SUPPORTING INFORMATION

Dissociation of dinitrogen on iron clusters: A detailed study of the Fe_{16} + N_2 case

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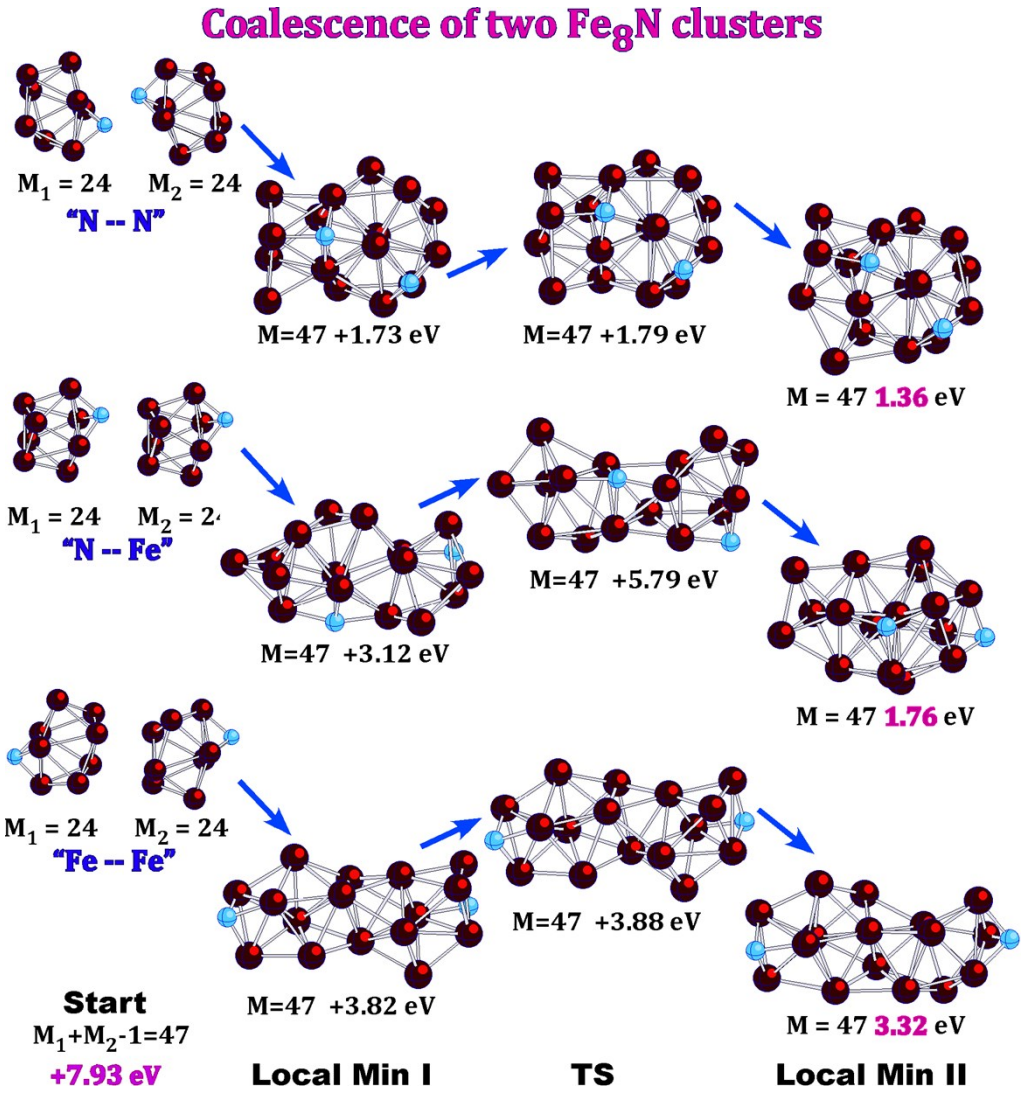


Figure S1. Coalescence pathways of two ground-state Fe_8N clusters via transition states. Local minima were found using the Intrinsic Reaction Coordinate (IRC) method. All total energies are given with respect to the total energy of the ground-state $Fe_{16}N_2$ cluster.

