444317	0.315004
H	-3.311483	6.967128	0.719091
H	-5.621685	1.199621	-3.297916
C	-5.270270	-0.694753	-2.320730
C	-4.994697	0.313502	-3.249879
C	-3.904681	0.174851	-4.114567
H	-3.677813	0.955832	-4.835343
C	-3.095998	-0.962750	-4.046360

H	-2.237510	-1.057702	-4.706769
H	-1.560526	-3.055838	-3.579257
C	-2.513832	-3.224609	-3.070159
H	-3.023792	-4.063341	-3.554632
C	-3.372869	-1.979059	-3.124248
H	-4.670587	-2.604480	-1.523710
C	-4.466645	-1.835664	-2.261358
H	-6.111837	-0.594443	-1.640583
O	-2.284166	-3.690839	-1.728676
C	-1.482057	-2.881970	-0.959457
C	-1.856248	-4.612163	0.905474
H	-2.378182	-4.516223	1.866996
H	-1.025755	-5.317895	1.065634
H	-2.546127	-5.064001	0.191912
C	-1.374030	-3.275207	0.403743
N	-0.566256	-2.466781	1.187036
C	-0.211394	-2.808992	2.397816
H	-0.457344	-3.794756	2.793219
C	0.502602	-1.912516	3.302375
C	0.362130	-0.509694	3.235990
H	-0.326250	-0.080664	2.516313
H	0.932075	1.397062	4.048065
C	1.062885	0.320133	4.110695
C	1.918044	-0.225495	5.074350
H	2.464964	0.423015	5.752765
C	2.044597	-1.616313	5.170022
H	2.696825	-2.052079	5.922249
C	1.337440	-2.449095	4.303843
H	1.443460	-3.528522	4.382968
O	-0.945228	-1.878657	-1.481266
H	-3.169933	-2.492891	0.757513
O	-4.140126	-2.391794	0.957770
C	-4.330942	-2.094406	2.242043
O	-3.159264	-1.968385	2.891582
O	-5.428789	-1.967336	2.742619
H	-3.786955	-0.709399	4.435694
C	-3.245486	-1.646507	4.290649
H	-3.745496	-2.449968	4.839147
H	-2.214206	-1.541176	4.626392

Int6-A_S_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.381649
Thermal and entropic correction, BS1 (a.u.)	1.473653
Electronic Energy, BS2 (a.u.)	-9902.746014
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	3.352627	0.347542	-0.431055
Fe	6.904098	-1.654043	1.198937
P	5.485920	0.618649	-1.026049
C	6.523837	0.212079	0.417827
C	6.029659	0.104454	1.777785
C	7.145572	-0.169768	2.637474
H	7.081596	-0.328563	3.703991
C	8.311939	-0.248346	1.831950

H	9.305555	-0.493894	2.180381
C	7.936101	-0.015855	0.477359
H	8.593358	-0.053600	-0.379383
C	5.685735	-3.047581	0.279872
H	4.822320	-2.792405	-0.316344
C	5.694005	-3.261953	1.690734
H	4.839940	-3.198112	2.349527
C	7.038631	-3.519254	2.093595
H	7.379646	-3.681167	3.107110
C	7.862439	-3.469135	0.928144
H	8.937589	-3.583327	0.906187
C	7.027595	-3.178260	-0.191874
H	7.352411	-3.025038	-1.211277
O	4.517950	0.418974	3.572596
C	4.649780	0.142781	2.251340
N	3.565205	-0.084592	1.591685
C	2.431089	0.089364	2.512074
C	3.131779	0.179187	3.930154
H	2.781764	1.060559	4.472501
H	1.962729	1.048380	2.265972
C	5.926463	2.350019	-1.449489
C	7.139470	2.969181	-1.114414
H	7.879005	2.439477	-0.522380
C	7.398931	4.275104	-1.534543
H	8.341154	4.747917	-1.272242
C	6.449644	4.973365	-2.283212
H	6.649479	5.992801	-2.598517
C	5.231374	4.370643	-2.601643
H	4.475919	4.923946	-3.150664
C	4.967861	3.067420	-2.184657
H	4.010354	2.605758	-2.411465
C	6.236022	-0.377643	-2.375338
C	5.528668	-1.502859	-2.819088
H	4.552686	-1.720305	-2.402444
C	6.069376	-2.339850	-3.796592
H	5.503724	-3.205674	-4.127112
C	7.321326	-2.052746	-4.344208
H	7.745733	-2.701184	-5.105220
C	8.021420	-0.915986	-3.926283
H	8.985655	-0.678879	-4.366645
C	7.479463	-0.076761	-2.952227
H	8.015268	0.819928	-2.654667
C	1.402569	-1.011475	2.407387
C	0.073321	-0.748180	2.754601
C	1.772078	-2.321956	2.085455
C	-0.863731	-1.782526	2.822684
C	0.839464	-3.356709	2.147824
C	-0.476733	-3.092619	2.533360
H	-0.218191	0.270333	2.996699
H	2.795581	-2.520680	1.789799
H	-1.891497	-1.575709	3.107518
H	1.144274	-4.372127	1.911794
H	-1.199525	-3.899290	2.603634
C	3.029543	-1.051753	4.801350
C	1.886949	-1.244987	5.586334
C	4.025367	-2.034257	4.794040
C	1.727006	-2.414492	6.327841
C	3.867911	-3.203711	5.540251
C	2.715787	-3.401057	6.302616

H	1.112002	-0.483280	5.604256
H	4.928668	-1.878399	4.215249
H	0.833654	-2.554027	6.929428
H	4.649003	-3.958530	5.527659
H	2.593294	-4.311050	6.882202
H	5.916186	7.313188	0.142413
C	3.861344	7.299042	-0.509771
C	4.975122	6.770925	0.145466
C	4.879876	5.539121	0.796912
H	5.750782	5.115130	1.287440
C	3.674005	4.840175	0.800802
H	3.598267	3.870680	1.280165
H	0.392531	5.333535	0.096246
C	1.226879	4.633638	0.173695
H	1.117720	4.046894	1.089232
C	2.545508	5.368925	0.157966
H	1.782896	7.014046	-1.004591
C	2.653692	6.598790	-0.501984
H	3.930439	8.256362	-1.018675
O	1.050958	3.766227	-0.970005
C	1.652673	2.539914	-0.902447
C	0.768294	2.212617	-3.290607
H	0.491005	3.261811	-3.196017
H	-0.149970	1.627109	-3.466068
H	1.385213	2.098270	-4.193384
C	1.490969	1.739070	-2.065357
N	1.920166	0.448851	-1.941664
C	1.721784	-0.455525	-2.875178
H	1.309707	-0.176778	-3.844994
C	2.033496	-1.862712	-2.683808
C	2.126530	-2.447456	-1.401198
H	1.928054	-1.838287	-0.526701
H	2.476137	-4.225891	-0.252717
C	2.416125	-3.801582	-1.251103
C	2.612578	-4.617088	-2.371446
H	2.840834	-5.671717	-2.251444
C	2.500740	-4.056115	-3.648600
H	2.639735	-4.678269	-4.528592
C	2.210050	-2.702449	-3.802826
H	2.125635	-2.277960	-4.799743
Ni	-2.935742	-0.031276	-0.839531
P	-4.612944	-1.441524	-0.646004
C	-5.892907	-0.436693	-2.901436
H	-4.988563	0.154059	-3.015041
C	-5.317737	-1.182538	1.051618
C	-4.659538	-4.198192	-1.400698
H	-5.569838	-3.995640	-1.952164
C	-4.022421	-3.180747	-0.680130
C	-6.006010	-1.317473	-1.816550
C	-4.898987	-2.041621	2.105621
H	-4.309016	-2.920564	1.878967
C	-7.193765	-2.042604	-1.636591
H	-7.306740	-2.697936	-0.778194
C	-6.487918	0.205228	2.698763
C	-6.099197	-0.061738	1.342155
C	-4.105986	-5.479984	-1.442393
H	-4.602352	-6.257152	-2.015404
C	-6.029875	-0.656075	3.747523
C	-5.234655	-1.778977	3.411205

H	-4.901729	-2.445700	4.202298
C	-2.812317	-3.462896	-0.021976
H	-2.274280	-2.670785	0.490113
C	-8.121533	-1.025127	-3.624460
H	-8.946301	-0.906724	-4.320262
C	-6.946295	-0.292235	-3.802801
H	-6.855177	0.400937	-4.633349
C	-8.243884	-1.899302	-2.541911
H	-9.164985	-2.452602	-2.389964
C	-6.388044	-0.374256	5.092604
H	-6.029167	-1.035967	5.876214
C	-7.644847	1.556607	4.365294
H	-8.272013	2.408185	4.611377
C	-2.270717	-4.744817	-0.056747
H	-1.325830	-4.938706	0.440260
C	-7.180685	0.707830	5.398303
H	-7.454906	0.911625	6.428855
C	-7.304753	1.316191	3.053387
H	-7.660006	1.981749	2.276209
C	-2.918488	-5.758324	-0.766856
H	-2.487792	-6.754052	-0.810429
P	-3.880060	1.754641	0.061382
C	-2.902688	1.090203	2.564664
H	-2.355125	0.338237	2.009238
C	-5.691442	1.814316	-0.306383
C	-2.879687	4.433045	-0.002395
H	-3.084235	4.495816	1.060314
C	-3.181404	3.266348	-0.715858
C	-3.742583	1.965877	1.866602
C	-6.171494	2.710760	-1.299495
H	-5.497852	3.437612	-1.736956
C	-4.488464	2.922044	2.571856
H	-5.173031	3.578347	2.042820
C	-7.931717	0.841069	-0.140899
C	-6.559782	0.886953	0.273286
C	-2.292070	5.520391	-0.654286
H	-2.061073	6.419960	-0.091420
C	-8.389450	1.732794	-1.164519
C	-7.479255	2.666551	-1.717478
H	-7.829659	3.355378	-2.481368
C	-2.876805	3.204147	-2.087810
H	-3.072625	2.288172	-2.640917
C	-3.542451	2.125567	4.651079
H	-3.476085	2.181266	5.733191
C	-2.803358	1.168134	3.953314
H	-2.163016	0.474418	4.489850
C	-4.380639	3.003624	3.959220
H	-4.969453	3.735308	4.502985
C	-9.739376	1.661476	-1.600557
H	-10.071132	2.341547	-2.380311
C	-10.166445	-0.123399	-0.027536
H	-10.860289	-0.836056	0.408070
C	-2.291889	4.290261	-2.734115
H	-2.049342	4.222757	-3.789834
C	-10.611644	0.753778	-1.045672
H	-11.642512	0.709195	-1.383438
C	-8.862782	-0.083246	0.411798
H	-8.533892	-0.765882	1.186194
C	-1.995929	5.451735	-2.015669

H	-1.527151	6.294310	-2.514390
H	-0.938362	1.795300	-1.035531
C	-1.006110	0.779724	-0.663857
H	-0.521290	0.607684	0.295536
C	-1.096488	-0.268835	-1.554558
C	-1.805972	-1.144298	-2.128516
C	-1.942840	-2.261641	-3.032959
C	-1.055867	-3.349601	-2.953690
C	-1.191631	-4.422623	-3.830726
H	-0.493124	-5.250552	-3.763579
C	-2.208366	-4.429014	-4.788322
H	-2.309759	-5.268989	-5.469232
H	-3.888833	-3.351877	-5.610992
C	-3.095699	-3.352209	-4.869308
C	-2.967074	-2.275813	-3.995898
H	-3.658588	-1.443399	-4.050010
H	-0.269308	-3.346646	-2.209696
O	2.248636	2.187292	0.146345

TS67-A_S_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.376058
Thermal and entropic correction, BS1 (a.u.)	1.472831
Electronic Energy, BS2 (a.u.)	-9902.738519
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-175.5i

Molecular Geometry in Cartesian Coordinates

Cu	3.479610	0.299281	-0.445723
Fe	7.138774	-1.407114	1.304640
P	5.601877	0.796089	-0.902428
C	6.580901	0.441462	0.597071
C	6.020712	0.195525	1.914840
C	7.107838	0.004230	2.832209
H	6.997942	-0.224068	3.882159
C	8.321923	0.114752	2.105711
H	9.315027	-0.030131	2.507718
C	8.004523	0.380797	0.742575
H	8.714664	0.470707	-0.066491
C	6.223373	-2.866291	0.164927
H	5.425124	-2.671619	-0.533527
C	6.066150	-3.163365	1.550939
H	5.128910	-3.231489	2.084256
C	7.365480	-3.296838	2.125843
H	7.584708	-3.483203	3.168391
C	8.326985	-3.086755	1.090281
H	9.401254	-3.083346	1.214307
C	7.621610	-2.820273	-0.121523
H	8.058188	-2.570838	-1.078632
O	4.386807	0.182625	3.631876
C	4.621339	0.053728	2.302067
N	3.600660	-0.198363	1.555547
C	2.402507	-0.177790	2.412076
C	3.012244	-0.227579	3.867244
H	2.554283	0.535630	4.500374
H	1.918452	0.792136	2.251988
C	5.846368	2.588317	-1.218763

C	6.955991	3.329284	-0.786976
H	7.720253	2.862500	-0.173786
C	7.079016	4.674851	-1.137413
H	7.942043	5.242124	-0.800760
C	6.093669	5.292664	-1.909846
H	6.185234	6.342794	-2.168330
C	4.974791	4.567818	-2.323649
H	4.189699	5.054428	-2.893774
C	4.850399	3.223510	-1.978648
H	3.973545	2.660152	-2.286001
C	6.560203	-0.024752	-2.239890
C	6.025149	-1.186275	-2.813331
H	5.047468	-1.536139	-2.504650
C	6.740139	-1.892087	-3.782751
H	6.308578	-2.790645	-4.212863
C	7.992975	-1.435220	-4.195773
H	8.551633	-1.981562	-4.950057
C	8.519568	-0.258872	-3.652139
H	9.483132	0.112277	-3.989070
C	7.804869	0.448005	-2.684897
H	8.207660	1.376498	-2.291329
C	1.419362	-1.276187	2.089229
C	0.049862	-1.053596	2.264201
C	1.855504	-2.544715	1.690884
C	-0.870966	-2.085906	2.066428
C	0.940286	-3.575033	1.481544
C	-0.424232	-3.351339	1.680589
H	-0.291834	-0.068374	2.569722
H	2.917004	-2.715583	1.549460
H	-1.932362	-1.909034	2.217345
H	1.292106	-4.554791	1.172408
H	-1.136064	-4.158262	1.542196
C	2.979134	-1.574193	4.553723
C	1.795715	-1.997055	5.171072
C	4.083450	-2.432013	4.536409
C	1.707232	-3.268561	5.734522
C	3.996118	-3.705194	5.103909
C	2.806947	-4.129820	5.697531
H	0.933540	-1.335906	5.191184
H	5.013971	-2.099992	4.090383
H	0.781557	-3.586906	6.204652
H	4.860756	-4.362524	5.084616
H	2.739152	-5.120101	6.137622
H	5.378066	7.630906	0.568358
C	3.364716	7.402622	-0.167298
C	4.507110	6.983909	0.517275
C	4.531493	5.728849	1.130030
H	5.426414	5.392285	1.644206
C	3.414788	4.897324	1.067083
H	3.433014	3.911911	1.519485
H	0.120891	5.052723	0.300566
C	1.026258	4.446824	0.360607
H	0.972553	3.805491	1.243541
C	2.256685	5.317148	0.398479
H	1.349002	6.900741	-0.744992
C	2.245018	6.571078	-0.223814
H	3.341801	8.377440	-0.646037
O	0.952482	3.615663	-0.826914
C	1.613060	2.430081	-0.783216

C	0.707623	2.098038	-3.170458
H	0.281020	3.086130	-3.002808
H	-0.097719	1.433881	-3.512919
H	1.438376	2.169088	-3.988781
C	1.351450	1.579154	-1.913980
N	2.004508	0.362410	-1.896151
C	1.888003	-0.480009	-2.890099
H	1.352603	-0.199673	-3.796656
C	2.465810	-1.818057	-2.878592
C	2.747551	-2.505591	-1.681073
H	2.495775	-2.042247	-0.734614
H	3.480856	-4.307338	-0.770381
C	3.284355	-3.790041	-1.705493
C	3.562651	-4.417638	-2.925028
H	3.988454	-5.416233	-2.942645
C	3.270773	-3.753183	-4.120763
H	3.468992	-4.236384	-5.073075
C	2.717245	-2.474384	-4.097846
H	2.486517	-1.967859	-5.031224
Ni	-3.169962	-0.147023	-0.914280
P	-4.892297	-1.477658	-0.744139
C	-5.967515	-0.407014	-3.070503
H	-4.964274	-0.011569	-3.208319
C	-5.556142	-1.233317	0.972030
C	-5.445339	-4.199745	-1.440374
H	-6.410025	-3.873173	-1.809396
C	-4.548417	-3.281074	-0.877300
C	-6.254230	-1.161136	-1.923292
C	-5.109852	-2.142603	1.973403
H	-4.562957	-3.031165	1.681089
C	-7.555514	-1.648485	-1.727793
H	-7.799418	-2.198890	-0.824768
C	-6.577352	0.134326	2.731521
C	-6.271130	-0.092111	1.345194
C	-5.092288	-5.544857	-1.559629
H	-5.793726	-6.244743	-2.003962
C	-6.095920	-0.780600	3.722509
C	-5.359721	-1.916457	3.303786
H	-5.004196	-2.620139	4.051882
C	-3.291396	-3.734690	-0.446943
H	-2.572101	-3.021293	-0.059228
C	-8.255945	-0.643325	-3.811942
H	-9.035035	-0.437096	-4.539551
C	-6.964985	-0.150556	-4.011792
H	-6.736223	0.439669	-4.894082
C	-8.550092	-1.391428	-2.669452
H	-9.558686	-1.753163	-2.498192
C	-6.369773	-0.536945	5.094417
H	-5.992974	-1.239846	5.832556
C	-7.593031	1.461010	4.507840
H	-8.175253	2.323719	4.817720
C	-2.941741	-5.077478	-0.567486
H	-1.952467	-5.404664	-0.263925
C	-7.104827	0.559340	5.482857
H	-7.314894	0.733532	6.533767
C	-7.332663	1.258251	3.171282
H	-7.705358	1.964261	2.439324
C	-3.842435	-5.986968	-1.124797
H	-3.565151	-7.031072	-1.234369

P	-4.039094	1.686788	0.032599
C	-2.929636	0.920274	2.444908
H	-2.426088	0.192281	1.818859
C	-5.861804	1.840600	-0.237928
C	-3.019856	4.370255	0.009755
H	-3.229409	4.422637	1.072273
C	-3.325239	3.211045	-0.715453
C	-3.800694	1.835601	1.839383
C	-6.347775	2.793053	-1.174826
H	-5.663647	3.508521	-1.615153
C	-4.488505	2.762312	2.635811
H	-5.200302	3.446304	2.183211
C	-8.130953	0.955070	-0.004871
C	-6.740280	0.925259	0.344531
C	-2.426213	5.462552	-0.628283
H	-2.195996	6.356790	-0.056161
C	-8.593454	1.895288	-0.981265
C	-7.670884	2.812936	-1.540862
H	-8.024523	3.538636	-2.268273
C	-3.017846	3.163634	-2.087234
H	-3.218628	2.252926	-2.647135
C	-3.426637	1.857510	4.613663
H	-3.295456	1.859395	5.691387
C	-2.743390	0.928031	3.826426
H	-2.082161	0.199231	4.286321
C	-4.294303	2.775649	4.016703
H	-4.841629	3.483931	4.630448
C	-9.959378	1.883614	-1.370632
H	-10.293609	2.598951	-2.117141
C	-10.394468	0.065927	0.161442
H	-11.097592	-0.634778	0.601749
C	-2.426912	4.255100	-2.721427
H	-2.187835	4.200248	-3.779049
C	-10.843322	0.987553	-0.815286
H	-11.885655	0.987071	-1.119254
C	-9.075936	0.049961	0.556426
H	-8.745253	-0.665345	1.300129
C	-2.127161	5.407846	-1.990534
H	-1.657693	6.255716	-2.479944
H	-0.990392	1.963823	-1.049147
C	-0.698926	0.954930	-0.793467
H	-0.221800	0.797317	0.169373
C	-1.190081	-0.118940	-1.471104
C	-1.857600	-1.108510	-1.946248
C	-1.704329	-2.322092	-2.726822
C	-0.589197	-3.148570	-2.506043
C	-0.451353	-4.347268	-3.200595
H	0.424331	-4.965888	-3.028058
C	-1.432207	-4.742088	-4.114486
H	-1.329394	-5.679378	-4.653484
H	-3.321947	-4.243641	-5.028985
C	-2.552051	-3.932464	-4.329233
C	-2.691423	-2.731389	-3.637939
H	-3.570357	-2.110413	-3.781888
H	0.150840	-2.849759	-1.774762
O	2.295176	2.110746	0.210914

Int7-A_S_NiCu

Charge 1

Electronic Energy, BS1 (a.u.)	-5980.405504
Thermal and entropic correction, BS1 (a.u.)	1.475543
Electronic Energy, BS2 (a.u.)	-9902.772244
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	-3.367398	0.002811	0.425383
Fe	-7.740441	-0.864077	0.456652
P	-4.833152	0.056807	2.147349
C	-6.471651	0.418598	1.440763
C	-6.727479	0.871666	0.086065
C	-8.137113	1.108176	-0.041809
H	-8.629546	1.420824	-0.950409
C	-8.751995	0.804557	1.200786
H	-9.812986	0.836275	1.405982
C	-7.740510	0.376864	2.107233
H	-7.899369	0.032005	3.118717
C	-6.755214	-2.608416	-0.022151
H	-5.681280	-2.711975	0.010221
C	-7.522459	-2.158955	-1.139685
H	-7.137280	-1.861380	-2.104289
C	-8.891064	-2.103903	-0.742662
H	-9.715817	-1.761371	-1.352384
C	-8.971827	-2.524792	0.619064
H	-9.869706	-2.555322	1.220888
C	-7.654093	-2.837737	1.065127
H	-7.371959	-3.141599	2.062980
O	-6.366697	1.390697	-2.186528
C	-5.803971	0.967456	-1.039158
N	-4.550416	0.663372	-1.082838
C	-4.069293	0.846770	-2.475222
C	-5.345417	1.391268	-3.223180
H	-5.174734	2.440558	-3.476370
H	-3.309723	1.629825	-2.448165
C	-4.510113	1.457379	3.291312
C	-5.491499	2.343040	3.758034
H	-6.525983	2.222064	3.456129
C	-5.137270	3.406186	4.591678
H	-5.902065	4.093518	4.940708
C	-3.805293	3.591658	4.969432
H	-3.533453	4.424297	5.611021
C	-2.823826	2.704908	4.517888
H	-1.785990	2.844390	4.805526
C	-3.176133	1.646397	3.682413
H	-2.414943	0.966408	3.313683
C	-5.137818	-1.363144	3.270040
C	-4.708458	-2.635419	2.869324
H	-4.168410	-2.754231	1.938189
C	-4.978650	-3.752588	3.661615
H	-4.640004	-4.730857	3.335672
C	-5.672122	-3.605411	4.864398
H	-5.882258	-4.473364	5.482195
C	-6.081117	-2.335097	5.282616
H	-6.603624	-2.215067	6.227001
C	-5.810396	-1.217079	4.493805
H	-6.108409	-0.231059	4.837905
C	-3.422026	-0.427681	-2.976855

C	-2.036723	-0.450920	-3.162871
C	-4.154679	-1.605138	-3.187838
C	-1.388599	-1.628533	-3.541519
C	-3.514857	-2.774512	-3.595838
C	-2.126443	-2.791080	-3.763955
H	-1.466608	0.453454	-2.981215
H	-5.228410	-1.603463	-3.048373
H	-0.311101	-1.635921	-3.658340
H	-4.098098	-3.673250	-3.774826
H	-1.622162	-3.705452	-4.062583
C	-5.837403	0.650245	-4.442909
C	-5.037163	0.642095	-5.591953
C	-7.058006	-0.031940	-4.452635
C	-5.440417	-0.058666	-6.726728
C	-7.461731	-0.733154	-5.591601
C	-6.653465	-0.752751	-6.728434
H	-4.086250	1.168722	-5.591211
H	-7.691041	-0.007516	-3.572495
H	-4.808116	-0.064002	-7.609384
H	-8.411604	-1.259971	-5.589667
H	-6.967768	-1.298549	-7.612791
H	-7.020475	4.325916	-0.970161
C	-4.988290	4.459949	-1.678744
C	-5.969909	4.275745	-0.701573
C	-5.594712	4.030712	0.621599
H	-6.350786	3.890443	1.387433
C	-4.244201	3.984434	0.966832
H	-3.952016	3.827355	1.999194
H	-1.635068	4.777897	1.260444
C	-1.805579	4.148647	0.384863
H	-1.158083	4.482819	-0.427641
C	-3.257076	4.154107	-0.010563
H	-2.870415	4.505722	-2.097572
C	-3.636664	4.381271	-1.338214
H	-5.277123	4.675544	-2.703449
O	-1.332580	2.838914	0.832123
C	-1.037870	1.953569	-0.130452
C	0.216044	0.900249	1.826084
H	1.015532	1.640773	1.791610
H	0.636685	-0.026963	2.215647
H	-0.558780	1.249896	2.506367
C	-0.352504	0.678253	0.415810
N	-1.390485	-0.411065	0.441424
C	-0.950102	-1.584726	0.749318
H	0.087506	-1.719875	1.064737
C	-1.736218	-2.816010	0.700715
C	-2.753385	-2.998395	-0.250677
H	-2.952666	-2.222365	-0.979656
H	-4.214150	-4.347404	-1.058720
C	-3.453148	-4.202339	-0.298914
C	-3.160457	-5.222143	0.612057
H	-3.711478	-6.157125	0.574909
C	-2.137521	-5.050948	1.550946
H	-1.896492	-5.849920	2.245265
C	-1.411300	-3.862221	1.581130
H	-0.593167	-3.736205	2.285821
Ni	3.826070	0.881384	-0.533926
P	5.861955	1.504290	0.017188
C	6.910901	1.188933	-2.534170

H	5.862521	1.143895	-2.818056
C	6.303850	0.347635	1.417916
C	7.072242	4.081429	0.432657
H	7.892029	3.763873	-0.201263
C	6.019631	3.202766	0.724278
C	7.241025	1.363695	-1.183150
C	6.117188	0.802664	2.753604
H	5.929001	1.853688	2.935087
C	8.592252	1.394760	-0.805745
H	8.858848	1.498454	0.241817
C	6.664048	-1.914872	2.301747
C	6.583753	-1.004461	1.192401
C	7.066226	5.383685	0.938835
H	7.885698	6.054750	0.697673
C	6.432889	-1.437293	3.631565
C	6.172051	-0.058294	3.821744
H	6.024256	0.316595	4.831454
C	4.958052	3.664216	1.522568
H	4.110360	3.010805	1.703796
C	9.256040	1.080708	-3.108911
H	10.038222	0.959764	-3.852423
C	7.914260	1.047342	-3.493372
H	7.649006	0.900467	-4.536273
C	9.593965	1.256913	-1.764869
H	10.635895	1.260768	-1.460914
C	6.483159	-2.345725	4.722535
H	6.303195	-1.964595	5.724437
C	7.002568	-4.154113	3.208871
H	7.226813	-5.205256	3.052099
C	4.960562	4.957266	2.038912
H	4.121283	5.298725	2.636502
C	6.760933	-3.677670	4.519609
H	6.801786	-4.363450	5.360667
C	6.955156	-3.298706	2.131586
H	7.137521	-3.680025	1.134138
C	6.016228	5.823209	1.745252
H	6.012662	6.838428	2.131133
P	4.096107	-1.287145	-0.695315
C	2.896910	-1.575392	1.792642
H	2.724562	-0.510672	1.667760
C	5.817535	-1.856051	-1.071504
C	2.535995	-3.285507	-2.089484
H	2.598681	-3.915638	-1.209389
C	3.108668	-2.006142	-2.084870
C	3.593960	-2.259423	0.786208
C	6.123793	-2.409989	-2.345090
H	5.321364	-2.642514	-3.034860
C	3.897211	-3.616251	0.969171
H	4.488275	-4.143161	0.225925
C	8.208741	-1.829275	-0.546998
C	6.848401	-1.563124	-0.177513
C	1.879638	-3.763423	-3.226841
H	1.442454	-4.757844	-3.216609
C	8.498159	-2.350063	-1.849304
C	7.423185	-2.640219	-2.724679
H	7.640042	-3.051497	-3.707110
C	2.979564	-1.202092	-3.231031
H	3.382601	-0.192555	-3.213669
C	2.759276	-3.601225	3.105950

H	2.449744	-4.119673	4.008821
C	2.475605	-2.242252	2.944377
H	1.952835	-1.696889	3.725824
C	3.476124	-4.283778	2.119832
H	3.728760	-5.330649	2.258205
C	9.849229	-2.563746	-2.232126
H	10.052667	-2.951166	-3.226926
C	10.598735	-1.791751	-0.068643
H	11.415693	-1.582180	0.615572
C	2.342979	-1.686693	-4.373149
H	2.264980	-1.058966	-5.256090
C	10.880332	-2.290295	-1.363403
H	11.909730	-2.458904	-1.665241
C	9.300283	-1.566434	0.328440
H	9.099478	-1.175188	1.318633
C	1.799187	-2.975187	-4.376389
H	1.301946	-3.354335	-5.264567
H	0.298092	0.283550	-1.609701
C	0.752739	0.284003	-0.615308
H	1.045451	-0.748857	-0.416390
C	1.965499	1.136771	-0.590218
C	2.531014	2.294102	-0.554431
C	2.470177	3.740087	-0.473692
C	1.608026	4.395356	0.426163
C	1.617996	5.785893	0.537349
H	0.952783	6.274138	1.245400
C	2.480957	6.550782	-0.251040
H	2.489761	7.632957	-0.161252
H	4.027231	6.496168	-1.753833
C	3.341445	5.911071	-1.148088
C	3.343988	4.523031	-1.250759
H	4.036651	4.016734	-1.915786
H	0.944999	3.807612	1.051322
O	-1.260516	2.144663	-1.309038

Int6-A_R_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.390034
Thermal and entropic correction, BS1 (a.u.)	1.475505
Electronic Energy, BS2 (a.u.)	-9902.750083
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	2.979946	0.526329	0.138948
Fe	5.592677	-2.421720	-2.276847
P	2.495806	-0.991097	-1.372813
C	3.940717	-1.210469	-2.481582
C	5.165324	-0.422807	-2.415523
C	6.004198	-0.808956	-3.511038
H	6.991450	-0.413460	-3.698256
C	5.327897	-1.808641	-4.256390
H	5.717281	-2.328076	-5.120830
C	4.068588	-2.048327	-3.637869
H	3.329780	-2.752733	-3.990002
C	5.358396	-3.584601	-0.579399
H	4.487875	-3.553758	0.057511

C	6.516035	-2.760134	-0.458351
H	6.672033	-1.990587	0.284852
C	7.403343	-3.083121	-1.530553
H	8.353011	-2.609712	-1.738570
C	6.790779	-4.106565	-2.315307
H	7.196225	-4.541184	-3.218655
C	5.527375	-4.415527	-1.727291
H	4.806361	-5.127291	-2.102791
O	6.664076	1.312697	-1.758826
C	5.552349	0.594858	-1.444661
N	4.957675	0.907839	-0.350763
C	5.616727	2.119435	0.181799
C	6.990824	2.106826	-0.576039
H	7.242905	3.108959	-0.929120
H	5.023936	2.963147	-0.190695
C	1.141027	-0.534785	-2.537885
C	0.756896	0.815199	-2.569520
H	1.274150	1.543191	-1.948234
C	-0.301860	1.223014	-3.383196
H	-0.571372	2.272389	-3.402915
C	-0.994631	0.291990	-4.159425
H	-1.831288	0.613062	-4.773204
C	-0.605986	-1.050920	-4.145411
H	-1.135137	-1.779010	-4.753900
C	0.462938	-1.459026	-3.346836
H	0.756088	-2.503458	-3.338300
C	2.014446	-2.649135	-0.734272
C	1.536675	-2.668893	0.585836
H	1.469272	-1.739990	1.143590
C	1.198678	-3.874404	1.202490
H	0.874903	-3.869790	2.237848
C	1.320260	-5.075121	0.504587
H	1.066531	-6.014765	0.985814
C	1.780399	-5.066502	-0.815294
H	1.881158	-5.999539	-1.362654
C	2.126758	-3.863637	-1.429736
H	2.525265	-3.884386	-2.436298
C	5.591981	2.168381	1.689663
C	5.024287	3.273638	2.331292
C	6.042846	1.091780	2.463359
C	4.909084	3.307038	3.721981
C	5.925125	1.118389	3.850517
C	5.355474	2.225920	4.483707
H	4.642929	4.099971	1.737378
H	6.471407	0.223866	1.975573
H	4.458087	4.168545	4.205775
H	6.259174	0.265893	4.433675
H	5.256993	2.243419	5.565302
C	8.161676	1.495267	0.158270
C	8.815574	2.246773	1.141885
C	8.569573	0.179051	-0.079294
C	9.846301	1.682892	1.892036
C	9.600241	-0.387217	0.673825
C	10.237684	0.360975	1.664565
H	8.500631	3.268371	1.337080
H	8.087488	-0.394461	-0.861342
H	10.341686	2.274023	2.656310
H	9.905607	-1.412284	0.482938
H	11.038802	-0.078886	2.250832

H	-0.471070	4.747306	-5.261965
C	1.219373	4.261308	-4.011295
C	-0.050644	4.790489	-4.260571
C	-0.771787	5.380303	-3.219359
H	-1.760745	5.790920	-3.400783
C	-0.212584	5.464070	-1.942700
H	-0.765839	5.950228	-1.146151
H	1.451438	6.119861	0.064845
C	1.704013	5.130653	-0.326680
H	2.791562	5.055701	-0.415418
C	1.062288	4.944821	-1.685710
H	2.740943	3.900679	-2.524374
C	1.765954	4.329955	-2.729734
H	1.780540	3.791317	-4.813629
O	1.253811	4.231453	0.708988
C	1.860476	2.997216	0.746433
C	1.065004	2.889834	3.171105
H	0.720636	3.902953	2.967238
H	1.751698	2.931163	4.029177
H	0.195858	2.292277	3.489456
C	1.739218	2.303267	1.967009
N	2.331661	1.062029	2.013495
C	2.324823	0.348371	3.116480
H	1.786396	0.722202	3.986471
C	3.032950	-0.901851	3.346643
C	3.985581	-1.473617	2.475344
H	4.229992	-0.970746	1.546124
H	5.386862	-3.064258	2.136393
C	4.641177	-2.655691	2.810257
C	4.370210	-3.312628	4.013953
H	4.888776	-4.232512	4.266709
C	3.441657	-2.754897	4.896675
H	3.233307	-3.238676	5.847380
C	2.795375	-1.566451	4.570521
H	2.095685	-1.126638	5.274602
Ni	-2.778985	0.854338	0.352007
P	-4.723956	0.878032	-0.682013
C	-5.972928	2.053977	1.490453
H	-4.957434	2.291868	1.794260
C	-4.973302	-0.816458	-1.386510
C	-5.931878	2.425404	-2.751068
H	-6.892891	2.177214	-2.315978
C	-4.742814	1.965572	-2.164994
C	-6.188448	1.341117	0.301560
C	-4.568815	-1.031712	-2.734202
H	-4.261212	-0.190590	-3.343035
C	-7.498670	1.028085	-0.090467
H	-7.673652	0.436982	-0.983501
C	-5.370549	-3.222413	-1.154620
C	-5.350214	-1.901386	-0.593411
C	-5.885022	3.232482	-3.888044
H	-6.809904	3.591991	-4.328943
C	-4.957379	-3.417873	-2.512295
C	-4.553542	-2.293662	-3.273934
H	-4.236334	-2.440178	-4.302932
C	-3.513272	2.327647	-2.733189
H	-2.590880	1.995144	-2.272424
C	-8.357829	2.142343	1.874978
H	-9.200442	2.447106	2.488174

C	-7.056167	2.455151	2.272123
H	-6.882542	3.006502	3.191148
C	-8.578021	1.428546	0.694438
H	-9.586878	1.162252	0.396722
C	-4.959861	-4.726995	-3.062615
H	-4.641409	-4.858781	-4.093122
C	-5.776120	-5.618491	-0.970317
H	-6.091926	-6.473941	-0.380838
C	-3.470244	3.122257	-3.878377
H	-2.510645	3.400796	-4.299868
C	-5.364278	-5.806183	-2.311254
H	-5.369771	-6.802278	-2.743233
C	-5.772810	-4.363750	-0.404866
H	-6.079141	-4.238026	0.626434
C	-4.656458	3.578230	-4.456036
H	-4.624860	4.207238	-5.340672
P	-2.993185	-1.118652	1.318027
C	-1.801893	-2.525458	-0.772715
H	-1.553750	-1.549844	-1.179310
C	-4.756977	-1.422125	1.810536
C	-1.299582	-2.106988	3.391635
H	-1.210427	-3.022336	2.819146
C	-2.087217	-1.052228	2.915136
C	-2.471207	-2.631639	0.453953
C	-5.146395	-1.234569	3.165132
H	-4.397130	-1.025449	3.917613
C	-2.800475	-3.897790	0.963984
H	-3.348438	-3.981734	1.897868
C	-7.101497	-1.825227	1.226437
C	-5.723191	-1.716786	0.846764
C	-0.610141	-1.976644	4.599198
H	0.017357	-2.789879	4.948850
C	-7.477105	-1.591657	2.588469
C	-6.465869	-1.308469	3.538275
H	-6.746466	-1.149907	4.575950
C	-2.159111	0.141522	3.655972
H	-2.736798	0.979878	3.273734
C	-1.808365	-4.936304	-0.975320
H	-1.558657	-5.830264	-1.537868
C	-1.482702	-3.680091	-1.485455
H	-0.983627	-3.594681	-2.441975
C	-2.459168	-5.046294	0.255161
H	-2.724296	-6.022560	0.648334
C	-8.848556	-1.641754	2.954653
H	-9.117594	-1.457346	3.991023
C	-9.451116	-2.161420	0.672395
H	-10.219823	-2.384834	-0.061287
C	-1.479816	0.263612	4.866291
H	-1.544653	1.188880	5.430335
C	-9.817764	-1.918202	2.018446
H	-10.863532	-1.954916	2.307817
C	-8.130776	-2.116715	0.286279
H	-7.866839	-2.299430	-0.748506
C	-0.706905	-0.799575	5.341548
H	-0.172186	-0.703180	6.281524
H	-0.401778	0.537530	1.685066
C	-0.685396	0.867501	0.691076
H	-0.098010	0.437300	-0.116721
C	-1.255951	2.104522	0.529274

C	-2.280481	2.835049	0.367329
C	-2.779004	4.193677	0.428773
C	-1.957407	5.165482	1.040031
C	-2.398135	6.480295	1.160584
H	-1.756048	7.218593	1.632221
C	-3.655625	6.852029	0.673672
H	-3.995082	7.879204	0.766794
H	-5.451955	6.172352	-0.307185
C	-4.472834	5.894341	0.071246
C	-4.043884	4.572862	-0.045006
H	-4.689097	3.842610	-0.511515
H	-0.971503	4.876145	1.387141
O	2.469826	2.590840	-0.283075

TS67-A_R_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.387318
Thermal and entropic correction, BS1 (a.u.)	1.478311
Electronic Energy, BS2 (a.u.)	-9902.743583
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-63.0i

Molecular Geometry in Cartesian Coordinates

Cu	3.079226	0.504787	0.141978
Fe	5.608278	-2.467189	-2.277469
P	2.531386	-1.019100	-1.351264
C	3.955372	-1.257408	-2.483074
C	5.183989	-0.471793	-2.453641
C	6.003968	-0.884405	-3.554369
H	6.988869	-0.495780	-3.766818
C	5.312554	-1.897191	-4.266755
H	5.686194	-2.436331	-5.126030
C	4.062714	-2.119327	-3.623253
H	3.316937	-2.829461	-3.948007
C	5.397626	-3.593441	-0.552445
H	4.536990	-3.546646	0.096940
C	6.559735	-2.770471	-0.467719
H	6.730819	-1.985740	0.256025
C	7.428764	-3.119150	-1.546910
H	8.376501	-2.653659	-1.780134
C	6.800387	-4.157060	-2.299382
H	7.189846	-4.612318	-3.199566
C	5.545691	-4.449097	-1.684914
H	4.816396	-5.166025	-2.033497
O	6.702051	1.270180	-1.860764
C	5.590357	0.568416	-1.515766
N	5.010115	0.919174	-0.424303
C	5.677205	2.147527	0.057894
C	7.046294	2.097045	-0.704789
H	7.306689	3.084547	-1.091288
H	5.090231	2.980774	-0.345967
C	1.145200	-0.569242	-2.477711
C	0.747531	0.776461	-2.500108
H	1.287897	1.514502	-1.912904
C	-0.351023	1.171121	-3.265874
H	-0.636561	2.216235	-3.273384
C	-1.064842	0.230083	-4.009755

H	-1.932864	0.539900	-4.583830
C	-0.658921	-1.107692	-4.011630
H	-1.206879	-1.843341	-4.593556
C	0.445143	-1.503017	-3.256073
H	0.744988	-2.545488	-3.252335
C	2.057408	-2.663732	-0.675898
C	1.595680	-2.661011	0.650042
H	1.537138	-1.723187	1.193527
C	1.253684	-3.854887	1.286651
H	0.937148	-3.834539	2.324142
C	1.354765	-5.066050	0.603646
H	1.094616	-5.996084	1.099669
C	1.799597	-5.079547	-0.721169
H	1.882758	-6.020417	-1.257829
C	2.149978	-3.888519	-1.355941
H	2.532901	-3.926812	-2.367902
C	5.651746	2.254590	1.562608
C	5.082881	3.383650	2.161085
C	6.097699	1.206429	2.377452
C	4.961596	3.468791	3.549321
C	5.973596	1.284719	3.762312
C	5.402878	2.415519	4.352330
H	4.709868	4.190394	1.535301
H	6.528284	0.321140	1.923756
H	4.513057	4.349652	3.999447
H	6.306155	0.454903	4.378253
H	5.301585	2.473713	5.432193
C	8.214940	1.496038	0.041508
C	8.880310	2.270372	0.999502
C	8.611772	0.170691	-0.161543
C	9.911791	1.720241	1.758928
C	9.643199	-0.381647	0.601062
C	10.292183	0.389539	1.566392
H	8.575358	3.300012	1.166472
H	8.122250	-0.420474	-0.925626
H	10.417066	2.329302	2.502337
H	9.940889	-1.413475	0.436455
H	11.094508	-0.039187	2.159246
H	-0.527298	4.616744	-5.215681
C	1.193415	4.199706	-3.983054
C	-0.097933	4.680533	-4.219301
C	-0.829892	5.246469	-3.172430
H	-1.836343	5.616794	-3.342593
C	-0.260868	5.356812	-1.902331
H	-0.823663	5.823841	-1.101657
H	1.401275	6.091281	0.079778
C	1.689188	5.113454	-0.313282
H	2.777551	5.079270	-0.414203
C	1.036308	4.888678	-1.659471
H	2.746871	3.908928	-2.515043
C	1.751996	4.296387	-2.708627
H	1.762675	3.747918	-4.790011
O	1.294546	4.204497	0.744007
C	1.901486	2.985699	0.754110
C	1.118587	2.848467	3.188102
H	0.665520	3.810625	2.954446
H	1.888655	3.010676	3.956228
H	0.342867	2.211417	3.632909
C	1.716927	2.232950	1.954691

N	2.410264	1.035321	2.012040
C	2.447341	0.347770	3.125884
H	1.900305	0.714703	3.993198
C	3.185513	-0.883181	3.368876
C	4.126273	-1.456852	2.488026
H	4.338102	-0.973199	1.540314
H	5.544719	-3.034445	2.156621
C	4.808761	-2.619126	2.836636
C	4.570582	-3.250478	4.061278
H	5.108612	-4.156332	4.323675
C	3.648339	-2.692578	4.949855
H	3.463762	-3.161753	5.912259
C	2.976123	-1.522155	4.610230
H	2.278089	-1.080038	5.315185
Ni	-2.942828	0.940414	0.361765
P	-4.820490	0.869916	-0.748887
C	-6.143558	2.110605	1.346649
H	-5.139551	2.386626	1.656278
C	-5.050558	-0.855507	-1.383908
C	-6.019402	2.231814	-2.955365
H	-6.984005	1.933047	-2.561432
C	-4.838011	1.895002	-2.277234
C	-6.318750	1.343651	0.184672
C	-4.654371	-1.118198	-2.726047
H	-4.368363	-0.294585	-3.368896
C	-7.613322	0.978722	-0.213312
H	-7.757644	0.344640	-1.081996
C	-5.403651	-3.257844	-1.056358
C	-5.399845	-1.915936	-0.544523
C	-5.962995	2.972589	-4.136115
H	-6.882947	3.235052	-4.649934
C	-5.000960	-3.499420	-2.409656
C	-4.622633	-2.399007	-3.217980
H	-4.314582	-2.580103	-4.244433
C	-3.606403	2.320451	-2.794127
H	-2.695980	2.088486	-2.253433
C	-8.536212	2.145828	1.691784
H	-9.397040	2.449660	2.279741
C	-7.250273	2.511665	2.094837
H	-7.106915	3.103742	2.993662
C	-8.716447	1.379534	0.537948
H	-9.712337	1.071592	0.236511
C	-4.989802	-4.828358	-2.910069
H	-4.679320	-4.994302	-3.938183
C	-5.774426	-5.651299	-0.778557
H	-6.073433	-6.487809	-0.154056
C	-3.551439	3.046799	-3.983761
H	-2.589890	3.367620	-4.369467
C	-5.372042	-5.884181	-2.115114
H	-5.367661	-6.895844	-2.509458
C	-5.783134	-4.376020	-0.261027
H	-6.082240	-4.215434	0.767518
C	-4.730012	3.374176	-4.656563
H	-4.690307	3.947648	-5.577961
P	-3.047325	-1.059625	1.343361
C	-1.850630	-2.518224	-0.708050
H	-1.626108	-1.549848	-1.145531
C	-4.804933	-1.378934	1.853007
C	-1.228946	-1.969420	3.353348

H	-1.116345	-2.876117	2.771489
C	-2.106314	-0.964986	2.924153
C	-2.512094	-2.598592	0.524866
C	-5.197627	-1.163758	3.202127
H	-4.448745	-0.940058	3.951357
C	-2.812403	-3.855143	1.074455
H	-3.350483	-3.920064	2.015737
C	-7.148130	-1.801005	1.275214
C	-5.769840	-1.691893	0.892747
C	-0.484063	-1.802306	4.523139
H	0.207412	-2.579023	4.834239
C	-7.526901	-1.535960	2.630490
C	-6.517811	-1.227864	3.574998
H	-6.800559	-1.046534	4.608473
C	-2.211012	0.218186	3.679093
H	-2.854573	1.022379	3.331060
C	-1.811082	-4.934350	-0.837916
H	-1.548477	-5.840317	-1.375044
C	-1.511286	-3.688065	-1.386965
H	-1.019975	-3.623214	-2.349395
C	-2.454095	-5.018638	0.398778
H	-2.699900	-5.987413	0.822298
C	-8.898349	-1.587647	2.997066
H	-9.169503	-1.376378	4.027836
C	-9.494082	-2.181927	0.732012
H	-10.259534	-2.436856	0.005121
C	-1.478144	0.375695	4.854520
H	-1.574919	1.290691	5.431056
C	-9.864457	-1.901797	2.069651
H	-10.909939	-1.940823	2.359928
C	-8.174264	-2.132045	0.344793
H	-7.907937	-2.341809	-0.684213
C	-0.613313	-0.637325	5.279810
H	-0.038076	-0.512237	6.192399
H	-0.289249	0.648573	1.872961
C	-0.342846	1.198116	0.940927
H	0.288548	0.854740	0.128510
C	-1.304735	2.128668	0.729854
C	-2.364552	2.796723	0.432903
C	-2.803632	4.185401	0.452948
C	-1.996325	5.153379	1.086421
C	-2.403673	6.483263	1.146009
H	-1.772593	7.217095	1.639553
C	-3.615263	6.876799	0.566981
H	-3.929107	7.915431	0.610385
H	-5.363493	6.220345	-0.511518
C	-4.419832	5.925277	-0.062014
C	-4.023805	4.588783	-0.110456
H	-4.657214	3.858249	-0.595253
H	-1.042540	4.848388	1.504005
O	2.543019	2.600565	-0.251877

Int7-A_R_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-5980.421139
Thermal and entropic correction, BS1 (a.u.)	1.482591
Electronic Energy, BS2 (a.u.)	-9902.776940

Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	3.060139	0.372961	0.085117
Fe	5.705491	-2.506700	-2.188869
P	2.562621	-1.143378	-1.451059
C	4.035814	-1.354593	-2.521225
C	5.240114	-0.531691	-2.452423
C	6.128811	-0.954453	-3.495515
H	7.112124	-0.543723	-3.670002
C	5.503508	-2.006097	-4.210798
H	5.936523	-2.559837	-5.032000
C	4.227598	-2.244518	-3.627816
H	3.523282	-2.987979	-3.968834
C	5.429121	-3.577105	-0.438162
H	4.536730	-3.524298	0.167291
C	6.575184	-2.733968	-0.328273
H	6.702565	-1.922594	0.374549
C	7.498799	-3.106241	-1.352923
H	8.450379	-2.634972	-1.557174
C	6.920391	-4.178956	-2.096471
H	7.357738	-4.659132	-2.960956
C	5.642131	-4.468664	-1.531970
H	4.938115	-5.206181	-1.889220
O	6.683627	1.265395	-1.851742
C	5.572294	0.552974	-1.536663
N	4.929281	0.938637	-0.490061
C	5.543293	2.205725	-0.035720
C	6.954087	2.144326	-0.714914
H	7.225161	3.117852	-1.128076
H	4.970975	3.008425	-0.516017
C	1.205560	-0.689913	-2.603792
C	0.735213	0.630596	-2.555121
H	1.208367	1.353730	-1.899590
C	-0.346199	1.023853	-3.344742
H	-0.692969	2.048760	-3.287943
C	-0.969321	0.101851	-4.186440
H	-1.827931	0.402762	-4.779075
C	-0.491804	-1.210582	-4.257815
H	-0.971854	-1.929724	-4.915008
C	0.592777	-1.604004	-3.474448
H	0.940082	-2.631059	-3.521001
C	2.091782	-2.791858	-0.787835
C	1.593216	-2.799403	0.525330
H	1.503878	-1.863791	1.068720
C	1.231968	-3.998003	1.141391
H	0.867881	-3.987469	2.163130
C	1.351898	-5.203746	0.451673
H	1.069980	-6.136306	0.930335
C	1.834691	-5.206982	-0.859271
H	1.927950	-6.142763	-1.402791
C	2.202539	-4.011040	-1.474498
H	2.604198	-4.042090	-2.479035
C	5.436726	2.394780	1.456834
C	4.861310	3.564615	1.965515
C	5.831227	1.389943	2.348327
C	4.681570	3.731146	3.340416
C	5.650492	1.550083	3.720399

C	5.072608	2.719748	4.220763
H	4.540111	4.345051	1.280169
H	6.268568	0.475827	1.964037
H	4.235156	4.645308	3.720831
H	5.947944	0.754367	4.396384
H	4.930757	2.843635	5.290382
C	8.082078	1.589473	0.123955
C	8.679869	2.411202	1.087133
C	8.504663	0.262382	-0.000303
C	9.668287	1.905597	1.930127
C	9.492906	-0.245160	0.846060
C	10.072875	0.572921	1.816692
H	8.356548	3.443498	1.191443
H	8.071976	-0.365163	-0.769614
H	10.121948	2.551238	2.675841
H	9.812217	-1.278274	0.741398
H	10.842173	0.179329	2.473996
H	-0.526953	4.439347	-5.227549
C	1.177474	4.098640	-3.950682
C	-0.117117	4.548800	-4.227182
C	-0.879248	5.141164	-3.218179
H	-1.890047	5.481544	-3.418219
C	-0.342116	5.301351	-1.940261
H	-0.925835	5.789912	-1.169962
H	1.173312	5.995748	0.155092
C	1.535989	5.065464	-0.281991
H	2.628383	5.071443	-0.313509
C	0.950352	4.845849	-1.653190
H	2.701510	3.873294	-2.443891
C	1.704755	4.239053	-2.667572
H	1.771171	3.632558	-4.731268
O	1.130490	4.071362	0.725201
C	1.667726	2.865857	0.642878
C	0.806208	2.623539	3.019413
H	0.099145	3.415082	2.787403
H	1.688113	3.061406	3.495858
H	0.306585	1.949017	3.716562
C	1.186176	1.894182	1.729245
N	2.249537	0.858991	1.880461
C	2.369286	0.286311	3.027721
H	1.750185	0.618352	3.859882
C	3.256972	-0.822988	3.381894
C	4.139342	-1.470292	2.498206
H	4.192155	-1.156728	1.460008
H	5.638656	-2.992562	2.268961
C	4.956781	-2.500815	2.953287
C	4.906783	-2.909203	4.290348
H	5.548730	-3.713912	4.635839
C	4.030275	-2.281076	5.176698
H	3.984895	-2.592414	6.215710
C	3.214277	-1.247906	4.722922
H	2.535131	-0.754518	5.412287
Ni	-2.984020	0.997152	0.407802
P	-4.893297	0.927679	-0.700407
C	-6.312193	2.015396	1.408859
H	-5.316482	2.246700	1.778847
C	-5.142803	-0.799428	-1.361721
C	-5.999932	2.688536	-2.702277
H	-6.951697	2.637310	-2.185354

C	-4.898545	1.964927	-2.228128
C	-6.442098	1.358103	0.176474
C	-4.819850	-1.070834	-2.720975
H	-4.588495	-0.250102	-3.388410
C	-7.720853	1.038133	-0.302580
H	-7.829377	0.498989	-1.239056
C	-5.456824	-3.208293	-1.010795
C	-5.445465	-1.862723	-0.507617
C	-5.872204	3.505134	-3.829996
H	-6.730116	4.071033	-4.181425
C	-5.107806	-3.455908	-2.377112
C	-4.790541	-2.354158	-3.208222
H	-4.535798	-2.535637	-4.249450
C	-3.669891	2.078920	-2.900588
H	-2.807079	1.558447	-2.498283
C	-8.715390	2.022545	1.669139
H	-9.597944	2.268671	2.252068
C	-7.445629	2.346819	2.151461
H	-7.337232	2.848140	3.108779
C	-8.852041	1.371559	0.440676
H	-9.837241	1.100815	0.074249
C	-5.097059	-4.788807	-2.867695
H	-4.826374	-4.957821	-3.906756
C	-5.787898	-5.604956	-0.702351
H	-6.053854	-6.439869	-0.060664
C	-3.548843	2.874988	-4.037016
H	-2.590172	2.956765	-4.540201
C	-5.432198	-5.843987	-2.051088
H	-5.429076	-6.858740	-2.437903
C	-5.794181	-4.325519	-0.194946
H	-6.058137	-4.160130	0.842499
C	-4.652732	3.595812	-4.502889
H	-4.560117	4.231004	-5.379105
P	-3.046956	-0.998967	1.335947
C	-1.876372	-2.409763	-0.761738
H	-1.682408	-1.421702	-1.171318
C	-4.790486	-1.362056	1.886800
C	-1.143491	-1.998620	3.251258
H	-1.032106	-2.868209	2.615129
C	-2.069408	-1.002187	2.910532
C	-2.518558	-2.532091	0.478460
C	-5.161901	-1.175971	3.246837
H	-4.399856	-0.978078	3.989975
C	-2.788681	-3.809833	0.992812
H	-3.312474	-3.909946	1.939182
C	-7.151087	-1.752425	1.345845
C	-5.778597	-1.644688	0.940007
C	-0.351855	-1.875600	4.397043
H	0.372657	-2.648639	4.637506
C	-7.504533	-1.518796	2.713317
C	-6.475141	-1.238307	3.644091
H	-6.736272	-1.081340	4.687467
C	-2.176628	0.128086	3.742487
H	-2.847052	0.934029	3.457324
C	-1.797402	-4.819901	-0.963181
H	-1.530135	-5.706339	-1.530185
C	-1.524228	-3.553357	-1.479380
H	-1.048790	-3.450728	-2.446854
C	-2.423298	-4.948535	0.278563

H	-2.653409	-5.932810	0.674859
C	-8.868228	-1.583760	3.105775
H	-9.119315	-1.395159	4.146181
C	-9.505940	-2.134965	0.842039
H	-10.284432	-2.377217	0.124554
C	-1.410697	0.235949	4.902457
H	-1.523086	1.106245	5.542848
C	-9.851160	-1.885698	2.192073
H	-10.890408	-1.937220	2.502585
C	-8.194803	-2.066584	0.429388
H	-7.947890	-2.248232	-0.609628
C	-0.491287	-0.765765	5.231824
H	0.106389	-0.681126	6.135119
H	-0.211931	0.292477	1.868632
C	-0.037900	1.094414	1.146496
H	0.303219	0.595328	0.232244
C	-1.317020	1.769100	0.855418
C	-2.123709	2.722038	0.543969
C	-2.422178	4.141761	0.461678
C	-1.786566	5.076252	1.304816
C	-2.080919	6.436595	1.222912
H	-1.579062	7.135236	1.887246
C	-3.013859	6.903714	0.291937
H	-3.238363	7.963974	0.224508
H	-4.400007	6.330561	-1.261069
C	-3.663451	5.987206	-0.539982
C	-3.382606	4.625751	-0.446190
H	-3.895197	3.923669	-1.087285
H	-1.053104	4.730611	2.021168
O	2.442742	2.539410	-0.249925

IntIi-C_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-6284.749139
Thermal and entropic correction, BS1 (a.u.)	1.541143
Electronic Energy, BS2 (a.u.)	-10207.233168
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

xyz

Cu	2.727462	0.256524	0.061092
Fe	6.711016	-0.609811	-1.193251
P	3.951331	1.572618	-1.247177
C	5.689575	1.148529	-0.919791
C	6.197163	0.650593	0.341668
C	7.626560	0.577352	0.247469
H	8.280433	0.210015	1.024700
C	8.003409	1.021558	-1.048215
H	9.009968	1.037063	-1.442401
C	6.822973	1.377292	-1.762234
H	6.772432	1.724593	-2.784316
C	5.413611	-2.061790	-1.899486
H	4.345500	-1.933493	-1.955297
C	6.120646	-2.551079	-0.762109
H	5.679433	-2.858576	0.174961
C	7.516689	-2.512704	-1.056423

H	8.318030	-2.785255	-0.383224
C	7.671525	-2.000629	-2.381056
H	8.611100	-1.814773	-2.883080
C	6.371934	-1.719859	-2.901088
H	6.148774	-1.277909	-3.862379
O	6.154340	0.094299	2.640787
C	5.431733	0.226510	1.505843
N	4.175377	-0.056829	1.572471
C	3.874701	-0.433526	2.966562
C	5.313385	-0.594427	3.607096
H	5.377978	-0.037719	4.544359
H	3.363116	0.412687	3.439633
C	3.914270	3.363323	-0.827806
C	4.994475	4.004291	-0.202800
H	5.928919	3.476746	-0.047726
C	4.873306	5.325792	0.233623
H	5.717395	5.810721	0.715077
C	3.673120	6.015071	0.059948
H	3.573084	7.036034	0.415631
C	2.593203	5.384262	-0.564422
H	1.648998	5.906442	-0.663941
C	2.713672	4.068899	-1.011459
H	1.864875	3.585492	-1.486575
C	3.843971	1.468059	-3.073582
C	3.349621	0.275092	-3.623519
H	2.997006	-0.509458	-2.962730
C	3.282952	0.109088	-5.006528
H	2.887139	-0.815230	-5.416876
C	3.698040	1.142788	-5.851377
H	3.641494	1.019998	-6.928953
C	4.173691	2.340750	-5.310123
H	4.485202	3.148014	-5.966296
C	4.249329	2.505372	-3.925352
H	4.612574	3.439956	-3.507997
C	3.006435	-1.662603	3.085754
C	2.195644	-1.827657	4.212552
C	3.075116	-2.690904	2.139149
C	1.487973	-3.015023	4.408790
C	2.360457	-3.873332	2.327747
C	1.572673	-4.043916	3.469504
H	2.128667	-1.027054	4.944669
H	3.681034	-2.550564	1.252195
H	0.870757	-3.134834	5.292816
H	2.419688	-4.663641	1.585183
H	1.017722	-4.965074	3.618216
C	5.803188	-2.012086	3.794840
C	5.409925	-2.728792	4.931020
C	6.593574	-2.643961	2.828882
C	5.773828	-4.065641	5.084220
C	6.961603	-3.981754	2.984240
C	6.546703	-4.698396	4.107442
H	4.801704	-2.244922	5.690114
H	6.933252	-2.086892	1.963381
H	5.457865	-4.612035	5.967714
H	7.576492	-4.461559	2.227998
H	6.832370	-5.738946	4.227948
H	-0.304155	-3.320524	-6.912521
C	0.334397	-2.397161	-5.069821
C	0.095146	-3.483817	-5.916081

C	0.362206	-4.779076	-5.472751
H	0.172289	-5.628937	-6.121228
C	0.860354	-4.988251	-4.184304
H	1.052669	-6.000974	-3.838786
H	2.703695	-3.840295	-1.855942
C	1.660663	-4.151771	-1.949722
H	1.573207	-5.202469	-1.669365
C	1.111719	-3.905995	-3.334397
H	1.019976	-1.747101	-3.149209
C	0.846232	-2.605056	-3.789441
H	0.113636	-1.385692	-5.393432
O	0.867770	-3.434817	-0.957530
C	1.286570	-2.232102	-0.578779
C	-0.639187	-2.306385	1.118288
H	-1.571804	-1.791198	1.343863
H	-0.115902	-2.527754	2.049042
H	-0.899008	-3.241328	0.627047
C	0.227065	-1.452730	0.187533
N	0.865605	-0.265731	0.782161
C	0.312489	0.252286	1.821208
H	-0.572526	-0.199076	2.264225
C	0.862051	1.409694	2.531744
C	1.526301	2.451763	1.870856
H	1.551163	2.468858	0.788595
H	2.578431	4.308470	2.067025
C	2.098676	3.493216	2.595513
C	2.010435	3.502678	3.990085
H	2.451590	4.318143	4.555224
C	1.322045	2.484264	4.658170
H	1.233798	2.504364	5.740300
C	0.736978	1.448462	3.931408
H	0.205535	0.651349	4.441032
O	2.370846	-1.766288	-0.910690
H	-0.418719	-1.090944	-0.626184
Ni	-3.019947	1.255658	0.468738
P	-3.445580	0.217064	-1.418150
C	-5.869737	1.569688	-1.619461
H	-5.470139	2.147922	-0.790542
C	-3.388577	-1.630468	-1.265704
C	-2.461404	0.586295	-4.108096
H	-3.456676	0.362787	-4.474678
C	-2.195403	0.576129	-2.732889
C	-5.091030	0.540505	-2.170008
C	-2.360811	-2.356731	-1.927983
H	-1.707791	-1.844343	-2.624811
C	-5.623439	-0.239232	-3.207583
H	-5.057172	-1.077302	-3.602663
C	-4.100751	-3.707532	-0.184049
C	-4.283342	-2.301379	-0.425278
C	-1.457561	0.923117	-5.020526
H	-1.685635	0.946138	-6.082483
C	-3.021237	-4.405575	-0.819067
C	-2.189333	-3.703357	-1.723041
H	-1.403250	-4.234564	-2.249206
C	-0.903106	0.909505	-2.294377
H	-0.703028	0.978827	-1.229489
C	-7.667368	1.051393	-3.149907
H	-8.668810	1.241442	-3.524135
C	-7.150795	1.825115	-2.108533

H	-7.748375	2.617517	-1.667825
C	-6.902367	0.019768	-3.698455
H	-7.312461	-0.602149	-4.487896
C	-2.825600	-5.788980	-0.555316
H	-1.995500	-6.295465	-1.041054
C	-4.764588	-5.802681	0.882712
H	-5.447635	-6.351999	1.523780
C	0.101380	1.228023	-3.203644
H	1.087201	1.492426	-2.841214
C	-3.669362	-6.474676	0.286028
H	-3.511694	-7.531002	0.481638
C	-4.980489	-4.464543	0.644376
H	-5.840409	-3.974552	1.086567
C	-0.173108	1.239860	-4.573378
H	0.608914	1.503869	-5.278752
P	-4.203812	0.094604	1.921739
C	-2.420088	-0.654479	3.926072
H	-2.166870	0.402786	3.926429
C	-5.666537	-0.752794	1.120727
C	-5.393221	0.835393	4.419659
H	-5.219060	-0.186278	4.741897
C	-5.003968	1.243781	3.134326
C	-3.432370	-1.122771	3.068622
C	-6.956940	-0.267060	1.485113
H	-7.050640	0.418352	2.316252
C	-3.771888	-2.477337	3.100357
H	-4.567995	-2.846652	2.470825
C	-6.745531	-2.050621	-0.666678
C	-5.559290	-1.661869	0.060519
C	-6.005266	1.737096	5.291565
H	-6.297620	1.410099	6.285266
C	-8.018307	-1.506369	-0.302646
C	-8.089063	-0.625231	0.800609
H	-9.054669	-0.225859	1.099271
C	-5.250974	2.567671	2.737971
H	-4.931578	2.896443	1.753368
C	-2.083847	-2.893537	4.781441
H	-1.563116	-3.579292	5.442883
C	-1.758315	-1.532575	4.780916
H	-0.987598	-1.160276	5.449946
C	-3.091680	-3.362404	3.940453
H	-3.360460	-4.414667	3.935592
C	-9.178320	-1.852458	-1.045997
H	-10.130902	-1.421889	-0.749324
C	-7.848522	-3.259987	-2.481675
H	-7.784875	-3.937071	-3.328478
C	-5.866099	3.466991	3.609353
H	-6.036770	4.491184	3.291559
C	-9.100570	-2.713074	-2.115195
H	-9.992358	-2.973949	-2.677012
C	-6.707771	-2.939313	-1.781395
H	-5.762527	-3.361740	-2.095851
C	-6.242603	3.053632	4.889130
H	-6.715139	3.754334	5.571166
H	-2.718335	3.270938	3.292898
C	-2.010385	3.560451	2.514923
H	-0.990154	3.423634	2.883197
O	-0.122456	5.324465	1.608399
C	-2.235035	2.796816	1.266816

C	-2.266114	2.928198	-0.018257
C	-1.978058	3.717541	-1.202384
C	-0.749052	4.389502	-1.334888
C	-0.438794	5.078197	-2.507480
H	0.522361	5.575266	-2.605952
C	-1.352846	5.124398	-3.563329
H	-1.107646	5.658797	-4.476445
H	-3.302325	4.505642	-4.248908
C	-2.583696	4.476665	-3.434881
C	-2.889709	3.774959	-2.271491
H	-3.834935	3.251605	-2.185868
H	-0.057632	4.361291	-0.502883
C	-1.272311	5.689409	1.771806
O	-2.263346	4.985538	2.324593
O	-1.757024	6.890462	1.428665
C	-0.826866	7.739199	0.738543
H	-1.332382	8.698290	0.628114
H	0.096818	7.855038	1.311604
H	-0.595777	7.318579	-0.245135

TS12i-C_NiCu

	Value
Charge	1
Electronic Energy, BS1 (a.u.)	-6284.703438
Thermal and entropic correction, BS1 (a.u.)	1.537871
Electronic Energy, BS2 (a.u.)	-10207.209589
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-75.7i

Molecular Geometry in Cartesian Coordinates

Cu	2.823490	0.246504	-0.036425
Fe	6.692822	-1.125043	-1.285501
P	3.851556	0.878104	-1.903335
C	5.631435	0.614759	-1.609387
C	6.286046	0.639132	-0.316845
C	7.700300	0.528419	-0.533617
H	8.444535	0.489794	0.248035
C	7.924762	0.427074	-1.931742
H	8.884022	0.282776	-2.409010
C	6.663244	0.477343	-2.591978
H	6.493593	0.389468	-3.655924
C	5.404057	-2.740922	-1.138424
H	4.334465	-2.643758	-1.051957
C	6.314793	-2.745148	-0.042214
H	6.050467	-2.665179	1.001989
C	7.639769	-2.821697	-0.565644
H	8.554591	-2.805242	0.010947
C	7.546360	-2.870008	-1.990325
H	8.379044	-2.893229	-2.679890
C	6.164839	-2.817348	-2.344999
H	5.762252	-2.785567	-3.347802
O	6.535868	0.895534	2.023015
C	5.675134	0.659992	1.006795
N	4.442723	0.447351	1.319914
C	4.325839	0.561890	2.787770
C	5.832412	0.612020	3.263963
H	5.988527	1.470625	3.920972

H	3.858692	1.525925	3.009716
C	3.750647	2.659744	-2.333642
C	4.828191	3.372932	-2.887904
H	5.772948	2.876069	-3.080662
C	4.695888	4.730445	-3.179072
H	5.534807	5.272573	-3.605791
C	3.496296	5.393062	-2.904948
H	3.403490	6.455643	-3.109916
C	2.424922	4.696478	-2.344316
H	1.510814	5.200250	-2.056798
C	2.549022	3.334306	-2.067998
H	1.705121	2.818233	-1.621550
C	3.582789	-0.024077	-3.486051
C	3.153131	-1.357700	-3.414004
H	2.940722	-1.794430	-2.445737
C	2.979337	-2.111913	-4.574150
H	2.634927	-3.138808	-4.499920
C	3.217052	-1.532666	-5.823907
H	3.077272	-2.114919	-6.729877
C	3.617218	-0.196337	-5.906069
H	3.787105	0.262595	-6.875575
C	3.799520	0.557549	-4.743345
H	4.101249	1.597652	-4.816986
C	3.487706	-0.535624	3.400165
C	2.737287	-0.276274	4.551466
C	3.482569	-1.826620	2.860862
C	2.005296	-1.294508	5.166452
C	2.749180	-2.844480	3.469999
C	2.013457	-2.583765	4.629750
H	2.720603	0.729626	4.961299
H	4.037220	-2.020503	1.950535
H	1.430715	-1.080629	6.063311
H	2.753707	-3.842808	3.042007
H	1.445661	-3.377530	5.106050
C	6.385683	-0.643379	3.899912
C	6.057205	-0.937562	5.229226
C	7.190891	-1.534054	3.183606
C	6.497708	-2.119918	5.820737
C	7.634798	-2.717994	3.777409
C	7.283754	-3.017996	5.093759
H	5.440408	-0.247524	5.797917
H	7.482094	-1.293586	2.167867
H	6.231111	-2.338552	6.850382
H	8.260385	-3.401715	3.210548
H	7.628949	-3.938098	5.555482
H	-1.106511	-5.406410	-4.897707
C	-0.138310	-3.948922	-3.634917
C	-0.574173	-5.235063	-3.966945
C	-0.326454	-6.297375	-3.097228
H	-0.665371	-7.298210	-3.346833
C	0.347905	-6.073886	-1.894047
H	0.526463	-6.902569	-1.213427
H	2.553069	-4.273179	-0.389071
C	1.506929	-4.553815	-0.249571
H	1.452783	-5.428409	0.400337
C	0.792883	-4.791312	-1.557360
H	0.874754	-2.723504	-2.200335
C	0.545718	-3.728666	-2.440320
H	-0.330985	-3.110969	-4.296496

O	0.831018	-3.491741	0.489960
C	1.321020	-2.257241	0.396636
C	-0.510604	-1.667216	2.082859
H	-1.374921	-1.017009	2.214543
H	0.066941	-1.689405	3.008569
H	-0.889181	-2.666946	1.881160
C	0.350551	-1.196583	0.907124
N	1.082930	0.074420	1.061786
C	0.709079	0.882604	1.997000
H	-0.106616	0.598083	2.661347
C	1.337360	2.156538	2.322358
C	2.154763	2.868336	1.431272
H	2.248392	2.541084	0.406043
H	3.411850	4.576336	1.132094
C	2.812190	4.020053	1.844414
C	2.645016	4.490249	3.149433
H	3.130838	5.409762	3.458668
C	1.809909	3.809280	4.039361
H	1.649986	4.196248	5.040305
C	1.149296	2.659682	3.623368
H	0.491062	2.133622	4.309503
O	2.387189	-2.000541	-0.146030
H	-0.311717	-1.074034	0.036610
Ni	-3.467205	1.624135	0.025579
P	-3.688088	-0.030513	-1.380301
C	-6.078207	1.077711	-2.272274
H	-5.767912	1.935525	-1.681756
C	-3.621073	-1.681305	-0.535816
C	-2.386372	-0.538120	-3.883320
H	-3.346757	-0.836434	-4.288705
C	-2.280598	-0.106145	-2.556616
C	-5.243447	-0.048164	-2.339279
C	-2.511922	-2.536694	-0.786322
H	-1.782026	-2.266968	-1.538719
C	-5.652454	-1.168578	-3.077654
H	-5.036909	-2.062877	-3.095755
C	-4.449631	-3.304745	1.100605
C	-4.605641	-2.073020	0.375230
C	-1.257839	-0.547462	-4.707919
H	-1.355736	-0.856804	-5.744583
C	-3.296997	-4.122520	0.868934
C	-2.362515	-3.724738	-0.115771
H	-1.516176	-4.364209	-0.336944
C	-1.030961	0.311438	-2.070109
H	-0.948227	0.717354	-1.065598
C	-7.698107	-0.029811	-3.682592
H	-8.654112	-0.027910	-4.197083
C	-7.300772	1.086061	-2.942720
H	-7.944685	1.957849	-2.879692
C	-6.872625	-1.154355	-3.751469
H	-7.190580	-2.030146	-4.307962
C	-3.127415	-5.326038	1.605975
H	-2.242045	-5.927473	1.417889
C	-5.223670	-4.938377	2.740812
H	-5.972760	-5.266937	3.454907
C	0.095609	0.272112	-2.884569
H	1.048616	0.592763	-2.482932
C	-4.063443	-5.724017	2.530925
H	-3.925911	-6.643866	3.091002

C	-5.416599	-3.770382	2.038907
H	-6.320470	-3.193717	2.198187
C	-0.014312	-0.151605	-4.211583
H	0.861755	-0.158514	-4.850917
P	-4.647773	0.910937	1.765239
C	-2.665192	0.727599	3.706563
H	-2.331712	1.676359	3.298275
C	-6.073551	-0.138328	1.198269
C	-5.814657	2.325991	3.938425
H	-5.588382	1.457293	4.548527
C	-5.465639	2.343535	2.581032
C	-3.789609	0.083676	3.158670
C	-7.372255	0.441695	1.293875
H	-7.507321	1.360353	1.848669
C	-4.215575	-1.130948	3.703364
H	-5.099317	-1.617064	3.313951
C	-7.048216	-1.957908	-0.129841
C	-5.911234	-1.341573	0.505952
C	-6.447573	3.430056	4.512340
H	-6.708370	3.412174	5.566230
C	-8.331907	-1.328397	-0.055081
C	-8.460564	-0.130095	0.685824
H	-9.437245	0.338849	0.768774
C	-5.764679	3.476971	1.807018
H	-5.481264	3.501829	0.757206
C	-2.384017	-1.088537	5.282636
H	-1.832752	-1.547214	6.098032
C	-1.978045	0.148367	4.771733
H	-1.115652	0.653527	5.196131
C	-3.503916	-1.725336	4.747952
H	-3.832732	-2.683107	5.139640
C	-9.445526	-1.913000	-0.715505
H	-10.409099	-1.415639	-0.647280
C	-8.046481	-3.717467	-1.495905
H	-7.940913	-4.642239	-2.055318
C	-6.400847	4.575920	2.382236
H	-6.618232	5.451042	1.777637
C	-9.309967	-3.084688	-1.422215
H	-10.166948	-3.526650	-1.921208
C	-6.948639	-3.171265	-0.871014
H	-5.990686	-3.668412	-0.953747
C	-6.741364	4.553823	3.737425
H	-7.228089	5.412934	4.188821
H	-3.195058	4.000762	1.891392
C	-2.413441	3.502608	1.328254
H	-1.482190	3.292105	1.844479
O	0.266360	4.795835	-0.069150
C	-2.440881	3.470708	-0.024013
C	-2.652154	3.011302	-1.200596
C	-2.285163	3.270821	-2.580052
C	-1.054848	3.910368	-2.830112
C	-0.643444	4.129038	-4.142178
H	0.310837	4.613367	-4.327726
C	-1.446260	3.722167	-5.212649
H	-1.119149	3.891855	-6.234596
H	-3.302845	2.789284	-5.794871
C	-2.673351	3.101247	-4.966423
C	-3.091787	2.873425	-3.656959
H	-4.038957	2.381422	-3.465366

H	-0.461854	4.227763	-1.976989
C	0.185494	5.364081	1.050618
O	-0.395797	4.999990	2.095783
O	0.859472	6.583824	1.216881
C	1.552094	7.085799	0.089536
H	1.922594	8.076763	0.369135
H	2.402584	6.449982	-0.188972
H	0.899073	7.176263	-0.787304

Int2i-C_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-6284.760989
Thermal and entropic correction, BS1 (a.u.)	1.539075
Electronic Energy, BS2 (a.u.)	-10207.241700
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	3.486703	-0.013330	0.371536
Fe	6.900098	1.479564	-1.652274
P	4.049425	2.128328	0.224954
C	5.857771	2.170380	-0.020120
C	6.791133	1.126899	0.360986
C	8.115190	1.571463	0.032224
H	9.014945	0.991202	0.174032
C	8.013847	2.862111	-0.549427
H	8.834474	3.443104	-0.946640
C	6.638786	3.231830	-0.581615
H	6.235159	4.141820	-1.001126
C	5.596985	0.499404	-2.929869
H	4.584691	0.231799	-2.668199
C	6.744024	-0.311619	-2.691874
H	6.743663	-1.286809	-2.227810
C	7.897255	0.410102	-3.121383
H	8.923370	0.078745	-3.038337
C	7.460299	1.670238	-3.632889
H	8.098687	2.461084	-4.002306
C	6.039122	1.727303	-3.512894
H	5.409429	2.568236	-3.766900
O	7.567749	-0.887052	1.342724
C	6.499141	-0.209883	0.860292
N	5.368920	-0.827486	0.858363
C	5.584305	-2.154431	1.465436
C	7.157632	-2.273742	1.508865
H	7.482392	-2.582583	2.505075
H	5.217236	-2.109452	2.495507
C	3.774826	3.128852	1.741395
C	4.763597	3.933881	2.326636
H	5.747510	4.008032	1.874720
C	4.489939	4.636158	3.502959
H	5.261513	5.255505	3.951118
C	3.232209	4.539341	4.102584
H	3.024881	5.081462	5.020590
C	2.246033	3.734514	3.525524
H	1.270973	3.637066	3.992389
C	2.511642	3.030571	2.350773
H	1.744006	2.379157	1.944611

C	3.458333	3.197773	-1.148858
C	2.937589	2.575956	-2.291760
H	2.835810	1.496986	-2.306160
C	2.538146	3.335253	-3.392220
H	2.119904	2.840242	-4.263536
C	2.649592	4.727303	-3.355965
H	2.335881	5.321074	-4.209261
C	3.144255	5.357317	-2.209759
H	3.214283	6.440417	-2.171415
C	3.542195	4.597686	-1.107147
H	3.909797	5.092424	-0.212756
C	4.851336	-3.256917	0.739491
C	4.426963	-4.388381	1.443445
C	4.605147	-3.178207	-0.635279
C	3.783799	-5.436679	0.782393
C	3.954499	-4.219091	-1.297047
C	3.548551	-5.355550	-0.592088
H	4.599812	-4.446624	2.514953
H	4.898186	-2.286049	-1.176040
H	3.464098	-6.312430	1.339588
H	3.766574	-4.144000	-2.364333
H	3.047133	-6.168698	-1.108477
C	7.809014	-3.141072	0.454135
C	7.756408	-4.534637	0.587882
C	8.449115	-2.588039	-0.659113
C	8.302055	-5.360212	-0.393045
C	8.997824	-3.415889	-1.641671
C	8.919879	-4.802757	-1.515731
H	7.271809	-4.975844	1.453840
H	8.528970	-1.511257	-0.751044
H	8.247986	-6.438757	-0.279693
H	9.491053	-2.973532	-2.502563
H	9.346238	-5.446006	-2.279504
H	-2.844498	1.665417	-5.137254
C	-1.029878	1.446152	-3.992851
C	-2.009917	1.014602	-4.891336
C	-1.914567	-0.250279	-5.473645
H	-2.675512	-0.591620	-6.168996
C	-0.843654	-1.086984	-5.152713
H	-0.780624	-2.078551	-5.593674
H	2.234262	-1.106881	-3.871801
C	1.254294	-1.585277	-3.835497
H	1.271771	-2.500781	-4.428982
C	0.140122	-0.663526	-4.253262
H	0.779937	0.942790	-2.958696
C	0.039708	0.610208	-3.677675
H	-1.100657	2.421124	-3.524706
O	1.003885	-2.028563	-2.460724
C	1.708347	-1.481873	-1.468763
C	0.504726	-3.181226	0.024245
H	-0.144786	-3.198281	0.898803
H	1.285478	-3.941499	0.108686
H	-0.117905	-3.400036	-0.841899
C	1.106517	-1.779125	-0.105678
N	2.057845	-1.377633	0.940408
C	1.948030	-1.915556	2.100978
H	1.229869	-2.713481	2.283370
C	2.766554	-1.528616	3.253984
C	3.218210	-0.211992	3.425103

H	2.848337	0.556629	2.762029
H	4.393371	1.138284	4.608447
C	4.063021	0.111207	4.483868
C	4.457581	-0.879361	5.388996
H	5.119373	-0.630869	6.213492
C	3.971647	-2.184563	5.254366
H	4.253884	-2.947088	5.974044
C	3.115430	-2.504633	4.201110
H	2.734092	-3.516550	4.093569
O	2.676862	-0.753190	-1.655106
H	0.265794	-1.071653	-0.005203
Ni	-4.079196	0.470254	1.803132
P	-3.926062	1.125265	-0.302325
C	-6.275929	2.605022	-0.054292
H	-6.185242	2.366928	1.001939
C	-3.818522	-0.419827	-1.332446
C	-2.492486	3.382942	-1.282479
H	-3.442556	3.809535	-1.579768
C	-2.429984	2.114844	-0.685460
C	-5.320362	2.109841	-0.951113
C	-2.538004	-0.900716	-1.718565
H	-1.662749	-0.287063	-1.569107
C	-5.444384	2.393233	-2.319916
H	-4.716239	1.996805	-3.021594
C	-4.809072	-2.485729	-2.213218
C	-4.946112	-1.208510	-1.570546
C	-1.323345	4.121152	-1.472412
H	-1.383047	5.112052	-1.912935
C	-3.505215	-2.961346	-2.558868
C	-2.387590	-2.134509	-2.298570
H	-1.397952	-2.473422	-2.579999
C	-1.192025	1.619839	-0.248874
H	-1.140380	0.695450	0.317979
C	-7.463125	3.649162	-1.881712
H	-8.299734	4.237776	-2.245548
C	-7.344780	3.371642	-0.518514
H	-8.088442	3.741760	0.180735
C	-6.511242	3.161596	-2.780942
H	-6.612615	3.361823	-3.842763
C	-3.361376	-4.238608	-3.162659
H	-2.361510	-4.584636	-3.411686
C	-5.755449	-4.550333	-3.099963
H	-6.621945	-5.169222	-3.313184
C	-0.026243	2.345141	-0.479815
H	0.916304	1.935167	-0.135212
C	-4.461589	-5.019563	-3.430688
H	-4.342905	-5.993674	-3.895705
C	-5.925032	-3.321096	-2.504216
H	-6.921638	-2.983666	-2.247036
C	-0.086397	3.597615	-1.091247
H	0.816346	4.177267	-1.239420
P	-5.529042	-1.168458	1.512813
C	-3.472251	-3.037372	1.308349
H	-2.806094	-2.233150	1.616464
C	-6.741359	-0.803720	0.155482
C	-6.990066	-2.573528	3.532582
H	-6.660365	-3.497302	3.070800
C	-6.599971	-1.339037	3.000362
C	-4.850422	-2.821458	1.155724

C	-8.069392	-0.413709	0.482718
H	-8.406704	-0.460413	1.510182
C	-5.682740	-3.860372	0.707742
H	-6.742682	-3.679921	0.554214
C	-7.221300	-0.325453	-2.198738
C	-6.322191	-0.769911	-1.174364
C	-7.795999	-2.622601	4.673651
H	-8.087956	-3.585885	5.081105
C	-8.539924	0.102408	-1.842421
C	-8.937315	0.029361	-0.485098
H	-9.945574	0.330684	-0.213903
C	-7.020473	-0.156367	3.635833
H	-6.694789	0.805364	3.245498
C	-3.775165	-5.333278	0.582962
H	-3.354151	-6.307742	0.353251
C	-2.947425	-4.300310	1.024023
H	-1.882930	-4.472908	1.138748
C	-5.145724	-5.113308	0.424516
H	-5.789908	-5.908018	0.061827
C	-9.413173	0.588276	-2.851766
H	-10.409575	0.913971	-2.565714
C	-7.708772	0.212498	-4.524257
H	-7.396800	0.256597	-5.563579
C	-7.831765	-0.208016	4.766977
H	-8.149476	0.712822	5.246813
C	-9.008664	0.644170	-4.165607
H	-9.684158	1.015526	-4.930334
C	-6.837948	-0.258568	-3.568194
H	-5.842045	-0.576694	-3.853233
C	-8.221956	-1.445406	5.288513
H	-8.847578	-1.488981	6.174844
H	-4.541183	-0.289352	4.385041
C	-3.662356	-0.133929	3.766747
H	-2.894653	-0.904667	3.799344
O	0.247035	0.828582	2.358070
C	-3.261238	1.153646	3.480802
C	-3.148259	2.104469	2.659704
C	-2.683115	3.424802	2.310827
C	-1.308033	3.713003	2.366878
C	-0.858768	4.993440	2.052921
H	0.205349	5.206659	2.090548
C	-1.765524	5.989621	1.680992
H	-1.408785	6.986399	1.437946
H	-3.836992	6.470756	1.312673
C	-3.131031	5.700939	1.610119
C	-3.590638	4.422155	1.915816
H	-4.647641	4.185679	1.848138
H	-0.620757	2.911700	2.617996
C	-0.455706	-0.187142	2.536749
O	-1.079794	-0.883744	1.689157
O	-0.587853	-0.676212	3.839458
C	-0.080797	0.166847	4.873629
H	-0.244566	-0.371549	5.810107
H	0.984473	0.371649	4.743192
H	-0.618777	1.121699	4.900050

Int3i-C_NiCu

Charge 1

Electronic Energy, BS1 (a.u.)	-6284.759259
Thermal and entropic correction, BS1 (a.u.)	1.539711
Electronic Energy, BS2 (a.u.)	-10207.237381
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	3.787460	-0.407812	0.168337
Fe	6.689408	2.581460	-0.343519
P	3.588581	1.708570	0.788607
C	5.282750	2.307367	1.123428
C	6.449068	1.467668	1.352826
C	7.589585	2.323570	1.514677
H	8.601473	1.979828	1.669957
C	7.153971	3.667008	1.385979
H	7.786980	4.543023	1.411222
C	5.749917	3.661876	1.152258
H	5.141678	4.533648	0.966224
C	5.908303	1.878775	-2.129887
H	5.000614	1.298944	-2.205601
C	7.210917	1.339778	-1.924238
H	7.451419	0.292067	-1.819282
C	8.131714	2.425236	-1.823370
H	9.192738	2.344713	-1.630061
C	7.394521	3.640179	-1.972194
H	7.800530	4.640466	-1.908198
C	6.019776	3.303258	-2.159152
H	5.196086	3.996875	-2.253945
O	7.723495	-0.487371	1.787429
C	6.557441	0.015755	1.312402
N	5.704522	-0.834847	0.857014
C	6.261944	-2.183785	1.075151
C	7.776281	-1.886558	1.385417
H	8.100393	-2.454014	2.260659
H	5.802992	-2.581396	1.986857
C	2.670383	1.914961	2.363587
C	3.245638	2.364016	3.559195
H	4.280144	2.694309	3.577706
C	2.485519	2.379336	4.733690
H	2.934171	2.729749	5.659035
C	1.158681	1.941758	4.720500
H	0.579453	1.942712	5.639749
C	0.580325	1.492860	3.528068
H	-0.438776	1.122047	3.491164
C	1.332695	1.482176	2.354605
H	0.889803	1.110410	1.435035
C	2.893043	3.012346	-0.298111
C	2.642548	2.698549	-1.639016
H	2.768152	1.678434	-1.982536
C	2.223687	3.688351	-2.530609
H	2.018928	3.427586	-3.563383
C	2.050185	4.998161	-2.083245
H	1.730337	5.770638	-2.776505
C	2.254475	5.311096	-0.734053
H	2.089734	6.324318	-0.378272
C	2.658104	4.319717	0.159514
H	2.787978	4.558023	1.211489
C	5.966639	-3.132060	-0.061270

C	5.814457	-4.498436	0.197029
C	5.836538	-2.668362	-1.374283
C	5.543471	-5.392004	-0.840803
C	5.557100	-3.556643	-2.412096
C	5.412997	-4.921859	-2.149947
H	5.901459	-4.861980	1.217586
H	5.919232	-1.606506	-1.574306
H	5.430779	-6.451104	-0.627814
H	5.453056	-3.182011	-3.426340
H	5.200404	-5.614222	-2.959256
C	8.758984	-2.070000	0.248888
C	9.119098	-3.367433	-0.139165
C	9.312089	-0.979075	-0.428494
C	9.990349	-3.569680	-1.207517
C	10.186226	-1.182341	-1.499390
C	10.522973	-2.476317	-1.895927
H	8.702398	-4.222781	0.384274
H	9.066595	0.028363	-0.113727
H	10.255157	-4.580819	-1.501650
H	10.606534	-0.326084	-2.019232
H	11.202333	-2.633892	-2.728126
H	-1.397080	3.659869	-4.407581
C	-0.627859	1.992208	-3.288680
C	-0.710849	2.818309	-4.407501
C	0.097674	2.561996	-5.518756
H	0.041259	3.198194	-6.397343
C	0.975676	1.478356	-5.504599
H	1.595221	1.275266	-6.375493
H	3.074319	-0.152349	-4.333708
C	2.043499	-0.506513	-4.423208
H	1.944835	-1.066481	-5.356628
C	1.059607	0.643961	-4.380425
H	0.308395	0.294697	-2.375183
C	0.255866	0.909470	-3.267622
H	-1.240396	2.196648	-2.421211
O	1.786108	-1.472753	-3.378802
C	2.502192	-1.394669	-2.251055
C	1.699148	-3.739172	-1.679989
H	1.028027	-4.277415	-1.006641
H	2.643643	-4.286193	-1.760328
H	1.222005	-3.710427	-2.660452
C	1.935317	-2.306756	-1.182049
N	2.708621	-2.146274	0.051788
C	2.630254	-3.060210	0.946127
H	2.135917	-4.009661	0.735659
C	3.176897	-2.919741	2.301272
C	3.187886	-1.679366	2.957860
H	2.718183	-0.825058	2.487927
H	3.746935	-0.591567	4.719678
C	3.754995	-1.557720	4.224171
C	4.309104	-2.677600	4.852206
H	4.755208	-2.583656	5.837905
C	4.260508	-3.927231	4.225138
H	4.667634	-4.802226	4.722881
C	3.680844	-4.051370	2.962797
H	3.642369	-5.019899	2.471342
O	3.436060	-0.616450	-2.099325
H	0.968577	-1.823273	-0.936229
O	-0.095613	-0.458923	-0.052588

C	-0.551772	-0.876329	1.035258
O	-0.016857	-2.116946	1.432847
O	-1.395355	-0.351227	1.798933
H	-0.070287	-1.732901	3.484517
C	-0.300987	-2.528293	2.770227
H	-1.347907	-2.824345	2.890419
H	0.341787	-3.390000	2.965435
Ni	-4.427598	0.316337	1.855770
P	-4.455740	1.212718	-0.158684
C	-6.990740	2.267073	0.299070
H	-6.787312	2.006759	1.334566
C	-4.065049	-0.179929	-1.316753
C	-3.416113	3.622127	-1.267455
H	-4.364156	3.748529	-1.774849
C	-3.175797	2.499720	-0.459824
C	-6.035894	1.968002	-0.683068
C	-2.693820	-0.380363	-1.626413
H	-1.942458	0.301308	-1.257471
C	-6.312349	2.273099	-2.024946
H	-5.600296	2.006213	-2.799383
C	-4.601914	-2.267628	-2.477985
C	-5.014256	-1.127885	-1.707075
C	-2.444598	4.614728	-1.394434
H	-2.646334	5.485245	-2.012083
C	-3.214662	-2.440525	-2.793616
C	-2.282147	-1.480178	-2.336019
H	-1.225912	-1.615830	-2.546777
C	-1.947604	2.382992	0.213835
H	-1.751448	1.521812	0.847716
C	-8.458807	3.184749	-1.387556
H	-9.399997	3.650857	-1.662793
C	-8.196728	2.874941	-0.051824
H	-8.932424	3.097100	0.715247
C	-7.516534	2.881377	-2.373285
H	-7.729219	3.093960	-3.415880
C	-2.802485	-3.580227	-3.534396
H	-1.745244	-3.695599	-3.758855
C	-5.088842	-4.349477	-3.651609
H	-5.807956	-5.091793	-3.985072
C	-0.981458	3.379491	0.077612
H	-0.037990	3.284857	0.603713
C	-3.717271	-4.515005	-3.959910
H	-3.392638	-5.380556	-4.529789
C	-5.518373	-3.261540	-2.926115
H	-6.570130	-3.158489	-2.688481
C	-1.230250	4.498851	-0.717225
H	-0.477626	5.273119	-0.808842
P	-5.596405	-1.503540	1.344167
C	-3.258836	-2.910337	0.854296
H	-2.773708	-2.016869	1.230054
C	-6.856298	-1.228882	0.011736
C	-6.783945	-3.321853	3.206714
H	-6.323524	-4.130348	2.650293
C	-6.602086	-1.993235	2.804200
C	-4.656615	-2.970120	0.806117
C	-8.230467	-1.121275	0.359795
H	-8.544295	-1.308284	1.378932
C	-5.290179	-4.105410	0.274946
H	-6.372537	-4.139294	0.191197

C	-7.429928	-0.667814	-2.300172
C	-6.454742	-1.013473	-1.307919
C	-7.548192	-3.612705	4.340187
H	-7.679052	-4.646265	4.646477
C	-8.803166	-0.523625	-1.921018
C	-9.172326	-0.774934	-0.577250
H	-10.217022	-0.686171	-0.291732
C	-7.186762	-0.961730	3.561226
H	-7.022631	0.073887	3.271831
C	-3.128530	-5.108529	-0.140696
H	-2.538176	-5.935009	-0.525185
C	-2.496557	-3.978206	0.377976
H	-1.414809	-3.896238	0.400788
C	-4.524702	-5.173626	-0.187290
H	-5.015788	-6.044076	-0.610818
C	-9.758100	-0.122336	-2.892801
H	-10.795620	-0.013172	-2.588952
C	-8.024223	-0.024015	-4.574262
H	-7.731740	0.169283	-5.602049
C	-7.955970	-1.255412	4.685044
H	-8.402507	-0.449644	5.259846
C	-9.379506	0.125701	-4.191990
H	-10.116834	0.433002	-4.927450
C	-7.075546	-0.410989	-3.655101
H	-6.040741	-0.515685	-3.958783
C	-8.138517	-2.585282	5.076351
H	-8.731299	-2.816626	5.956104
H	-4.606109	-0.931745	4.296702
C	-3.808699	-0.506853	3.694251
H	-2.919623	-1.115232	3.540970
C	-3.663682	0.858176	3.610676
C	-3.745924	1.928653	2.941520
C	-3.435833	3.335788	2.844491
C	-2.280923	3.833940	3.477187
C	-1.946089	5.179894	3.367014
H	-1.049071	5.550534	3.854352
C	-2.753101	6.046431	2.624686
H	-2.486320	7.095138	2.533161
H	-4.529804	6.227585	1.415073
C	-3.902332	5.559930	1.997555
C	-4.244142	4.214359	2.105975
H	-5.126893	3.833380	1.604902
H	-1.644376	3.154750	4.032456

TS34i-C_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-6284.743587
Thermal and entropic correction, BS1 (a.u.)	1.535600
Electronic Energy, BS2 (a.u.)	-10207.220600
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-1278.0i

Molecular Geometry in Cartesian Coordinates

Cu	3.777248	-0.437572	0.183745
Fe	6.614212	2.610493	-0.119645
P	3.560943	1.598806	1.003157
C	5.253440	2.191998	1.355948

C	6.436135	1.350389	1.477119
C	7.570271	2.204730	1.682756
H	8.589949	1.862632	1.779582
C	7.116379	3.548598	1.684594
H	7.740430	4.427379	1.768775
C	5.706560	3.545132	1.490510
H	5.084507	4.422075	1.398539
C	5.792725	2.044772	-1.938341
H	4.891765	1.458066	-2.039704
C	7.106184	1.509115	-1.810235
H	7.359416	0.459216	-1.795614
C	8.017092	2.594910	-1.643613
H	9.083624	2.513006	-1.484021
C	7.262319	3.807953	-1.673175
H	7.658408	4.805114	-1.537473
C	5.886971	3.468270	-1.852381
H	5.053545	4.156450	-1.869928
O	7.748417	-0.619901	1.693400
C	6.561682	-0.090835	1.301294
N	5.704899	-0.907115	0.796560
C	6.280339	-2.264265	0.884132
C	7.801453	-1.974312	1.156266
H	8.170083	-2.616229	1.959520
H	5.863189	-2.731814	1.783058
C	2.661071	1.682829	2.600959
C	3.290192	1.841425	3.842492
H	4.356910	2.040727	3.889752
C	2.545768	1.737428	5.022349
H	3.039117	1.866227	5.981609
C	1.176492	1.467079	4.970987
H	0.605882	1.376549	5.890768
C	0.543570	1.306846	3.732960
H	-0.514599	1.074036	3.666703
C	1.281674	1.417898	2.556312
H	0.785961	1.279284	1.600642
C	2.824296	2.964064	0.021871
C	2.545631	2.729568	-1.331309
H	2.662669	1.731531	-1.738464
C	2.126370	3.775557	-2.155976
H	1.914613	3.580591	-3.201364
C	1.973980	5.058620	-1.628870
H	1.664198	5.876329	-2.273560
C	2.185520	5.287064	-0.264159
H	2.028316	6.277110	0.154428
C	2.598623	4.241581	0.561638
H	2.746321	4.416404	1.623616
C	5.931094	-3.128988	-0.302573
C	5.799795	-4.511720	-0.134769
C	5.702827	-2.570830	-1.564054
C	5.440935	-5.326419	-1.209418
C	5.330803	-3.380634	-2.636625
C	5.198592	-4.760451	-2.463687
H	5.960867	-4.948215	0.847463
H	5.768447	-1.496887	-1.693784
H	5.341129	-6.398570	-1.066111
H	5.138218	-2.931008	-3.606376
H	4.909286	-5.390633	-3.299634
C	8.739073	-2.032635	-0.031370
C	9.072155	-3.279314	-0.578297

C	9.285080	-0.875525	-0.595305
C	9.908735	-3.363343	-1.689370
C	10.124185	-0.960380	-1.709347
C	10.433763	-2.202245	-2.263086
H	8.660920	-4.186133	-0.145492
H	9.059676	0.090758	-0.159836
H	10.151696	-4.335829	-2.106928
H	10.538145	-0.052944	-2.139872
H	11.085660	-2.267955	-3.128950
H	-1.191299	3.867766	-4.589886
C	-0.640837	2.085254	-3.516583
C	-0.514492	3.019859	-4.542911
C	0.493099	2.863445	-5.499729
H	0.603872	3.587512	-6.301907
C	1.356845	1.770232	-5.430003
H	2.132281	1.646802	-6.183008
H	3.203030	-0.038456	-4.253818
C	2.169401	-0.365112	-4.398942
H	2.103597	-0.899899	-5.351224
C	1.227251	0.822351	-4.404744
H	0.132312	0.286762	-2.627410
C	0.229023	0.993970	-3.442111
H	-1.412968	2.209480	-2.767796
O	1.829765	-1.342164	-3.402578
C	2.453220	-1.259667	-2.198896
C	1.238839	-3.442560	-1.663289
H	0.505887	-3.790299	-0.927477
H	1.969564	-4.247338	-1.826130
H	0.713229	-3.272417	-2.603300
C	1.906880	-2.160202	-1.199385
N	2.682781	-2.170266	-0.005689
C	2.658882	-3.177563	0.798372
H	2.168054	-4.108503	0.511304
C	3.255801	-3.156288	2.137377
C	3.321190	-1.978259	2.902629
H	2.864154	-1.072187	2.523685
H	3.974343	-1.054371	4.723997
C	3.940350	-1.975873	4.150315
C	4.491311	-3.154305	4.663598
H	4.976361	-3.152703	5.635255
C	4.388950	-4.342994	3.933631
H	4.795164	-5.265916	4.337314
C	3.763233	-4.346759	2.687327
H	3.692088	-5.268227	2.115446
O	3.339070	-0.409671	-1.997736
H	0.843691	-1.304790	-0.692142
O	0.005018	-0.582593	-0.248864
C	-0.457881	-0.907490	0.913481
O	0.051681	-2.080651	1.386337
O	-1.277868	-0.258647	1.567391
H	0.005598	-1.520463	3.395907
C	-0.207844	-2.385902	2.765351
H	-1.244121	-2.704060	2.906414
H	0.469654	-3.202571	3.013603
Ni	-4.364506	0.407255	1.789288
P	-4.473548	1.228176	-0.257465
C	-7.000387	2.275947	0.248167
H	-6.750957	2.076969	1.287266
C	-4.082085	-0.210856	-1.357469

C	-3.553017	3.628295	-1.475805
H	-4.528582	3.716949	-1.936674
C	-3.239618	2.530803	-0.659794
C	-6.085461	1.929324	-0.755914
C	-2.715408	-0.395648	-1.699965
H	-1.979216	0.341601	-1.416796
C	-6.418853	2.159558	-2.099775
H	-5.734250	1.861587	-2.887392
C	-4.596446	-2.376696	-2.378563
C	-5.017682	-1.200711	-1.668703
C	-2.618922	4.645810	-1.669778
H	-2.877569	5.498029	-2.291506
C	-3.213068	-2.539918	-2.715379
C	-2.293740	-1.527830	-2.350386
H	-1.242148	-1.650053	-2.589354
C	-1.973773	2.462925	-0.051468
H	-1.724536	1.625448	0.593191
C	-8.546357	3.087304	-1.423130
H	-9.502494	3.530939	-1.683519
C	-8.225738	2.854778	-0.084458
H	-8.930375	3.115325	0.699479
C	-7.642975	2.737397	-2.429840
H	-7.900122	2.891894	-3.472617
C	-2.789986	-3.714831	-3.392076
H	-1.735455	-3.822813	-3.631129
C	-5.061976	-4.534978	-3.413027
H	-5.771538	-5.310430	-3.685944
C	-1.043824	3.480432	-0.256256
H	-0.069480	3.424037	0.216600
C	-3.693476	-4.692368	-3.738613
H	-3.361861	-5.584913	-4.260595
C	-5.500650	-3.413611	-2.746209
H	-6.549461	-3.316744	-2.493427
C	-1.369762	4.578009	-1.054325
H	-0.648099	5.373885	-1.193973
P	-5.564536	-1.422721	1.399887
C	-3.249563	-2.889301	0.957339
H	-2.749759	-1.977261	1.258658
C	-6.841992	-1.232282	0.074026
C	-6.727277	-3.094996	3.408631
H	-6.286487	-3.945477	2.901040
C	-6.543328	-1.799752	2.909685
C	-4.648724	-2.931388	0.942449
C	-8.213876	-1.127793	0.431463
H	-8.513600	-1.260943	1.463296
C	-5.306566	-4.090364	0.500497
H	-6.390771	-4.115142	0.442097
C	-7.445277	-0.810877	-2.258807
C	-6.455693	-1.086380	-1.259140
C	-7.468708	-3.297447	4.575971
H	-7.601825	-4.305404	4.957232
C	-8.817320	-0.669024	-1.873554
C	-9.170084	-0.851608	-0.514231
H	-10.213486	-0.764332	-0.223762
C	-7.102592	-0.711313	3.603601
H	-6.938304	0.299757	3.237702
C	-3.167367	-5.150584	0.110382
H	-2.594405	-6.008303	-0.228538
C	-2.510684	-3.997030	0.540330

H	-1.427499	-3.939042	0.537907
C	-4.564425	-5.197779	0.095038
H	-5.075372	-6.087683	-0.258717
C	-9.787763	-0.334861	-2.855221
H	-10.824203	-0.227282	-2.547313
C	-8.070694	-0.293597	-4.556516
H	-7.790905	-0.148145	-5.595594
C	-7.848741	-0.917454	4.761902
H	-8.276087	-0.068933	5.287594
C	-9.424876	-0.146915	-4.168910
H	-10.173732	0.110336	-4.911821
C	-7.107416	-0.619017	-3.628665
H	-6.074162	-0.723404	-3.937794
C	-8.033498	-2.214562	5.250176
H	-8.608503	-2.377321	6.156619
H	-4.465208	-0.743115	4.275785
C	-3.681846	-0.363837	3.625871
H	-2.816314	-1.005708	3.477499
C	-3.505838	0.993408	3.484943
C	-3.602704	2.044314	2.788374
C	-3.292766	3.445370	2.630372
C	-2.098306	3.956262	3.173255
C	-1.771396	5.298111	3.003610
H	-0.845506	5.681278	3.422257
C	-2.623941	6.145133	2.290357
H	-2.362912	7.190164	2.152594
H	-4.473700	6.297418	1.191191
C	-3.811444	5.644666	1.751438
C	-4.146502	4.303772	1.919534
H	-5.059254	3.909533	1.486365
H	-1.427049	3.291840	3.705755

Int4i-C_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-6284.747216
Thermal and entropic correction, BS1 (a.u.)	1.539250
Electronic Energy, BS2 (a.u.)	-10207.227303
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

xyz

Cu	3.661845	-0.416810	0.195268
Fe	6.515679	2.591100	-0.084957
P	3.477458	1.572893	1.136216
C	5.192956	2.141273	1.416421
C	6.369835	1.286997	1.480817
C	7.517048	2.125745	1.677407
H	8.535893	1.772269	1.734991
C	7.075206	3.473009	1.729313
H	7.709387	4.343963	1.819285
C	5.660444	3.486406	1.575418
H	5.041749	4.369437	1.527294
C	5.636041	2.107291	-1.901884
H	4.719307	1.546036	-2.002296
C	6.936876	1.533111	-1.822040
H	7.160101	0.476501	-1.846778

C	7.881109	2.587962	-1.641477
H	8.948357	2.472616	-1.509422
C	7.159342	3.821103	-1.613189
H	7.585706	4.802210	-1.453958
C	5.771375	3.523799	-1.770980
H	4.956802	4.234067	-1.746012
O	7.656981	-0.705099	1.632069
C	6.472467	-0.151077	1.268186
N	5.597076	-0.941709	0.755120
C	6.154489	-2.308839	0.802973
C	7.683640	-2.045092	1.058638
H	8.058202	-2.713681	1.836874
H	5.742276	-2.791478	1.696529
C	2.694513	1.643129	2.797550
C	3.437631	1.532838	3.981520
H	4.523081	1.534648	3.942484
C	2.786586	1.416359	5.212852
H	3.372199	1.339772	6.124598
C	1.391381	1.396737	5.274080
H	0.889720	1.296499	6.232044
C	0.644526	1.506148	4.096544
H	-0.440691	1.470741	4.122284
C	1.291687	1.635373	2.868234
H	0.699852	1.718928	1.962773
C	2.715913	2.980723	0.234702
C	2.428899	2.810742	-1.127014
H	2.534717	1.830534	-1.579574
C	2.023247	3.899869	-1.901578
H	1.811680	3.756084	-2.955253
C	1.885414	5.159195	-1.315320
H	1.590713	6.011056	-1.921884
C	2.097687	5.320979	0.058567
H	1.951700	6.292078	0.523026
C	2.505353	4.234614	0.833444
H	2.665711	4.360619	1.900430
C	5.788637	-3.147977	-0.396632
C	5.690797	-4.537065	-0.257531
C	5.523378	-2.565984	-1.639587
C	5.329758	-5.334706	-1.343431
C	5.147497	-3.360050	-2.722859
C	5.050530	-4.745851	-2.579744
H	5.875249	-4.991182	0.712730
H	5.556687	-1.487630	-1.744804
H	5.255153	-6.411745	-1.222737
H	4.919348	-2.892805	-3.676435
H	4.758175	-5.363102	-3.424294
C	8.597674	-2.080718	-0.147872
C	8.933239	-3.317481	-0.714964
C	9.112839	-0.911046	-0.714973
C	9.741979	-3.379890	-1.847905
C	9.924148	-0.974080	-1.850680
C	10.236372	-2.206538	-2.423784
H	8.544494	-4.233503	-0.280773
H	8.885538	0.048224	-0.265234
H	9.987097	-4.345093	-2.280854
H	10.314030	-0.057035	-2.283416
H	10.866600	-2.255357	-3.306674
H	-1.133264	4.048258	-4.571325
C	-0.643289	2.200115	-3.582366

C	-0.446718	3.208285	-4.525218
C	0.643033	3.134462	-5.398208
H	0.808989	3.916804	-6.133413
C	1.518374	2.049984	-5.331732
H	2.358134	1.991305	-6.020800
H	3.284769	0.167599	-4.180387
C	2.262764	-0.158025	-4.395055
H	2.250697	-0.637170	-5.379347
C	1.318133	1.027529	-4.393732
H	0.091647	0.347877	-2.766804
C	0.238489	1.119204	-3.512235
H	-1.481335	2.258662	-2.898689
O	1.879157	-1.188118	-3.478346
C	2.423552	-1.145143	-2.221562
C	1.240034	-3.379363	-1.857605
H	0.422156	-3.678736	-1.188081
H	1.915283	-4.243085	-1.956168
H	0.818138	-3.180013	-2.842685
C	1.971574	-2.166535	-1.345676
N	2.598724	-2.180479	-0.102927
C	2.566087	-3.225714	0.669830
H	2.131205	-4.160240	0.313196
C	3.129329	-3.261874	2.016486
C	3.252037	-2.118012	2.830189
H	2.852049	-1.173434	2.481888
H	3.928981	-1.296931	4.690003
C	3.854237	-2.194574	4.083461
C	4.335312	-3.416939	4.563899
H	4.806041	-3.475138	5.540779
C	4.181920	-4.569276	3.786523
H	4.535894	-5.526966	4.157689
C	3.575884	-4.494315	2.533421
H	3.472349	-5.389894	1.926082
O	3.235795	-0.230492	-1.927294
H	0.739332	-0.962976	-0.438689
O	0.069262	-0.308665	-0.074164
C	-0.366523	-0.614611	1.135573
O	0.198851	-1.724638	1.631379
O	-1.202855	0.048953	1.728838
H	0.073743	-1.179258	3.641303
C	-0.105484	-2.046748	3.004278
H	-1.141654	-2.379755	3.094442
H	0.577815	-2.853413	3.261077
Ni	-4.372431	0.481427	1.763173
P	-4.478211	1.219228	-0.320432
C	-7.050230	2.171880	0.134325
H	-6.795546	2.030369	1.181678
C	-4.000395	-0.234646	-1.368192
C	-3.658666	3.610130	-1.630779
H	-4.632601	3.636569	-2.102874
C	-3.306865	2.564232	-0.764124
C	-6.117519	1.823569	-0.852915
C	-2.622076	-0.362206	-1.694377
H	-1.930907	0.428840	-1.442496
C	-6.454481	1.983516	-2.205905
H	-5.753440	1.685557	-2.978842
C	-4.394068	-2.457825	-2.320214
C	-4.880796	-1.280282	-1.655925
C	-2.764547	4.655252	-1.864624

H	-3.051996	5.466400	-2.527222
C	-3.000566	-2.565448	-2.634533
C	-2.136985	-1.495143	-2.298610
H	-1.079617	-1.576126	-2.530272
C	-2.046004	2.579464	-0.143904
H	-1.771106	1.789462	0.546618
C	-8.624507	2.841117	-1.573208
H	-9.598546	3.229956	-1.853990
C	-8.298957	2.680484	-0.225130
H	-9.017333	2.943151	0.545505
C	-7.702159	2.490991	-2.562491
H	-7.961412	2.590661	-3.611394
C	-2.511828	-3.741433	-3.263499
H	-1.450936	-3.806937	-3.485975
C	-4.741351	-4.671371	-3.281342
H	-5.409177	-5.489255	-3.535000
C	-1.155424	3.622010	-0.388339
H	-0.184832	3.626714	0.094444
C	-3.362738	-4.773473	-3.584590
H	-2.981243	-5.666596	-4.070135
C	-5.242664	-3.549361	-2.661184
H	-6.298379	-3.494656	-2.425417
C	-1.517492	4.665614	-1.240833
H	-0.824997	5.480662	-1.416791
P	-5.457809	-1.428592	1.412937
C	-3.033082	-2.737446	1.060478
H	-2.611921	-1.784163	1.352693
C	-6.723398	-1.354063	0.064590
C	-6.527634	-3.131778	3.445908
H	-6.013543	-3.959021	2.969760
C	-6.434259	-1.839803	2.914720
C	-4.425431	-2.878492	1.012214
C	-8.104130	-1.313410	0.401455
H	-8.411734	-1.433052	1.432460
C	-4.985915	-4.093277	0.587209
H	-6.063560	-4.198212	0.503487
C	-7.316210	-1.036754	-2.287775
C	-6.327641	-1.227136	-1.267486
C	-7.274007	-3.360027	4.605428
H	-7.336801	-4.364843	5.012111
C	-8.699057	-0.957861	-1.924130
C	-9.060245	-1.117929	-0.564160
H	-10.110768	-1.079336	-0.289338
C	-7.089276	-0.779833	3.567882
H	-6.997375	0.230646	3.175788
C	-2.766600	-5.006948	0.279160
H	-2.124881	-5.829636	-0.020812
C	-2.204654	-3.798776	0.694308
H	-1.127650	-3.668726	0.718973
C	-4.155693	-5.154287	0.230443
H	-4.592363	-6.087151	-0.111561
C	-9.672469	-0.708547	-2.927788
H	-10.717418	-0.648210	-2.636299
C	-7.936478	-0.628115	-4.608548
H	-7.650579	-0.501110	-5.648347
C	-7.839931	-1.012489	4.718131
H	-8.342100	-0.186239	5.212133
C	-9.301917	-0.543181	-4.242391
H	-10.053113	-0.351214	-5.002438

C	-6.969990	-0.870661	-3.658926
H	-5.928484	-0.928517	-3.952233
C	-7.933461	-2.306744	5.239201
H	-8.511838	-2.489516	6.139621
H	-4.518200	-0.552414	4.299010
C	-3.725573	-0.181118	3.656123
H	-2.837328	-0.803437	3.574664
C	-3.582838	1.171691	3.454677
C	-3.681410	2.185656	2.706689
C	-3.382063	3.580081	2.487835
C	-2.181621	4.115340	2.992902
C	-1.858592	5.448493	2.760136
H	-0.927788	5.850987	3.148466
C	-2.721550	6.261422	2.020194
H	-2.463717	7.299342	1.832278
H	-4.583763	6.363199	0.936714
C	-3.914777	5.736441	1.518104
C	-4.245819	4.403969	1.749023
H	-5.161673	3.987822	1.342801
H	-1.503232	3.474975	3.546212

Int1ii-A_NiCu

	Value
Charge	1
Electronic Energy, BS1 (a.u.)	-6284.753729
Thermal and entropic correction, BS1 (a.u.)	1.545787
Electronic Energy, BS2 (a.u.)	-10207.236843
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

xyz

Cu	2.874873	-0.363599	-0.077219
Fe	6.947875	-1.996587	0.850449
P	3.500755	-2.412288	0.440901
C	5.230750	-2.630052	-0.083862
C	5.970417	-1.700347	-0.926380
C	7.263740	-2.268705	-1.177958
H	8.045522	-1.790903	-1.749544
C	7.334819	-3.522198	-0.514861
H	8.199421	-4.170242	-0.479785
C	6.097603	-3.745809	0.154618
H	5.859232	-4.596296	0.776771
C	6.452505	-1.163980	2.677261
H	5.446332	-1.090297	3.058395
C	7.117046	-0.201343	1.859346
H	6.699443	0.730675	1.504984
C	8.412752	-0.711802	1.541249
H	9.150323	-0.234505	0.910808
C	8.545364	-1.990296	2.162858
H	9.398496	-2.649486	2.079866
C	7.333704	-2.270194	2.863259
H	7.103206	-3.177432	3.404119
O	6.438037	0.184634	-2.292868
C	5.556308	-0.402879	-1.451689
N	4.454098	0.230707	-1.241610
C	4.434376	1.400527	-2.156751

C	5.939912	1.531046	-2.570840
H	6.010876	1.670192	-3.651261
H	3.889300	1.072300	-3.044790
C	2.562257	-3.655745	-0.523952
C	3.113411	-4.460466	-1.528856
H	4.178390	-4.425940	-1.736102
C	2.288331	-5.313368	-2.270447
H	2.720340	-5.933018	-3.050790
C	0.919436	-5.372418	-2.005218
H	0.278673	-6.033866	-2.579425
C	0.367343	-4.577580	-0.994456
H	-0.695553	-4.618123	-0.785851
C	1.182625	-3.718178	-0.266333
H	0.746638	-3.096943	0.509030
C	3.369529	-3.032468	2.160134
C	3.072151	-2.104579	3.168417
H	2.936785	-1.058765	2.909769
C	2.941921	-2.520909	4.494643
H	2.717714	-1.792266	5.268068
C	3.087048	-3.871542	4.818463
H	2.976877	-4.199289	5.847715
C	3.358888	-4.806362	3.813595
H	3.454685	-5.859109	4.062192
C	3.497024	-4.390749	2.488827
H	3.674137	-5.125468	1.708639
C	3.686182	2.574167	-1.571560
C	2.507101	2.993749	-2.200215
C	4.060294	3.176541	-0.362726
C	1.696285	3.972045	-1.620530
C	3.258041	4.159355	0.213038
C	2.066057	4.550275	-0.404959
H	2.198264	2.522631	-3.128327
H	4.967637	2.861579	0.139460
H	0.765945	4.255999	-2.101923
H	3.546112	4.598084	1.163191
H	1.422782	5.280734	0.075216
C	6.773020	2.557035	-1.841767
C	6.651439	3.905601	-2.197429
C	7.617826	2.201058	-0.785789
C	7.344318	4.886389	-1.489350
C	8.310408	3.183679	-0.074900
C	8.170454	4.528735	-0.420547
H	5.995813	4.190106	-3.016142
H	7.742556	1.155016	-0.534585
H	7.238366	5.929710	-1.770447
H	8.962764	2.896024	0.744813
H	8.708642	5.293158	0.131494
H	5.465704	0.279749	-6.215239
C	3.382053	0.543238	-5.718833
C	4.634872	-0.067660	-5.607965
C	4.813556	-1.136098	-4.724750
H	5.784586	-1.612525	-4.635227
C	3.741690	-1.589359	-3.954034
H	3.875563	-2.421651	-3.269594
H	1.486108	-2.473167	-2.856599
C	1.350646	-1.443149	-3.184797
H	0.387917	-1.335492	-3.686300
C	2.487101	-0.975200	-4.050916
H	1.340624	0.571816	-5.008195

C	2.312205	0.093087	-4.942813
H	3.238061	1.367822	-6.410657
O	1.274196	-0.692326	-1.927961
C	0.525881	0.432237	-1.915172
C	-0.765938	-0.075606	0.100539
H	-1.625160	-0.204443	-0.559643
H	-1.130293	0.329629	1.041287
H	-0.299820	-1.046307	0.278518
C	0.253110	0.904174	-0.496458
H	-0.185595	1.902636	-0.579087
N	1.447048	0.935715	0.375458
C	1.349938	1.733338	1.384624
H	0.458630	2.357732	1.484885
C	2.313842	1.873229	2.481919
C	3.648970	1.428088	2.438534
H	4.039505	0.972347	1.533688
H	5.518803	1.286478	3.491556
C	4.485424	1.609239	3.537526
C	4.005908	2.218511	4.701618
H	4.665472	2.353453	5.553725
C	2.686655	2.668385	4.754672
H	2.310114	3.156611	5.648359
C	1.853326	2.510478	3.649181
H	0.846149	2.907916	3.667947
Ni	-3.735173	1.260378	0.714091
P	-4.648765	0.775163	-1.214204
C	-7.192211	1.164843	-0.153941
H	-6.643461	1.601874	0.675940
C	-4.050788	-0.910763	-1.743541
C	-5.154423	2.405365	-3.527883
H	-6.203905	2.147782	-3.444758
C	-4.219600	1.878156	-2.626565
C	-6.479608	0.661211	-1.251208
C	-3.072969	-1.001588	-2.775701
H	-2.767324	-0.107310	-3.303435
C	-7.182162	0.079018	-2.316960
H	-6.639067	-0.334584	-3.161310
C	-3.852617	-3.333221	-1.418314
C	-4.438696	-2.066546	-1.057458
C	-4.743760	3.284761	-4.532784
H	-5.480251	3.694534	-5.218097
C	-2.902838	-3.402454	-2.488329
C	-2.524600	-2.205184	-3.141649
H	-1.813556	-2.253466	-3.962441
C	-2.874345	2.263008	-2.746317
H	-2.146084	1.899943	-2.031961
C	-9.275322	0.497835	-1.182437
H	-10.358266	0.423455	-1.152190
C	-8.584418	1.081964	-0.118893
H	-9.126894	1.463870	0.740892
C	-8.573311	0.000167	-2.282793
H	-9.106717	-0.471238	-3.102098
C	-2.392503	-4.663771	-2.898632
H	-1.687374	-4.691413	-3.724943
C	-3.690197	-5.762104	-1.185633
H	-3.992190	-6.676485	-0.683951
C	-2.461023	3.114730	-3.765592
H	-1.411912	3.380383	-3.841846
C	-2.775652	-5.823038	-2.265202

H	-2.384808	-6.782987	-2.589617
C	-4.220281	-4.556578	-0.783239
H	-4.946877	-4.536524	0.020685
C	-3.399071	3.635316	-4.659451
H	-3.085854	4.318692	-5.443369
P	-4.165576	-0.552811	1.895199
C	-1.704158	-1.089720	3.091049
H	-1.793414	-0.066959	3.445463
C	-5.539557	-1.630859	1.235891
C	-4.633578	-0.931074	4.696724
H	-4.163824	-1.903710	4.587829
C	-4.761786	-0.086096	3.583164
C	-2.743202	-1.650022	2.325996
C	-6.690036	-1.780283	2.064891
H	-6.653135	-1.441053	3.091179
C	-2.616025	-2.970514	1.885115
H	-3.412182	-3.429414	1.315734
C	-6.815063	-2.664187	-0.592504
C	-5.589867	-2.093934	-0.084908
C	-5.105065	-0.527681	5.946625
H	-4.997618	-1.188698	6.801794
C	-7.965491	-2.755811	0.253849
C	-7.858374	-2.321308	1.595048
H	-8.720243	-2.409423	2.251174
C	-5.372287	1.166744	3.746596
H	-5.442532	1.836069	2.893236
C	-0.434159	-3.142697	2.929216
H	0.461725	-3.712510	3.157426
C	-0.562440	-1.828020	3.391131
H	0.234137	-1.380933	3.977810
C	-1.466291	-3.710428	2.180040
H	-1.384367	-4.733043	1.822575
C	-9.185938	-3.269664	-0.260333
H	-10.045091	-3.324489	0.402746
C	-8.149036	-3.604240	-2.411210
H	-8.224386	-3.929076	-3.444788
C	-5.847746	1.567599	4.996124
H	-6.311285	2.543250	5.109000
C	-9.280985	-3.687524	-1.566650
H	-10.217658	-4.079064	-1.951772
C	-6.954443	-3.109188	-1.939857
H	-6.110502	-3.041175	-2.613891
C	-5.713897	0.720802	6.098640
H	-6.077608	1.033587	7.072962
H	-3.010773	2.447673	3.927542
C	-2.318372	2.807022	3.163945
H	-1.337444	2.351333	3.343863
O	-0.269457	4.381217	2.276870
C	-2.810705	2.504348	1.806873
C	-3.059567	3.042954	0.659962
C	-2.947020	4.185260	-0.226522
C	-1.690684	4.749160	-0.520535
C	-1.582164	5.815071	-1.413542
H	-0.603822	6.238163	-1.630254
C	-2.721314	6.338834	-2.030040
H	-2.635390	7.166045	-2.728306
H	-4.861770	6.172876	-2.233612
C	-3.972218	5.782772	-1.748094
C	-4.084224	4.713436	-0.863400

H	-5.050195	4.259012	-0.667205
H	-0.809046	4.345439	-0.038866
C	-1.240762	4.889864	2.816683
O	-2.233732	4.242081	3.423045
O	-1.464470	6.200619	2.913200
C	-0.503206	7.037873	2.246591
H	-0.769512	8.058416	2.519501
H	0.512010	6.803103	2.576569
H	-0.581411	6.901724	1.164432
O	0.019065	0.922513	-2.901578

TS12ii-A_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-6284.718446
Thermal and entropic correction, BS1 (a.u.)	1.542539
Electronic Energy, BS2 (a.u.)	-10207.216594
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-44.3i

Molecular Geometry in Cartesian Coordinates

xyz

Cu	2.905125	-0.339948	-0.086192
Fe	6.976090	-2.014185	0.711866
P	3.531540	-2.412414	0.301450
C	5.256487	-2.605565	-0.244634
C	5.988195	-1.631997	-1.043829
C	7.281718	-2.183028	-1.329637
H	8.059024	-1.674442	-1.880361
C	7.360786	-3.467888	-0.729927
H	8.228055	-4.113332	-0.731163
C	6.127911	-3.729152	-0.066000
H	5.895168	-4.609764	0.515163
C	6.488566	-1.281436	2.583636
H	5.485438	-1.232868	2.976314
C	7.138584	-0.272207	1.812044
H	6.709976	0.673373	1.511185
C	8.435631	-0.754400	1.457854
H	9.164348	-0.238740	0.847684
C	8.583602	-2.062467	2.010666
H	9.441477	-2.709086	1.887178
C	7.379778	-2.388521	2.704805
H	7.161670	-3.324516	3.199940
O	6.442865	0.318444	-2.320874
C	5.566468	-0.311215	-1.503881
N	4.463825	0.307914	-1.258267
C	4.437892	1.522523	-2.116396
C	5.942142	1.678211	-2.523420
H	6.012596	1.877002	-3.594582
H	3.896524	1.232098	-3.019458
C	2.583957	-3.599373	-0.727569
C	3.129458	-4.348021	-1.777958
H	4.193779	-4.302543	-1.986417
C	2.301839	-5.158674	-2.562826
H	2.731212	-5.734619	-3.377342
C	0.934034	-5.233385	-2.295879
H	0.293426	-5.867162	-2.901293
C	0.386539	-4.494054	-1.241401

H	-0.675287	-4.546814	-1.029394
C	1.204800	-3.675254	-0.470552
H	0.772628	-3.095401	0.338493
C	3.399361	-3.128016	1.983277
C	3.109315	-2.252948	3.040315
H	2.986343	-1.192441	2.840078
C	2.976476	-2.739716	4.342406
H	2.763095	-2.050381	5.154094
C	3.110205	-4.107257	4.592452
H	2.999250	-4.489058	5.602880
C	3.376204	-4.988574	3.538642
H	3.466858	-6.053646	3.730532
C	3.518696	-4.502876	2.238258
H	3.694794	-5.195227	1.419894
C	3.680390	2.662535	-1.480182
C	2.496366	3.099148	-2.089015
C	4.045687	3.209038	-0.242417
C	1.669597	4.031667	-1.457370
C	3.223501	4.141859	0.385645
C	2.023258	4.544911	-0.208761
H	2.198288	2.674319	-3.042916
H	4.958012	2.882851	0.243576
H	0.734356	4.330333	-1.923153
H	3.496201	4.527091	1.363013
H	1.351383	5.204281	0.328188
C	6.773797	2.664044	-1.739460
C	6.644988	4.030253	-2.016560
C	7.623314	2.252007	-0.708120
C	7.335419	4.971841	-1.255027
C	8.313572	3.195244	0.056339
C	8.166386	4.557228	-0.210846
H	5.983916	4.358368	-2.814212
H	7.752422	1.193942	-0.517049
H	7.222202	6.029192	-1.473890
H	8.968464	2.864042	0.857389
H	8.701262	5.291253	0.383970
H	5.413315	0.620351	-6.242222
C	3.335773	0.857860	-5.709414
C	4.589611	0.242760	-5.643399
C	4.779359	-0.866475	-4.814446
H	5.751981	-1.344655	-4.758141
C	3.717149	-1.356832	-4.053281
H	3.860062	-2.218962	-3.408960
H	1.472830	-2.292898	-2.974769
C	1.335862	-1.247318	-3.248740
H	0.368508	-1.111698	-3.734905
C	2.461704	-0.739274	-4.105644
H	1.304118	0.852869	-4.970745
C	2.275810	0.370537	-4.942563
H	3.184115	1.715916	-6.357452
O	1.276486	-0.561238	-1.955296
C	0.527479	0.558342	-1.872811
C	-0.744753	-0.032362	0.122212
H	-1.621110	-0.100185	-0.524585
H	-1.069910	0.292534	1.107187
H	-0.297106	-1.023711	0.213486
C	0.285186	0.968031	-0.427678
H	-0.134904	1.977578	-0.452214
N	1.481783	0.930032	0.435879

C	1.415935	1.702259	1.470313
H	0.580156	2.405571	1.582077
C	2.366785	1.733558	2.586397
C	3.712262	1.325089	2.511967
H	4.126176	0.989894	1.565613
H	5.573116	1.118317	3.572637
C	4.528950	1.401486	3.637972
C	4.013992	1.860863	4.855436
H	4.658881	1.917293	5.727760
C	2.681739	2.265461	4.937406
H	2.276209	2.639676	5.872460
C	1.864581	2.222248	3.807782
H	0.837097	2.576160	3.877438
Ni	-3.724181	1.234703	0.812866
P	-4.635370	0.818432	-1.126427
C	-7.123962	1.394378	-0.025719
H	-6.538949	1.836092	0.776257
C	-4.067300	-0.865192	-1.680552
C	-5.082281	2.367238	-3.488984
H	-6.124508	2.074598	-3.445260
C	-4.172398	1.919495	-2.521122
C	-6.463643	0.795324	-1.108254
C	-3.050627	-0.929237	-2.678064
H	-2.684289	-0.019042	-3.134430
C	-7.217356	0.216381	-2.140382
H	-6.716853	-0.270970	-2.970818
C	-3.977687	-3.308055	-1.502470
C	-4.522275	-2.041708	-1.079449
C	-4.655668	3.222248	-4.506190
H	-5.370865	3.573670	-5.244002
C	-2.986368	-3.348100	-2.534360
C	-2.532897	-2.129516	-3.093191
H	-1.780216	-2.155807	-3.876329
C	-2.838532	2.348530	-2.588904
H	-2.130256	2.037780	-1.831413
C	-9.260847	0.828852	-1.003185
H	-10.345729	0.833555	-0.959577
C	-8.517938	1.410581	0.026055
H	-9.021174	1.870760	0.870948
C	-8.609738	0.234222	-2.086589
H	-9.184097	-0.235885	-2.878141
C	-2.494327	-4.600244	-2.992332
H	-1.754052	-4.604350	-3.787301
C	-3.896783	-5.748503	-1.398445
H	-4.244800	-6.678898	-0.960320
C	-2.409975	3.182952	-3.616454
H	-1.368964	3.484607	-3.652535
C	-2.934937	-5.778875	-2.437456
H	-2.553505	-6.731083	-2.793604
C	-4.410627	-4.551325	-0.953111
H	-5.166357	-4.553314	-0.176486
C	-3.322026	3.629094	-4.574270
H	-2.997486	4.297618	-5.366063
P	-4.144776	-0.685944	1.914079
C	-1.686757	-1.403930	3.034251
H	-1.728970	-0.423277	3.493952
C	-5.584339	-1.645985	1.223486
C	-4.548270	-1.118127	4.704267
H	-4.083804	-2.088749	4.563081

C	-4.697897	-0.244888	3.616323
C	-2.756602	-1.854497	2.239923
C	-6.727003	-1.770158	2.066822
H	-6.662101	-1.464906	3.102144
C	-2.696266	-3.141577	1.696726
H	-3.522929	-3.525026	1.117315
C	-6.921192	-2.574178	-0.614860
C	-5.669858	-2.067406	-0.108076
C	-4.989588	-0.740556	5.973279
H	-4.863964	-1.420790	6.810331
C	-8.063481	-2.640794	0.244713
C	-7.921989	-2.249289	1.596192
H	-8.778296	-2.321078	2.261192
C	-5.301912	1.006001	3.820976
H	-5.401571	1.697570	2.988094
C	-0.505555	-3.485058	2.675447
H	0.371577	-4.105210	2.835708
C	-0.572822	-2.211428	3.249783
H	0.247901	-1.848763	3.859653
C	-1.574237	-3.948892	1.906390
H	-1.545096	-4.942269	1.468097
C	-9.311202	-3.085960	-0.268023
H	-10.164159	-3.124087	0.403896
C	-8.314722	-3.401554	-2.442130
H	-8.416590	-3.694625	-3.482781
C	-5.744374	1.380145	5.089397
H	-6.197302	2.355757	5.236544
C	-9.439403	-3.458956	-1.585149
H	-10.396671	-3.797592	-1.969428
C	-7.093537	-2.974600	-1.972199
H	-6.253516	-2.927876	-2.653204
C	-5.587149	0.506785	6.168190
H	-5.922696	0.800197	7.158171
H	-2.812857	2.016002	3.729844
C	-2.228904	2.110932	2.823568
H	-1.251438	1.650619	2.804299
O	-0.160909	4.284869	1.985971
C	-2.695896	2.771617	1.746898
C	-3.256233	3.128592	0.651424
C	-3.317627	4.292429	-0.216964
C	-2.156900	5.069699	-0.396798
C	-2.181504	6.157597	-1.266697
H	-1.284596	6.756404	-1.401059
C	-3.351802	6.483951	-1.958959
H	-3.364533	7.329526	-2.640551
H	-5.419776	5.974423	-2.302730
C	-4.508525	5.723658	-1.768347
C	-4.492829	4.632218	-0.902945
H	-5.382535	4.025322	-0.766935
H	-1.266732	4.816798	0.172291
C	-0.595923	4.521535	3.143004
O	-0.939307	3.687546	4.025514
O	-0.735530	5.834362	3.541109
C	-0.342690	6.823276	2.595597
H	-0.487880	7.787312	3.089047
H	0.709808	6.712887	2.308686
H	-0.954740	6.779800	1.687663
O	-0.010843	1.084749	-2.824651

Int2ii-A_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-6284.736646
Thermal and entropic correction, BS1 (a.u.)	1.541198
Electronic Energy, BS2 (a.u.)	-10207.227850
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	3.050672	-0.223768	-0.083937
Fe	7.124268	-1.921123	0.623179
P	3.703352	-2.323283	0.085187
C	5.443412	-2.442227	-0.435566
C	6.179268	-1.385922	-1.114943
C	7.489024	-1.886192	-1.416902
H	8.271707	-1.313812	-1.892243
C	7.575240	-3.221609	-0.941390
H	8.453428	-3.850918	-0.980500
C	6.329610	-3.564928	-0.341548
H	6.098009	-4.501097	0.145283
C	6.562481	-1.367772	2.534006
H	5.545818	-1.368348	2.892944
C	7.224853	-0.284269	1.882860
H	6.792423	0.680391	1.656168
C	8.539847	-0.719428	1.533857
H	9.283240	-0.142485	1.001277
C	8.686287	-2.071535	1.969047
H	9.556695	-2.695022	1.817588
C	7.463497	-2.472717	2.586082
H	7.239693	-3.452545	2.984388
O	6.629593	0.695011	-2.165464
C	5.752006	-0.025686	-1.430884
N	4.649717	0.556856	-1.112725
C	4.632033	1.884298	-1.779056
C	6.130074	2.068199	-2.212981
H	6.168758	2.374906	-3.260030
H	4.046218	1.752626	-2.691911
C	2.792648	-3.385696	-1.099605
C	3.378199	-4.055259	-2.180989
H	4.451146	-4.007019	-2.338403
C	2.577465	-4.786644	-3.065212
H	3.035750	-5.298729	-3.906239
C	1.198767	-4.863959	-2.864294
H	0.578126	-5.432309	-3.549434
C	0.611275	-4.203215	-1.779604
H	-0.459585	-4.256180	-1.620269
C	1.402001	-3.456638	-0.913178
H	0.939632	-2.920181	-0.091303
C	3.555187	-3.264935	1.653266
C	3.241714	-2.554073	2.820565
H	3.104326	-1.477853	2.772318
C	3.094218	-3.223414	4.037256
H	2.857114	-2.661093	4.935605
C	3.239945	-4.611183	4.092090
H	3.118092	-5.134375	5.035720
C	3.529059	-5.329845	2.927157
H	3.627127	-6.410759	2.965312

C	3.682967	-4.661438	1.711971
H	3.873779	-5.228256	0.805201
C	3.942075	2.928167	-0.933650
C	2.734380	3.473641	-1.388862
C	4.400793	3.269441	0.345631
C	1.978734	4.316179	-0.570878
C	3.659187	4.127379	1.154370
C	2.436539	4.636373	0.708901
H	2.358454	3.196145	-2.370518
H	5.325632	2.845819	0.719786
H	1.006298	4.672150	-0.891924
H	4.012712	4.359400	2.154313
H	1.825120	5.243202	1.368736
C	6.998696	2.964069	-1.363635
C	6.876930	4.351935	-1.498744
C	7.877782	2.443698	-0.408766
C	7.605135	5.206993	-0.673176
C	8.606432	3.300147	0.419345
C	8.467674	4.683195	0.293439
H	6.191651	4.763455	-2.235019
H	7.995347	1.370344	-0.324154
H	7.496893	6.281849	-0.781536
H	9.283792	2.885365	1.160633
H	9.032544	5.349650	0.938072
H	5.585201	1.547485	-5.983044
C	3.508171	1.678317	-5.411767
C	4.770620	1.077854	-5.439216
C	4.980862	-0.133911	-4.775347
H	5.960578	-0.600575	-4.790281
C	3.930065	-0.741772	-4.086356
H	4.088597	-1.683939	-3.569432
H	1.726990	-1.852367	-3.120986
C	1.548005	-0.790105	-3.278121
H	0.586717	-0.644263	-3.770149
C	2.665140	-0.143257	-4.048710
H	1.478966	1.536067	-4.678783
C	2.458946	1.071644	-4.718868
H	3.340736	2.617107	-5.931349
O	1.436805	-0.248391	-1.922785
C	0.624107	0.821771	-1.743519
C	-0.741080	0.315485	0.237475
H	-1.585773	0.351221	-0.450527
H	-1.065865	0.716639	1.199369
H	-0.432352	-0.724816	0.357031
C	0.423941	1.175084	-0.282085
H	0.121692	2.227123	-0.256241
N	1.621379	0.967338	0.573702
C	1.532851	1.595445	1.698772
H	0.633929	2.189520	1.893744
C	2.479958	1.608111	2.814058
C	3.780644	1.071670	2.803991
H	4.163116	0.595943	1.904924
H	5.606235	0.798594	3.909910
C	4.597121	1.195521	3.925504
C	4.129868	1.850850	5.070724
H	4.775643	1.947308	5.938811
C	2.844576	2.394719	5.087746
H	2.484755	2.919305	5.967711
C	2.025727	2.282768	3.965233

H	1.037846	2.739116	3.945202
Ni	-3.998742	0.919814	1.352792
P	-4.698333	0.894141	-0.766868
C	-7.310807	0.884091	0.179368
H	-6.842217	1.131513	1.127785
C	-3.920957	-0.530575	-1.674970
C	-4.967763	2.879641	-2.803117
H	-5.965276	2.504676	-2.999906
C	-4.194449	2.345549	-1.761276
C	-6.506421	0.701139	-0.955155
C	-2.915045	-0.253390	-2.644632
H	-2.638983	0.769714	-2.863514
C	-7.107764	0.360598	-2.175564
H	-6.493709	0.179005	-3.051846
C	-3.563272	-2.926177	-2.049573
C	-4.243923	-1.853938	-1.370711
C	-4.457935	3.916574	-3.583742
H	-5.064629	4.332293	-4.382952
C	-2.600479	-2.622502	-3.065577
C	-2.289290	-1.266441	-3.326384
H	-1.562430	-1.026960	-4.096409
C	-2.930451	2.888460	-1.490468
H	-2.347089	2.567747	-0.635035
C	-9.285372	0.396744	-1.124725
H	-10.361689	0.269875	-1.190416
C	-8.694169	0.732178	0.095415
H	-9.307748	0.867227	0.981132
C	-8.491599	0.213243	-2.258807
H	-8.946340	-0.068858	-3.202865
C	-2.011027	-3.677605	-3.813575
H	-1.292905	-3.425151	-4.588677
C	-3.257836	-5.301157	-2.531559
H	-3.506683	-6.338171	-2.327847
C	-2.417423	3.911088	-2.287058
H	-1.446512	4.319599	-2.034839
C	-2.338374	-4.989730	-3.562477
H	-1.894406	-5.788752	-4.148647
C	-3.856930	-4.299045	-1.801640
H	-4.586407	-4.556292	-1.042403
C	-3.175965	4.418772	-3.340837
H	-2.783652	5.221819	-3.958357
P	-4.143450	-1.203568	1.882680
C	-1.539212	-1.675163	2.701096
H	-1.641001	-0.709934	3.186149
C	-5.430222	-2.117282	0.890261
C	-4.399208	-2.415009	4.448599
H	-3.678073	-3.151317	4.109824
C	-4.783556	-1.365181	3.604309
C	-2.599985	-2.189315	1.936167
C	-6.578606	-2.571517	1.604703
H	-6.586040	-2.537578	2.684630
C	-2.455802	-3.430533	1.306563
H	-3.271421	-3.844127	0.727577
C	-6.581558	-2.708336	-1.196916
C	-5.415459	-2.216890	-0.504338
C	-4.942674	-2.518006	5.731403
H	-4.634626	-3.332064	6.380666
C	-7.739562	-3.101176	-0.453791
C	-7.690629	-3.045053	0.958182

H	-8.551887	-3.375608	1.532310
C	-5.723762	-0.426419	4.061178
H	-6.016947	0.396025	3.413570
C	-0.210316	-3.632136	2.195858
H	0.718907	-4.184923	2.294895
C	-0.354655	-2.395508	2.832937
H	0.462034	-1.991263	3.421318
C	-1.260461	-4.143959	1.430074
H	-1.154286	-5.100966	0.928114
C	-8.906294	-3.537572	-1.136410
H	-9.773162	-3.827660	-0.549165
C	-7.797932	-3.210562	-3.254018
H	-7.825653	-3.251037	-4.338806
C	-6.269877	-0.535545	5.338234
H	-6.992034	0.198985	5.681557
C	-8.939219	-3.592540	-2.509771
H	-9.834464	-3.927673	-3.024538
C	-6.654512	-2.782850	-2.618792
H	-5.801848	-2.482547	-3.213668
C	-5.877185	-1.582415	6.177436
H	-6.295793	-1.664683	7.175858
H	-3.737444	1.155499	4.056484
C	-3.262225	1.578166	3.176090
H	-2.174403	1.637349	3.194841
O	-1.059446	4.166872	0.448152
C	-3.875600	2.669152	2.554016
C	-4.470576	3.333098	1.689689
C	-5.069875	4.318081	0.854395
C	-4.249352	5.229297	0.159631
C	-4.833088	6.176271	-0.676534
H	-4.199650	6.868893	-1.221744
C	-6.221207	6.226342	-0.829847
H	-6.668014	6.966500	-1.487236
H	-8.116112	5.358227	-0.266546
C	-7.037921	5.321301	-0.144168
C	-6.469056	4.368630	0.694395
H	-7.093487	3.656213	1.222812
H	-3.171727	5.148638	0.259549
C	-0.853066	4.172239	1.687104
O	-0.817109	3.201593	2.482958
O	-0.595062	5.397012	2.301965
C	-0.726129	6.556120	1.486153
H	-0.409707	7.399710	2.105016
H	-0.102156	6.500725	0.587731
H	-1.764202	6.713226	1.170112
O	0.028529	1.369388	-2.647913

Int3ii-A_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-6284.750164
Thermal and entropic correction, BS1 (a.u.)	1.539648
Electronic Energy, BS2 (a.u.)	-10207.230602
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Ni	-4.307092	1.031961	1.557478

P	-4.499816	1.014431	-0.645777
C	-7.049648	2.098746	-0.426203
H	-6.744068	2.311986	0.595032
C	-4.063390	-0.707607	-1.172797
C	-3.746516	2.826958	-2.715991
H	-4.732118	2.693103	-3.144202
C	-3.357929	2.119876	-1.567763
C	-6.163595	1.427337	-1.280756
C	-2.696723	-0.950759	-1.482453
H	-1.972577	-0.147185	-1.485755
C	-6.564733	1.132896	-2.592869
H	-5.900440	0.584172	-3.252667
C	-4.502711	-3.112010	-1.350546
C	-4.956029	-1.777360	-1.072804
C	-2.879173	3.755103	-3.293197
H	-3.195889	4.311218	-4.170662
C	-3.128703	-3.331034	-1.687646
C	-2.246278	-2.224935	-1.722934
H	-1.195790	-2.388396	-1.936291
C	-2.083998	2.335529	-1.020442
H	-1.781360	1.797726	-0.125529
C	-8.704606	2.181543	-2.186171
H	-9.691843	2.467318	-2.536371
C	-8.315035	2.475580	-0.878240
H	-8.996588	2.990500	-0.207841
C	-7.828856	1.509152	-3.042212
H	-8.137561	1.256381	-4.051328
C	-2.677270	-4.649506	-1.962707
H	-1.637100	-4.791196	-2.242081
C	-4.894694	-5.511213	-1.547656
H	-5.571346	-6.358653	-1.490101
C	-1.226601	3.265019	-1.602315
H	-0.258642	3.449602	-1.153361
C	-3.538870	-5.719745	-1.896505
H	-3.184706	-6.723421	-2.112152
C	-5.363413	-4.244582	-1.281141
H	-6.403472	-4.104938	-1.012894
C	-1.626133	3.988901	-2.725239
H	-0.969355	4.741679	-3.150006
P	-5.364729	-0.895145	1.906465
C	-2.918789	-2.188654	1.934673
H	-2.514118	-1.183345	1.910133
C	-6.699632	-1.265064	0.673269
C	-6.332738	-1.909610	4.398559
H	-5.828758	-2.841475	4.168040
C	-6.269877	-0.832647	3.506401
C	-4.305358	-2.380799	1.941689
C	-8.061352	-1.102027	1.049839
H	-8.312711	-0.875582	2.077995
C	-4.829439	-3.683304	1.919451
H	-5.903361	-3.840715	1.881699
C	-7.424196	-1.726981	-1.618875
C	-6.379532	-1.583868	-0.647067
C	-7.034216	-1.783756	5.600889
H	-7.072610	-2.623287	6.288562
C	-8.785552	-1.518054	-1.228213
C	-9.070353	-1.220864	0.126686
H	-10.104440	-1.082262	0.430346
C	-6.910990	0.373699	3.841211

H	-6.840438	1.222448	3.164559
C	-2.581714	-4.581066	1.897264
H	-1.916581	-5.439492	1.866995
C	-2.059342	-3.287673	1.915916
H	-0.989550	-3.106467	1.900912
C	-3.966590	-4.777638	1.901351
H	-4.374139	-5.782960	1.865147
C	-9.813917	-1.600073	-2.204379
H	-10.841709	-1.435087	-1.892807
C	-8.173152	-2.094758	-3.908962
H	-7.944923	-2.318501	-4.946795
C	-7.617789	0.492881	5.035837
H	-8.109152	1.429366	5.282022
C	-9.517175	-1.879054	-3.518461
H	-10.310067	-1.937903	-4.257923
C	-7.155041	-2.023053	-2.985403
H	-6.130426	-2.184690	-3.298479
C	-7.680353	-0.589138	5.919302
H	-8.223984	-0.496445	6.854579
H	-4.386907	0.926954	4.306299
C	-3.623542	1.082828	3.550436
H	-2.711270	0.496211	3.636050
C	-3.535664	2.289364	2.898150
C	-3.651775	2.975456	1.843634
C	-3.330754	4.198511	1.148337
C	-2.098456	4.827845	1.408815
C	-1.735374	5.978749	0.717739
H	-0.771137	6.438220	0.908493
C	-2.596481	6.518285	-0.241318
H	-2.307791	7.409802	-0.790346
H	-4.491220	6.316017	-1.252118
C	-3.824044	5.903859	-0.501307
C	-4.191220	4.749315	0.186028
H	-5.131948	4.254888	-0.033091
H	-1.424710	4.390181	2.136023
Cu	3.797042	-1.031810	-0.020485
Fe	7.573212	1.464583	0.102672
P	5.908705	-1.514202	-0.616173
C	6.705382	0.048234	-1.102673
C	6.026773	1.323726	-1.248129
C	6.987796	2.280136	-1.718883
H	6.783318	3.327100	-1.886221
C	8.234049	1.618311	-1.871496
H	9.164700	2.083375	-2.165885
C	8.064777	0.254802	-1.499807
H	8.839704	-0.497255	-1.472776
C	7.120014	1.129869	2.091399
H	6.316594	0.489393	2.427374
C	7.026503	2.526021	1.798086
H	6.138469	3.137794	1.869534
C	8.300836	2.966583	1.335780
H	8.541163	3.964297	0.995152
C	9.185006	1.846093	1.346622
H	10.213571	1.846611	1.012717
C	8.457586	0.711779	1.813459
H	8.831080	-0.299135	1.893072
O	4.305180	2.941623	-1.280910
C	4.637494	1.672815	-0.960599
N	3.701693	0.945805	-0.442914

C	2.514022	1.811910	-0.238540
C	2.841131	3.010202	-1.191083
H	2.470196	2.736334	-2.184106
H	1.621183	1.284299	-0.583635
C	5.843382	-2.449730	-2.196033
C	5.815128	-1.790568	-3.432205
H	5.974751	-0.717930	-3.479658
C	5.567215	-2.504428	-4.606501
H	5.553231	-1.983286	-5.559636
C	5.344395	-3.882130	-4.558213
H	5.155433	-4.436883	-5.472520
C	5.377877	-4.546652	-3.328415
H	5.215225	-5.619804	-3.284793
C	5.620818	-3.834923	-2.154380
H	5.637498	-4.356912	-1.201035
C	7.175320	-2.375172	0.388384
C	6.977721	-2.429997	1.775027
H	6.071942	-2.017855	2.204796
C	7.943078	-3.006885	2.602166
H	7.776187	-3.040090	3.674181
C	9.107844	-3.541984	2.048364
H	9.859492	-3.991806	2.690336
C	9.299941	-3.513395	0.662992
H	10.197662	-3.944228	0.229367
C	8.336930	-2.937139	-0.165327
H	8.479815	-2.936197	-1.241997
C	2.338466	2.156114	1.229511
C	1.081336	2.544618	1.705037
C	3.423134	2.150598	2.115105
C	0.915094	2.923393	3.037612
C	3.264918	2.560090	3.440605
C	2.007041	2.947167	3.907701
H	0.221350	2.528050	1.046814
H	4.389221	1.815410	1.760424
H	-0.074706	3.183815	3.399503
H	4.123808	2.578627	4.106211
H	1.877604	3.254196	4.941253
C	2.422914	4.419742	-0.876828
C	1.637564	5.108363	-1.809482
C	2.827336	5.086399	0.288953
C	1.227123	6.420919	-1.573794
C	2.426922	6.400924	0.522628
C	1.621885	7.070640	-0.403896
H	1.347004	4.607451	-2.728401
H	3.452715	4.578427	1.012759
H	0.611476	6.935616	-2.305392
H	2.746095	6.905362	1.429786
H	1.313629	8.095411	-0.217806
H	0.543994	2.942353	-4.426449
C	-0.383431	1.022117	-4.139960
C	0.705846	1.871376	-4.349956
C	1.994364	1.342890	-4.464139
H	2.842665	2.001726	-4.629818
C	2.195939	-0.034162	-4.355110
H	3.197823	-0.449621	-4.401287
H	2.338587	-2.667682	-4.285468
C	1.315892	-2.378550	-4.031300
H	0.609515	-2.944251	-4.641452
C	1.107253	-0.891745	-4.163171

H	-1.030328	-1.013714	-3.905113
C	-0.182254	-0.354579	-4.062285
H	-1.381634	1.434362	-4.036033
O	1.026531	-2.852884	-2.673352
C	1.892995	-2.459009	-1.731672
C	0.943645	-4.288600	-0.246842
H	0.408799	-4.477099	0.685856
H	1.775129	-4.996929	-0.326411
H	0.244415	-4.481091	-1.059024
C	1.439410	-2.840287	-0.330436
N	2.476570	-2.439831	0.632344
C	2.542253	-3.036859	1.764570
H	1.934429	-3.918923	1.977070
C	3.415658	-2.581994	2.854473
C	3.606830	-1.210561	3.095447
H	3.059126	-0.484631	2.503797
H	4.570322	0.262166	4.322731
C	4.446618	-0.797396	4.128609
C	5.104352	-1.741325	4.923769
H	5.760400	-1.413922	5.724852
C	4.897940	-3.106145	4.702527
H	5.396101	-3.841621	5.326795
C	4.044072	-3.524477	3.682504
H	3.880157	-4.585249	3.511014
O	2.894614	-1.816788	-1.990206
H	0.614854	-2.128981	-0.147738
O	-0.022232	-0.194784	-0.085563
C	-0.415688	-0.095797	1.096828
O	0.315956	-0.895631	1.997926
O	-1.351503	0.590578	1.573185
H	0.075412	0.339770	3.662741
C	0.040239	-0.716799	3.385886
H	-0.937709	-1.127046	3.661821
H	0.821375	-1.263039	3.920647

TS34ii-A_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-6284.733137
Thermal and entropic correction, BS1 (a.u.)	1.534587
Electronic Energy, BS2 (a.u.)	-10207.214406
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-1227.4i

Molecular Geometry in Cartesian Coordinates

Ni	-4.496236	0.934695	1.583164
P	-4.670983	1.039323	-0.618375
C	-7.198794	2.177649	-0.415946
H	-6.913904	2.348893	0.619040
C	-4.250197	-0.668108	-1.198058
C	-3.854629	2.950836	-2.566230
H	-4.826602	2.835416	-3.029171
C	-3.492388	2.177460	-1.452712
C	-6.310044	1.511911	-1.271633
C	-2.882322	-0.920678	-1.492353
H	-2.161530	-0.114994	-1.496828
C	-6.685853	1.269573	-2.601853
H	-6.019126	0.726263	-3.263698

C	-4.709710	-3.063429	-1.423793
C	-5.157960	-1.728805	-1.138469
C	-2.979708	3.917019	-3.064414
H	-3.275633	4.517894	-3.919124
C	-3.326629	-3.294651	-1.718587
C	-2.433790	-2.195975	-1.732904
H	-1.378981	-2.363173	-1.927444
C	-2.233813	2.370980	-0.861124
H	-1.949826	1.782198	0.006330
C	-8.807508	2.360350	-2.210636
H	-9.778221	2.683374	-2.574251
C	-8.442718	2.602056	-0.884913
H	-9.127177	3.112747	-0.214329
C	-7.929060	1.692528	-3.067684
H	-8.219472	1.480595	-4.091487
C	-2.878009	-4.616895	-1.979980
H	-1.826364	-4.772106	-2.203349
C	-5.122748	-5.453715	-1.669115
H	-5.811364	-6.293213	-1.650580
C	-1.371643	3.345971	-1.355450
H	-0.422381	3.518292	-0.864264
C	-3.755336	-5.676092	-1.959449
H	-3.403859	-6.682600	-2.165523
C	-5.586564	-4.185371	-1.403604
H	-6.634213	-4.035471	-1.172876
C	-1.747191	4.129000	-2.447056
H	-1.084093	4.905896	-2.814568
P	-5.674749	-0.933599	1.839977
C	-3.342103	-2.435942	1.949871
H	-2.849458	-1.472137	1.932127
C	-6.966137	-1.220236	0.546355
C	-6.829481	-1.851957	4.289925
H	-6.396682	-2.824266	4.083186
C	-6.639615	-0.789019	3.398436
C	-4.740252	-2.497710	1.916145
C	-8.337477	-1.033699	0.871796
H	-8.624298	-0.819758	1.893629
C	-5.382139	-3.745715	1.874719
H	-6.464402	-3.801924	1.803488
C	-7.600206	-1.618080	-1.782189
C	-6.595023	-1.519748	-0.764879
C	-7.567001	-1.660454	5.461444
H	-7.704667	-2.489697	6.148792
C	-8.972633	-1.389593	-1.442703
C	-9.308951	-1.114046	-0.094870
H	-10.351938	-0.959196	0.167506
C	-7.190068	0.469030	3.702975
H	-7.022274	1.305548	3.028360
C	-3.229856	-4.850066	1.922217
H	-2.645039	-5.764834	1.910815
C	-2.589608	-3.610705	1.954454
H	-1.506979	-3.544545	1.966129
C	-4.625730	-4.916107	1.884699
H	-5.124286	-5.879192	1.838851
C	-9.960499	-1.427628	-2.462377
H	-10.997140	-1.249532	-2.189918
C	-8.259100	-1.913118	-4.109783
H	-7.992174	-2.115932	-5.142612
C	-7.932147	0.654274	4.867504

H	-8.352403	1.630179	5.091032
C	-9.613982	-1.679941	-3.769675
H	-10.376057	-1.704667	-4.542651
C	-7.279309	-1.886156	-3.143306
H	-6.246012	-2.062674	-3.417538
C	-8.122227	-0.413447	5.749925
H	-8.694119	-0.269864	6.661565
H	-4.535864	0.633539	4.310114
C	-3.769775	0.791234	3.556359
H	-2.898951	0.141022	3.600858
C	-3.612764	2.034024	2.988932
C	-3.733400	2.813650	2.001029
C	-3.420012	4.092090	1.407141
C	-2.202782	4.723361	1.728218
C	-1.856473	5.928528	1.124957
H	-0.903254	6.391460	1.360509
C	-2.719406	6.521452	0.199372
H	-2.445925	7.458443	-0.276986
H	-4.602087	6.360129	-0.841306
C	-3.932907	5.905373	-0.117521
C	-4.283011	4.697141	0.479616
H	-5.212222	4.203355	0.215429
H	-1.524963	4.249169	2.428805
Cu	4.133665	-1.055416	-0.191831
Fe	7.877654	1.444414	0.335687
P	6.266803	-1.533544	-0.602020
C	7.153200	0.020649	-0.971624
C	6.525141	1.309057	-1.205038
C	7.553058	2.248389	-1.550791
H	7.389338	3.297458	-1.748476
C	8.798436	1.567581	-1.529490
H	9.767438	2.016274	-1.699122
C	8.558804	0.209325	-1.172306
H	9.311881	-0.552355	-1.029853
C	7.111533	1.183317	2.233593
H	6.231466	0.592621	2.442610
C	7.141158	2.574201	1.904684
H	6.289552	3.235742	1.829824
C	8.493473	2.937960	1.635820
H	8.837212	3.912566	1.317525
C	9.302936	1.774884	1.805299
H	10.368988	1.713888	1.634348
C	8.452002	0.692634	2.175684
H	8.754479	-0.332794	2.330444
O	4.807031	2.931426	-1.464802
C	5.117086	1.669894	-1.076589
N	4.146393	0.946198	-0.636137
C	2.919244	1.759837	-0.639611
C	3.350944	3.013862	-1.487911
H	3.046212	2.839458	-2.523985
H	2.137813	1.214145	-1.174631
C	6.387474	-2.505108	-2.159652
C	7.275827	-2.228339	-3.207408
H	7.962238	-1.391300	-3.136126
C	7.273484	-3.019554	-4.359159
H	7.964285	-2.795137	-5.166800
C	6.388844	-4.092873	-4.472996
H	6.389945	-4.705949	-5.369515
C	5.496212	-4.371858	-3.434055

H	4.798416	-5.199730	-3.521484
C	5.489140	-3.577693	-2.289352
H	4.773092	-3.770555	-1.495282
C	7.390864	-2.399170	0.562227
C	7.029550	-2.427185	1.916614
H	6.092663	-1.982483	2.233072
C	7.872596	-3.020838	2.857892
H	7.578047	-3.033769	3.902517
C	9.077878	-3.597386	2.451539
H	9.733930	-4.060912	3.182539
C	9.432263	-3.594275	1.098557
H	10.360122	-4.059191	0.778118
C	8.590361	-3.003759	0.155748
H	8.857149	-3.026851	-0.897115
C	2.454449	2.039997	0.774861
C	1.092034	2.024720	1.076031
C	3.370832	2.328794	1.794011
C	0.644765	2.301655	2.370651
C	2.929833	2.624032	3.083131
C	1.562373	2.612255	3.375473
H	0.381909	1.753034	0.304997
H	4.430946	2.295153	1.575220
H	-0.416309	2.234263	2.584237
H	3.652083	2.856716	3.860779
H	1.218638	2.829691	4.382676
C	2.874249	4.361049	-1.028715
C	1.708262	4.889810	-1.591906
C	3.525545	5.068839	-0.012185
C	1.173553	6.089184	-1.118716
C	3.001294	6.274910	0.450585
C	1.818411	6.783101	-0.093338
H	1.217419	4.350405	-2.397086
H	4.443284	4.672004	0.407316
H	0.258242	6.483288	-1.549929
H	3.514441	6.818287	1.238485
H	1.410962	7.722100	0.270139
H	0.191176	3.215160	-4.399666
C	-0.527883	1.228479	-3.980192
C	0.450413	2.163076	-4.330308
C	1.753477	1.738798	-4.602155
H	2.513809	2.460624	-4.888581
C	2.081583	0.383888	-4.510890
H	3.100919	0.054404	-4.688425
H	2.475223	-2.213475	-4.394306
C	1.434807	-2.030920	-4.114518
H	0.777899	-2.613619	-4.765198
C	1.102189	-0.559318	-4.184604
H	-0.968756	-0.852247	-3.668664
C	-0.203499	-0.125765	-3.921676
H	-1.539360	1.555891	-3.763462
O	1.185760	-2.587638	-2.799278
C	2.061888	-2.201579	-1.832315
C	0.862396	-3.887583	-0.326458
H	0.202320	-3.832566	0.544556
H	1.510758	-4.767309	-0.202310
H	0.239039	-4.053879	-1.204011
C	1.666436	-2.609185	-0.491978
N	2.640509	-2.276738	0.490841
C	2.637198	-2.854372	1.647667

H	1.985074	-3.705748	1.846333
C	3.437153	-2.378532	2.779907
C	3.664226	-1.003860	2.977508
H	3.224118	-0.288941	2.291403
H	4.556889	0.501542	4.219656
C	4.410840	-0.563359	4.068948
C	4.946757	-1.482888	4.976085
H	5.531386	-1.136480	5.823088
C	4.705286	-2.848919	4.800674
H	5.107170	-3.568038	5.508507
C	3.943896	-3.292009	3.719706
H	3.757962	-4.354508	3.585100
O	3.031130	-1.485989	-2.111687
H	0.689466	-1.553354	-0.274748
O	-0.142462	-0.719234	-0.124052
C	-0.566879	-0.607969	1.089844
O	0.065504	-1.458820	1.951315
O	-1.444715	0.165634	1.479628
H	-0.027962	-0.189774	3.603225
C	-0.155244	-1.244624	3.351793
H	-1.153954	-1.579513	3.647417
H	0.603083	-1.842005	3.859038

Int4ii-A_NiCu

Charge	1
Electronic Energy, BS1 (a.u.)	-6284.736055
Thermal and entropic correction, BS1 (a.u.)	1.537480
Electronic Energy, BS2 (a.u.)	-10207.219949
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Ni	-4.488232	0.923534	1.579799
P	-4.691525	1.015093	-0.622418
C	-7.262547	2.047827	-0.391067
H	-6.978173	2.221577	0.643633
C	-4.218863	-0.676040	-1.209894
C	-3.953642	2.954681	-2.576170
H	-4.923467	2.806096	-3.034159
C	-3.559677	2.194143	-1.464664
C	-6.352799	1.427681	-1.258921
C	-2.851536	-0.882157	-1.542277
H	-2.164435	-0.047795	-1.577829
C	-6.728167	1.179498	-2.588321
H	-6.044823	0.668701	-3.259109
C	-4.603561	-3.085172	-1.427651
C	-5.088967	-1.766546	-1.130529
C	-3.114990	3.950934	-3.078361
H	-3.435840	4.540678	-3.931776
C	-3.221523	-3.270073	-1.757506
C	-2.366161	-2.141862	-1.796113
H	-1.313686	-2.276345	-2.028068
C	-2.305830	2.432819	-0.879987
H	-1.997590	1.856893	-0.013225
C	-8.890609	2.177278	-2.172800
H	-9.876657	2.462123	-2.526844
C	-8.526754	2.422910	-0.847547

H	-9.227364	2.898090	-0.167658
C	-7.991281	1.554065	-3.041714
H	-8.280258	1.338734	-4.065177
C	-2.737579	-4.576411	-2.035814
H	-1.688992	-4.697155	-2.290070
C	-4.945212	-5.486875	-1.669076
H	-5.605531	-6.348367	-1.636109
C	-1.480469	3.437201	-1.377192
H	-0.535456	3.644072	-0.891516
C	-3.579271	-5.663582	-1.995298
H	-3.200597	-6.657309	-2.214538
C	-5.443209	-4.234752	-1.389189
H	-6.489433	-4.118910	-1.133728
C	-1.887484	4.206121	-2.467339
H	-1.251105	5.004133	-2.837424
P	-5.584204	-0.992220	1.858518
C	-3.193640	-2.404517	1.957839
H	-2.742104	-1.421457	1.951211
C	-6.885112	-1.323496	0.586527
C	-6.667278	-1.962452	4.319919
H	-6.205772	-2.918506	4.099617
C	-6.526486	-0.887628	3.433563
C	-4.588367	-2.519313	1.919396
C	-8.256324	-1.183338	0.935158
H	-8.533430	-0.983075	1.962411
C	-5.180490	-3.791104	1.869491
H	-6.259617	-3.889060	1.797108
C	-7.543260	-1.734243	-1.733020
C	-6.525511	-1.605610	-0.731638
C	-7.393258	-1.803614	5.503430
H	-7.492919	-2.641518	6.186780
C	-8.916662	-1.550969	-1.370568
C	-9.239953	-1.291180	-0.016425
H	-10.283058	-1.171420	0.263199
C	-7.114909	0.348981	3.754446
H	-6.986526	1.194881	3.082758
C	-2.986846	-4.811739	1.913229
H	-2.366477	-5.702580	1.896805
C	-2.395188	-3.548447	1.956785
H	-1.315216	-3.444908	1.973635
C	-4.378811	-4.931301	1.872488
H	-4.839520	-5.912586	1.819040
C	-9.919314	-1.618413	-2.374147
H	-10.956547	-1.474324	-2.084470
C	-8.230410	-2.047013	-4.049982
H	-7.974125	-2.239979	-5.087362
C	-7.845163	0.501437	4.931169
H	-8.295058	1.460929	5.167597
C	-9.586228	-1.857529	-3.687411
H	-10.359629	-1.905510	-4.447915
C	-7.236196	-1.989777	-3.099698
H	-6.202556	-2.132712	-3.391474
C	-7.985605	-0.577854	5.808812
H	-8.548274	-0.459641	6.729760
H	-4.473659	0.636339	4.307629
C	-3.724503	0.820454	3.542900
H	-2.827009	0.207322	3.585214
C	-3.627819	2.065140	2.966008
C	-3.802632	2.836184	1.979188

C	-3.564141	4.127899	1.378868
C	-2.384112	4.829393	1.693088
C	-2.108169	6.048817	1.082434
H	-1.182972	6.566859	1.315165
C	-3.005813	6.587060	0.156445
H	-2.787229	7.535277	-0.325757
H	-4.880528	6.314838	-0.875166
C	-4.183877	5.902022	-0.152207
C	-4.463345	4.679085	0.452178
H	-5.364914	4.133494	0.194649
H	-1.680102	4.401013	2.397373
Cu	4.126847	-1.046320	-0.233169
Fe	7.853197	1.439160	0.439595
P	6.261475	-1.490625	-0.660989
C	7.144345	0.084685	-0.946437
C	6.510415	1.380914	-1.113998
C	7.534438	2.343088	-1.403263
H	7.365701	3.400198	-1.546621
C	8.783758	1.669368	-1.409968
H	9.751127	2.132001	-1.548695
C	8.549874	0.292428	-1.127890
H	9.307473	-0.470322	-1.019226
C	7.092719	1.044048	2.316573
H	6.228657	0.419209	2.489261
C	7.086865	2.452593	2.072979
H	6.218146	3.094911	2.036281
C	8.429696	2.866302	1.829062
H	8.748842	3.866962	1.571742
C	9.268451	1.715756	1.928658
H	10.335735	1.692456	1.756023
C	8.444972	0.591553	2.230600
H	8.771858	-0.434155	2.322092
O	4.770785	2.984538	-1.363415
C	5.098155	1.723980	-0.982905
N	4.136556	0.983288	-0.551230
C	2.898198	1.774910	-0.564640
C	3.313888	3.038740	-1.406462
H	3.026253	2.859977	-2.446584
H	2.132098	1.216148	-1.108371
C	6.394978	-2.384146	-2.263815
C	7.344914	-2.109990	-3.257329
H	8.073417	-1.318891	-3.114323
C	7.349361	-2.841194	-4.447681
H	8.088030	-2.619245	-5.212545
C	6.408628	-3.851318	-4.655318
H	6.414474	-4.417421	-5.582253
C	5.454063	-4.126005	-3.672138
H	4.712170	-4.902971	-3.833123
C	5.441326	-3.391624	-2.487749
H	4.678204	-3.578057	-1.737345
C	7.378597	-2.402359	0.475133
C	6.992321	-2.503961	1.819179
H	6.041430	-2.092314	2.138411
C	7.826748	-3.130686	2.746592
H	7.511908	-3.199738	3.783117
C	9.048777	-3.667455	2.335907
H	9.698784	-4.156376	3.055727
C	9.427968	-3.592411	0.991612
H	10.368735	-4.027409	0.666689

C	8.594463	-2.968786	0.062692
H	8.880959	-2.937257	-0.984733
C	2.413848	2.056691	0.843230
C	1.045918	2.175565	1.093941
C	3.313340	2.234334	1.901363
C	0.577757	2.472560	2.375559
C	2.852850	2.549000	3.179653
C	1.481353	2.671027	3.421154
H	0.343826	1.998995	0.288348
H	4.372354	2.097992	1.720197
H	-0.491805	2.508570	2.551612
H	3.563296	2.693149	3.988804
H	1.121674	2.905903	4.418810
C	2.802615	4.373332	-0.948480
C	1.658278	4.903904	-1.553362
C	3.399031	5.063525	0.113288
C	1.093233	6.090084	-1.080504
C	2.843333	6.254631	0.577218
C	1.683401	6.766262	-0.011567
H	1.205731	4.376837	-2.389040
H	4.296948	4.661841	0.569622
H	0.196668	6.487983	-1.546538
H	3.313547	6.783677	1.400837
H	1.252096	7.694710	0.351666
H	0.058422	3.350801	-4.389001
C	-0.609946	1.335667	-4.023709
C	0.348072	2.306269	-4.328143
C	1.671374	1.927008	-4.566689
H	2.416598	2.677313	-4.817712
C	2.038827	0.581617	-4.488232
H	3.072915	0.286632	-4.638390
H	2.508342	-1.999220	-4.438246
C	1.457183	-1.861898	-4.171710
H	0.833808	-2.437885	-4.861266
C	1.080840	-0.398370	-4.209718
H	-0.995312	-0.764422	-3.770454
C	-0.244853	-0.009248	-3.980651
H	-1.637554	1.628040	-3.832749
O	1.201052	-2.476646	-2.889964
C	2.075911	-2.122884	-1.892404
C	0.889995	-3.911137	-0.483535
H	0.181167	-3.799660	0.346872
H	1.462122	-4.832586	-0.294367
H	0.317186	-4.062300	-1.396926
C	1.792324	-2.712331	-0.623598
N	2.669230	-2.357199	0.396550
C	2.679341	-2.982977	1.540044
H	2.083435	-3.884585	1.686808
C	3.426561	-2.505722	2.700151
C	3.639178	-1.130333	2.925379
H	3.212818	-0.408536	2.237813
H	4.487004	0.367909	4.206439
C	4.351892	-0.696584	4.041659
C	4.868349	-1.619370	4.956765
H	5.426594	-1.277724	5.823155
C	4.638220	-2.984787	4.759198
H	5.023083	-3.709563	5.471094
C	3.914698	-3.422000	3.650944
H	3.745446	-4.485026	3.498835

O	2.988900	-1.306776	-2.131338
H	0.626423	-1.308131	-0.300896
O	-0.088167	-0.596515	-0.178697
C	-0.477898	-0.492427	1.075391
O	0.224832	-1.291985	1.896882
O	-1.377926	0.247325	1.444265
H	0.113483	-0.052023	3.568580
C	0.024391	-1.108792	3.310942
H	-0.954608	-1.491351	3.611668
H	0.820555	-1.681661	3.784138

Int1_κO_Ni

Charge	0
Electronic Energy, BS1 (a.u.)	-3200.696716
Thermal and entropic correction, BS1 (a.u.)	0.7238522
Electronic Energy, BS2 (a.u.)	-4539.065449
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Ni	0.054611	1.562464	0.608540
P	0.885816	-0.384172	0.454181
C	1.888702	0.197469	-2.081278
H	1.808561	1.222044	-1.729184
C	-0.393710	-1.697175	0.829562
C	3.105054	-2.006445	1.386062
H	2.948464	-2.663775	0.537719
C	2.291918	-0.875323	1.563780
C	1.504777	-0.849419	-1.227885
C	-0.247021	-2.489965	2.003346
H	0.676852	-2.437965	2.567133
C	1.603361	-2.168943	-1.692477
H	1.275672	-2.989796	-1.062312
C	-2.650004	-2.630154	0.558554
C	-1.592759	-1.769403	0.110023
C	4.126629	-2.295606	2.291496
H	4.754744	-3.167548	2.134089
C	-2.482750	-3.398025	1.756825
C	-1.253589	-3.308539	2.455422
H	-1.117854	-3.893735	3.361636
C	2.535791	-0.037022	2.662384
H	1.918983	0.849919	2.792417
C	2.474988	-1.386506	-3.812504
H	2.843844	-1.596159	-4.812658
C	2.370984	-0.066419	-3.364840
H	2.662016	0.755755	-4.012931
C	2.090303	-2.436189	-2.973535
H	2.151934	-3.462963	-3.322949
C	-3.548269	-4.216119	2.221605
H	-3.404497	-4.783302	3.137889
C	-4.905503	-3.539884	0.339961
H	-5.845419	-3.596873	-0.202066
C	3.556049	-0.325573	3.571994
H	3.732632	0.336087	4.415710
C	-4.736645	-4.289189	1.530257
H	-5.545560	-4.916470	1.893958
C	-3.892939	-2.733693	-0.131296

H	-4.043900	-2.156525	-1.036131
C	4.352869	-1.457535	3.387714
H	5.153849	-1.681152	4.086921
P	-2.036264	1.418666	0.425616
C	-2.309965	0.219086	2.928684
H	-1.271060	0.524521	3.027724
C	-2.120851	0.388480	-1.125949
C	-4.440370	2.683223	-0.636666
H	-4.719863	1.729037	-1.072841
C	-3.234575	2.805115	0.076137
C	-2.983433	0.497249	1.730274
C	-2.248258	1.086843	-2.364812
H	-2.455815	2.151142	-2.352993
C	-4.317953	0.085774	1.593928
H	-4.859458	0.283232	0.675182
C	-1.698439	-1.665529	-2.404784
C	-1.813057	-0.976145	-1.147698
C	-5.277839	3.785842	-0.813892
H	-6.204254	3.674909	-1.371297
C	-1.837513	-0.938938	-3.632347
C	-2.103737	0.452839	-3.573376
H	-2.198464	1.012344	-4.500825
C	-2.890758	4.061866	0.597738
H	-1.950613	4.168776	1.135035
C	-4.272883	-0.881575	3.813375
H	-4.770408	-1.423364	4.613002
C	-2.948431	-0.465528	3.965106
H	-2.408608	-0.682166	4.882955
C	-4.956196	-0.602642	2.625980
H	-5.983421	-0.932645	2.498706
C	-1.702818	-1.619337	-4.872478
H	-1.804350	-1.047165	-5.791356
C	-1.325573	-3.700061	-3.704812
H	-1.127615	-4.767863	-3.737905
C	-3.732212	5.165486	0.430905
H	-3.449752	6.129271	0.846122
C	-1.453958	-2.973211	-4.913075
H	-1.355241	-3.484911	-5.866219
C	-1.439081	-3.064443	-2.487695
H	-1.324636	-3.635279	-1.574150
C	-4.927921	5.029305	-0.277385
H	-5.581359	5.886145	-0.416720
H	3.153702	3.906229	1.852614
C	3.824346	3.957427	0.989726
H	4.560955	4.746433	1.160082
O	3.081710	4.405842	-0.180480
C	4.471329	2.675196	0.739957
C	5.012606	1.614448	0.510976
C	5.664818	0.369594	0.251130
C	6.723679	-0.062752	1.072806
C	7.346052	-1.284613	0.824258
H	8.158806	-1.612607	1.465940
C	6.925703	-2.087191	-0.240987
H	7.412235	-3.040131	-0.428757
H	5.542164	-2.279189	-1.889073
C	5.878431	-1.660192	-1.062490
C	5.249058	-0.440652	-0.822672
H	4.430146	-0.114142	-1.452534
H	7.041944	0.557706	1.904600

C	1.873131	3.859735	-0.350141
O	1.287188	3.193181	0.494729
O	1.433843	4.171469	-1.561608
C	0.075884	3.783458	-1.884657
H	-0.081030	4.126260	-2.907015
H	-0.034272	2.698620	-1.823209
H	-0.629073	4.265936	-1.204912

Int1_kOi_Ni

Charge	0
Electronic Energy, BS1 (a.u.)	-3200.692079
Thermal and entropic correction, BS1 (a.u.)	0.721837
Electronic Energy, BS2 (a.u.)	-4539.060200
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Ni	0.132678	1.762228	-0.194648
P	-0.907320	-0.039037	-0.492735
C	-1.708520	-0.035827	2.172387
H	-1.529912	1.032248	2.078262
C	0.310036	-1.233618	-1.261660
C	-3.090929	-1.412669	-1.831164
H	-2.778926	-2.329867	-1.343685
C	-2.394452	-0.214553	-1.599476
C	-1.476863	-0.864122	1.062570
C	0.178669	-1.495421	-2.656366
H	-0.702115	-1.141928	-3.180078
C	-1.695074	-2.243562	1.190390
H	-1.481395	-2.905901	0.358369
C	2.467425	-2.407879	-1.313749
C	1.461241	-1.674115	-0.595345
C	-4.186349	-1.441792	-2.693651
H	-4.718093	-2.374543	-2.858292
C	2.310382	-2.648472	-2.717452
C	1.143863	-2.169342	-3.363110
H	1.020463	-2.344673	-4.428990
C	-2.831918	0.950811	-2.243871
H	-2.308654	1.883853	-2.056116
C	-2.378555	-1.948435	3.494584
H	-2.722906	-2.370224	4.434716
C	-2.158578	-0.572872	3.380765
H	-2.333618	0.080871	4.230811
C	-2.143481	-2.782394	2.397304
H	-2.292713	-3.854596	2.485854
C	3.320492	-3.349654	-3.430181
H	3.182940	-3.514367	-4.495976
C	4.607709	-3.582795	-1.399728
H	5.499712	-3.943457	-0.894978
C	-3.932659	0.926648	-3.104800
H	-4.261187	1.842812	-3.588027
C	4.446881	-3.812475	-2.787800
H	5.213003	-4.349051	-3.340294
C	3.649374	-2.897737	-0.685454
H	3.798139	-2.718820	0.372676
C	-4.609797	-0.271875	-3.333193
H	-5.469396	-0.296188	-3.997257

P	2.148582	1.348049	0.263332
C	2.651832	1.109069	-2.472046
H	1.656094	1.539541	-2.549369
C	2.090975	-0.162012	1.350911
C	4.507073	2.136465	1.786464
H	4.803787	1.093331	1.831586
C	3.303225	2.501175	1.158237
C	3.188359	0.868115	-1.197848
C	2.225973	0.028885	2.757600
H	2.495164	1.008619	3.135983
C	4.461841	0.287398	-1.101166
H	4.891178	0.070068	-0.129313
C	1.499657	-2.503580	1.786484
C	1.693462	-1.414218	0.868498
C	5.317833	3.102605	2.383289
H	6.243403	2.804800	2.868850
C	1.658389	-2.287410	3.194283
C	2.013841	-0.992613	3.649548
H	2.118658	-0.818453	4.717592
C	2.929654	3.853823	1.156998
H	1.987069	4.137407	0.693555
C	4.629059	0.188338	-3.515142
H	5.183509	-0.085361	-4.408472
C	3.365034	0.771802	-3.624143
H	2.928462	0.952919	-4.602595
C	5.176478	-0.049794	-2.251025
H	6.153655	-0.515648	-2.160123
C	1.442898	-3.360942	4.100379
H	1.561070	-3.172036	5.164511
C	0.941240	-4.835783	2.254281
H	0.663041	-5.822937	1.895550
C	3.744570	4.824604	1.746562
H	3.440527	5.867839	1.733188
C	1.092918	-4.612275	3.644526
H	0.931826	-5.426704	4.345116
C	1.135116	-3.811695	1.353419
H	1.002105	-3.999665	0.294817
C	4.941363	4.449981	2.359820
H	5.575414	5.200200	2.824358
H	-4.002848	4.492304	1.190762
C	-3.506726	3.590404	1.561067
H	-3.445965	3.638929	2.650937
O	-2.111785	3.606329	1.135766
C	-4.208192	2.390087	1.128953
C	-4.801344	1.384089	0.802339
C	-5.505893	0.195529	0.438705
C	-5.137584	-1.042568	1.000578
C	-5.826380	-2.201039	0.649469
H	-5.528840	-3.151487	1.082946
C	-6.890928	-2.141330	-0.254938
H	-7.427621	-3.046564	-0.524589
H	-8.086616	-0.866232	-1.521055
C	-7.263139	-0.915126	-0.814438
C	-6.574138	0.248320	-0.477391
H	-6.850976	1.200349	-0.918802
H	-4.313999	-1.083976	1.702636
C	-1.908171	3.915705	-0.150638
O	-2.741161	4.254141	-0.960419
O	-0.578169	3.821717	-0.389079

C	-0.154374	4.281825	-1.701714
H	0.932529	4.229337	-1.676234
H	-0.552503	3.621493	-2.474112
H	-0.495346	5.306611	-1.861219

Int1_A_Cu

Charge	1
Electronic Energy, BS1 (a.u.)	-3084.090238
Thermal and entropic correction, BS1 (a.u.)	0.783699
Electronic Energy, BS2 (a.u.)	-5668.093430
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

Cu	-0.353057	0.687712	0.859657
Fe	-2.201067	-2.045556	-1.963220
P	-2.310451	0.916023	-0.154796
C	-2.214202	-0.008674	-1.725261
C	-0.979610	-0.451202	-2.356454
C	-1.321835	-1.097928	-3.590586
H	-0.615889	-1.559623	-4.265687
C	-2.733846	-1.060687	-3.731568
H	-3.300981	-1.508587	-4.536348
C	-3.281188	-0.393115	-2.599293
H	-4.332876	-0.239513	-2.406500
C	-2.411135	-2.917547	-0.098985
H	-2.483579	-2.360180	0.822150
C	-1.206709	-3.368024	-0.718459
H	-0.203313	-3.206084	-0.349106
C	-1.555228	-4.011740	-1.945549
H	-0.863228	-4.427926	-2.665366
C	-2.977010	-3.959203	-2.081596
H	-3.547722	-4.327278	-2.923930
C	-3.506279	-3.281135	-0.941355
H	-4.546490	-3.041528	-0.765378
O	1.349752	-0.601974	-2.784443
C	0.390212	-0.349248	-1.864360
N	0.792723	-0.060536	-0.675379
C	2.269453	0.011601	-0.701479
C	2.622673	-0.674625	-2.071432
H	3.333223	-0.057991	-2.621811
H	2.536452	1.070225	-0.771586
C	-2.568584	2.654952	-0.693033
C	-2.034230	3.119781	-1.903971
H	-1.555747	2.428407	-2.590995
C	-2.106687	4.475784	-2.231024
H	-1.694115	4.823138	-3.174196
C	-2.709165	5.380267	-1.353003
H	-2.765159	6.434394	-1.609059
C	-3.243004	4.922791	-0.144610
H	-3.716512	5.619573	0.541370
C	-3.170872	3.568989	0.186911
H	-3.588622	3.224118	1.128830
C	-3.894540	0.422855	0.621672
C	-3.837431	-0.274792	1.837679
H	-2.872826	-0.478293	2.294231
C	-5.010743	-0.707851	2.459768

H	-4.955255	-1.252366	3.397984
C	-6.250195	-0.433996	1.877099
H	-7.163734	-0.768663	2.360177
C	-6.316598	0.284967	0.678716
H	-7.280512	0.513154	0.232923
C	-5.145764	0.716551	0.054812
H	-5.204912	1.291730	-0.864092
C	2.913317	-0.568780	0.534117
C	3.978935	0.105338	1.141629
C	2.472746	-1.780417	1.082415
C	4.601024	-0.426545	2.274699
C	3.091301	-2.312986	2.212213
C	4.158989	-1.638250	2.811540
H	4.320763	1.048356	0.724466
H	1.636668	-2.299811	0.627808
H	5.426980	0.106721	2.737419
H	2.727691	-3.245095	2.634416
H	4.637978	-2.051861	3.694605
C	3.102216	-2.103791	-2.003078
C	4.459790	-2.347556	-1.759168
C	2.219958	-3.184725	-2.110027
C	4.925587	-3.653221	-1.603612
C	2.687356	-4.492498	-1.958942
C	4.039045	-4.730205	-1.699990
H	5.148170	-1.510577	-1.674530
H	1.170553	-3.006131	-2.314310
H	5.979630	-3.830397	-1.409526
H	1.993339	-5.324473	-2.041409
H	4.401662	-5.747101	-1.580001
H	5.078725	1.808475	-3.416465
C	5.202435	2.729964	-1.469139
C	4.559568	2.396883	-2.665177
C	3.247491	2.823420	-2.892986
H	2.740601	2.558594	-3.816485
C	2.580376	3.578096	-1.926101
H	1.553716	3.891258	-2.089280
H	1.568269	5.148212	-0.071687
C	2.510477	4.749026	0.310603
H	3.134132	5.568553	0.670953
C	3.222919	3.926383	-0.731368
H	5.040861	3.765342	0.416349
C	4.538088	3.497499	-0.509580
H	6.221618	2.400915	-1.288018
O	2.226396	3.988555	1.534770
C	1.259664	3.077878	1.448886
C	-0.287923	3.309584	3.357197
H	-0.553694	2.938204	4.350530
H	-1.152952	3.207137	2.695274
H	-0.018703	4.367140	3.433260
C	0.895284	2.490429	2.804623
H	1.753714	2.579054	3.477595
N	0.492718	1.081059	2.651740
C	0.722263	0.330437	3.674539
H	1.245596	0.761323	4.534134
C	0.353678	-1.076190	3.828796
C	-0.373471	-1.811887	2.874702
H	-0.711203	-1.330254	1.962155
H	-1.202502	-3.717985	2.336501
C	-0.647400	-3.160088	3.083769

C	-0.201655	-3.797539	4.247612
H	-0.413434	-4.851327	4.404026
C	0.513538	-3.076464	5.207325
H	0.859828	-3.565915	6.112592
C	0.786171	-1.725729	4.999798
H	1.348891	-1.165987	5.742293
O	0.670656	2.800506	0.416576

Int1_A_kOi_Cu

Charge	1
Electronic Energy, BS1 (a.u.)	-3084.091528
Thermal and entropic correction, BS1 (a.u.)	0.790204
Electronic Energy, BS2 (a.u.)	-5668.094387
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-3.9i

Molecular Geometry in Cartesian Coordinates

Cu	0.436009	-0.547091	0.859758
Fe	0.685958	2.960584	-1.643741
P	2.327064	0.273160	-0.063359
C	1.795271	1.232086	-1.515818
C	0.560006	1.003254	-2.244763
C	0.563688	1.856202	-3.398517
H	-0.241385	1.936581	-4.114591
C	1.772395	2.601661	-3.391429
H	2.046757	3.366661	-4.105077
C	2.528306	2.221184	-2.246142
H	3.484359	2.629768	-1.951315
C	0.291523	3.687645	0.258094
H	0.617346	3.217860	1.173254
C	-0.929909	3.427728	-0.433976
H	-1.689032	2.716873	-0.137870
C	-0.947025	4.232192	-1.614497
H	-1.721093	4.238008	-2.370172
C	0.266183	4.986071	-1.650706
H	0.571229	5.659219	-2.440943
C	1.033019	4.647706	-0.494419
H	2.019973	5.017899	-0.251287
O	-1.435496	-0.077946	-2.903202
C	-0.553992	0.126612	-1.900849
N	-0.806003	-0.461937	-0.779168
C	-2.005520	-1.307885	-0.979988
C	-2.587861	-0.771568	-2.337329
H	-2.813882	-1.609612	-2.998207
H	-1.649413	-2.323610	-1.150427
C	3.543127	-0.907358	-0.778100
C	3.683557	-1.093602	-2.162096
H	3.112185	-0.488542	-2.857709
C	4.561251	-2.061178	-2.657769
H	4.658825	-2.196353	-3.731223
C	5.310111	-2.846865	-1.779719
H	5.992160	-3.598403	-2.166833
C	5.177977	-2.663413	-0.400149
H	5.754467	-3.273106	0.289590
C	4.296434	-1.705682	0.099207
H	4.190573	-1.585363	1.171617
C	3.327878	1.430273	0.942832

C	2.779871	1.884999	2.152393
H	1.807719	1.517915	2.471929
C	3.478041	2.800790	2.942229
H	3.045369	3.150736	3.875072
C	4.734349	3.256494	2.534391
H	5.280866	3.965544	3.149564
C	5.295289	2.790491	1.340562
H	6.277301	3.135084	1.029285
C	4.597884	1.878337	0.547326
H	5.043362	1.508694	-0.371524
C	-2.945767	-1.327358	0.197489
C	-3.483763	-2.545661	0.628914
C	-3.320682	-0.147292	0.850375
C	-4.389731	-2.583313	1.692219
C	-4.225409	-0.180919	1.910002
C	-4.763019	-1.399619	2.333928
H	-3.190093	-3.464644	0.128328
H	-2.899129	0.796799	0.525888
H	-4.800046	-3.534783	2.019054
H	-4.495314	0.741486	2.414282
H	-5.464965	-1.426145	3.162795
C	-3.763236	0.172234	-2.246177
C	-5.054621	-0.358852	-2.136429
C	-3.587349	1.559870	-2.198908
C	-6.151628	0.484228	-1.957557
C	-4.686168	2.404367	-2.024049
C	-5.969875	1.869236	-1.896376
H	-5.197544	-1.435607	-2.172229
H	-2.594260	1.980942	-2.302622
H	-7.147876	0.060852	-1.866709
H	-4.536613	3.479906	-1.985772
H	-6.823991	2.525711	-1.756894
H	-0.568858	-3.077024	-4.483540
C	-1.348812	-4.367204	-2.939092
C	-0.436788	-3.453719	-3.473487
C	0.649242	-3.026032	-2.702957
H	1.366563	-2.322998	-3.113843
C	0.822471	-3.501756	-1.402874
H	1.673786	-3.171476	-0.816463
H	0.991171	-5.459922	0.684466
C	0.054634	-4.911888	0.557487
H	-0.781573	-5.555007	0.835201
C	-0.101555	-4.403396	-0.852027
H	-1.902146	-5.531618	-1.209760
C	-1.183376	-4.833926	-1.631664
H	-2.193421	-4.707019	-3.531624
O	0.024462	-3.827542	1.537409
C	1.206873	-3.359031	1.972669
C	2.369730	-1.802806	3.588359
H	2.218156	-1.221627	4.501957
H	2.799678	-1.146823	2.827707
H	3.069902	-2.615564	3.792233
C	1.025495	-2.356854	3.114178
H	0.553967	-2.925350	3.927690
N	0.146141	-1.226036	2.732491
C	-0.577966	-0.768420	3.697683
H	-0.597388	-1.328442	4.638113
C	-1.367537	0.460350	3.715618
C	-1.227100	1.503351	2.781906

H	-0.508974	1.418274	1.972807
H	-1.874651	3.461681	2.183325
C	-1.998132	2.656826	2.899569
C	-2.924418	2.783883	3.940592
H	-3.522960	3.686223	4.025115
C	-3.068609	1.756830	4.877400
H	-3.781880	1.853735	5.690256
C	-2.286758	0.609358	4.771426
H	-2.389224	-0.187581	5.503504
O	2.288022	-3.732379	1.563432

TS45_A_OEther_Cu

Charge	0
Electronic Energy, BS1 (a.u.)	-3387.904447
Thermal and entropic correction, BS1 (a.u.)	0.825534
Electronic Energy, BS2 (a.u.)	-5972.045807
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-1240.7i

Molecular Geometry in Cartesian Coordinates

Cu	0.238806	-0.768942	0.271653
Fe	3.174712	2.296805	-0.767666
P	2.201459	-1.028192	-0.777117
C	2.588310	0.530489	-1.639185
C	1.629347	1.587105	-1.908309
C	2.306061	2.626849	-2.628740
H	1.858820	3.559877	-2.940560
C	3.660778	2.234661	-2.799838
H	4.437544	2.828076	-3.263189
C	3.835379	0.953849	-2.200929
H	4.762416	0.401930	-2.140343
C	3.080717	2.082072	1.284801
H	2.628826	1.235475	1.779490
C	2.404134	3.274624	0.888976
H	1.353354	3.484461	1.032112
C	3.342553	4.114580	0.216244
H	3.126539	5.072396	-0.238475
C	4.603048	3.440874	0.199839
H	5.508630	3.799782	-0.271310
C	4.441584	2.184339	0.859703
H	5.198271	1.420256	0.975455
O	-0.515313	2.555111	-2.193113
C	0.234136	1.678360	-1.484655
N	-0.351921	1.050112	-0.525990
C	-1.774646	1.435013	-0.532231
C	-1.814004	2.652557	-1.534403
H	-2.574629	2.480053	-2.297077
H	-2.332720	0.601855	-0.970490
C	1.943666	-2.242594	-2.136559
C	2.226630	-1.986236	-3.484843
H	2.675035	-1.042577	-3.779511
C	1.923507	-2.941612	-4.460349
H	2.142855	-2.732289	-5.503750
C	1.341130	-4.157907	-4.097738
H	1.102429	-4.895534	-4.858701
C	1.058918	-4.421532	-2.752724
H	0.594407	-5.360364	-2.464561

C	1.352011	-3.467236	-1.780080
H	1.098268	-3.658171	-0.740618
C	3.811559	-1.518134	-0.038450
C	3.981799	-1.366932	1.345702
H	3.160119	-1.008044	1.955516
C	5.202360	-1.686083	1.945453
H	5.318800	-1.565774	3.018422
C	6.258879	-2.167430	1.168586
H	7.207378	-2.418576	1.635011
C	6.089312	-2.341225	-0.209099
H	6.904321	-2.728949	-0.813911
C	4.870922	-2.022647	-0.810685
H	4.742185	-2.170921	-1.878957
C	-2.317253	1.715289	0.849163
C	-3.694702	1.617320	1.079325
C	-1.477205	2.107825	1.897836
C	-4.226744	1.924930	2.332105
C	-2.005728	2.396540	3.158125
C	-3.383347	2.313043	3.376763
H	-4.348099	1.289763	0.276186
H	-0.408091	2.171264	1.726198
H	-5.296689	1.838033	2.497913
H	-1.341574	2.689024	3.966913
H	-3.795681	2.539841	4.355917
C	-1.981528	4.020742	-0.921260
C	-3.273455	4.518570	-0.710300
C	-0.880028	4.776811	-0.503479
C	-3.462433	5.745162	-0.072202
C	-1.068772	6.006906	0.130510
C	-2.359830	6.491922	0.352988
H	-4.131675	3.937484	-1.037394
H	0.124438	4.409609	-0.682624
H	-4.469539	6.118967	0.089609
H	-0.205864	6.584950	0.449985
H	-2.506624	7.447485	0.848423
H	-6.032184	1.453229	-2.206469
C	-5.595922	-0.523975	-1.452512
C	-5.410665	0.567603	-2.307565
C	-4.418119	0.514345	-3.291487
H	-4.267047	1.357907	-3.959828
C	-3.607040	-0.618015	-3.409273
H	-2.816565	-0.644842	-4.155394
H	-2.031508	-2.736534	-3.276444
C	-2.923857	-2.945551	-2.680357
H	-3.471011	-3.771730	-3.142954
C	-3.795051	-1.714772	-2.560610
H	-4.939952	-2.508965	-0.921500
C	-4.799737	-1.663200	-1.586481
H	-6.351242	-0.490954	-0.672751
O	-2.537909	-3.477355	-1.390169
C	-1.721613	-2.683080	-0.657322
C	-1.574025	-4.634473	0.989434
H	-1.865924	-4.831865	2.026274
H	-0.611301	-5.134726	0.808024
H	-2.330739	-5.089771	0.350779
C	-1.499323	-3.140492	0.710533
H	-2.647986	-2.722837	1.467704
N	-0.510899	-2.362896	1.383399
C	0.029413	-2.780748	2.484532

H	-0.158680	-3.788986	2.856926
C	0.909507	-1.945767	3.309088
C	0.795280	-0.542031	3.338603
H	0.007963	-0.059398	2.768492
H	1.554557	1.304746	4.136368
C	1.660449	0.223663	4.119367
C	2.654800	-0.395439	4.884639
H	3.330864	0.203005	5.488445
C	2.760402	-1.790305	4.882742
H	3.522724	-2.279057	5.482909
C	1.888125	-2.558852	4.112044
H	1.974633	-3.642564	4.111473
O	-5.040511	-3.648863	1.126841
C	-4.988649	-2.592810	1.721694
O	-5.650843	-1.625503	2.029494
O	-3.428559	-2.474074	2.329027
C	-3.052362	-1.284631	3.031324
H	-2.475421	-0.616202	2.386880
H	-3.957845	-0.770953	3.354979
H	-2.448695	-1.563857	3.901692
O	-1.281891	-1.631100	-1.140302

CO2

Charge	0
Electronic Energy, BS1 (a.u.)	-188.575589
Thermal and entropic correction, BS1 (a.u.)	-0.006986
Electronic Energy, BS2 (a.u.)	-188.669139
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

O	1.152839	0.002447	0.000000
C	-0.000000	0.000681	0.000000
O	-1.152839	-0.002958	-0.000000

45_MeOCO2

Charge	-1
Electronic Energy, BS1 (a.u.)	-303.817307
Thermal and entropic correction, BS1 (a.u.)	0.025829
Electronic Energy, BS2 (a.u.)	-303.791447
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

O	0.472485	1.298759	0.000026
C	0.650131	0.061889	-0.000003
O	1.687813	-0.625748	-0.000019
O	-0.539871	-0.750222	0.000028
C	-1.759400	-0.033323	-0.000058
H	-2.567895	-0.775402	0.001066
H	-1.869614	0.611531	0.883540
H	-1.870296	0.610161	-0.884512

MeOCO2H

Charge	0
Electronic Energy, BS1 (a.u.)	-304.314786
Thermal and entropic correction, BS1 (a.u.)	0.038855
Electronic Energy, BS2 (a.u.)	-304.275870
Number of Imaginary Frequencies	0
Imaginary frequencies (cm-1)	None

Molecular Geometry in Cartesian Coordinates

H	1.501082	-1.487327	0.001555
O	1.677293	-0.530371	-0.000031
C	0.515999	0.141409	-0.000072
O	0.455911	1.349017	0.000027
O	-0.528591	-0.704286	-0.000402
C	-1.829233	-0.076722	0.000192
H	-2.548167	-0.896097	0.002430
H	-1.954113	0.541744	0.892642
H	-1.956299	0.538674	-0.894099

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