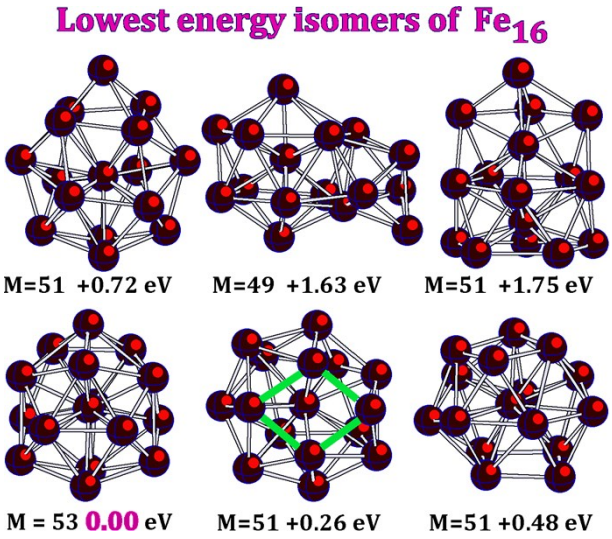


Figure S2. The lowest energy isomers of the Fe_{16} cluster. The spin multiplicities in all cases correspond to the lowest energy states among other states of an isomer with a given geometrical topology.

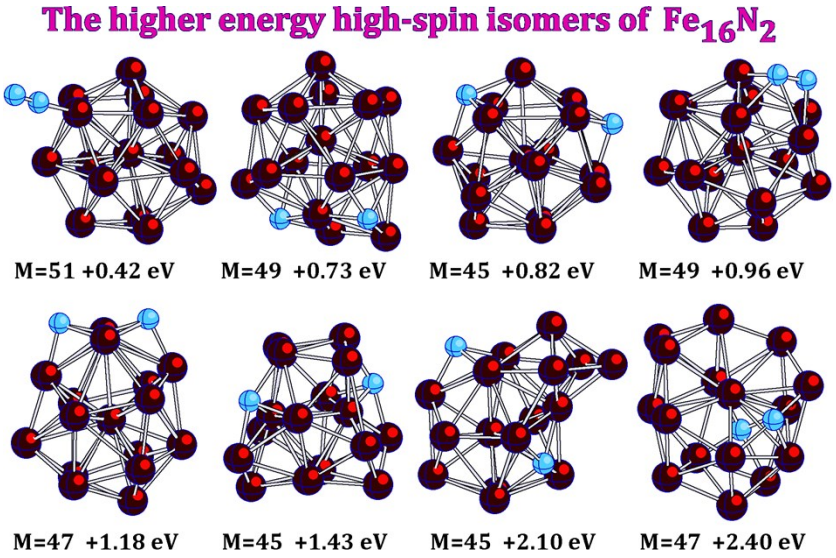


Figure S3. Some of higher energy representative isomers of $Fe_{16}N_2$. The spin multiplicities in all cases correspond to the lowest energy states among other states of an isomer with a given geometrical topology.

Table S1. Static electric polarizability of the Fe atom (Units: $Bohr^3$) computed using three basis set of an increasing quality and eight methods belonging to various groups.

Basis	BPW91	BLYP	B3LYP	CAM-B3LYP	ωB97XD	LC-BLYP	LC-BPW91	MP4
6-311+G*	57.32	56.27	60.14	60.87	61.50	61.23	64.02	62.22
6-311+G(3df)	57.57	56.47	60.27	61.05	61.57	61.42	63.98	53.74
aug-cc-PVQZ	59.68	58.43	61.63	62.08	62.19	61.29	64.69	51.38

The literature data are in the range 57–63.93 $Bohr^3$ collected by P. Schwerdtfeger in "Table of experimental and calculated static dipole polarizabilities for the electronic ground states of the neutral elements (in atomic units)", Massey University, Centre for Theoretical Chemistry and Physics, 2015.

Table S1A. Static electric polarizability of the Fe atom in $Å^3$

Basis	BPW91	BLYP	B3LYP	CAM-B3LYP	ωB97XD	LC-BLYP	LC-BPW91	MP4
6-311+G*	8.49	8.33	8.91	9.01	9.11	9.07	9.48	9.22
6-311+G(3df)	8.53	8.36	8.93	9.04	9.12	9.10	9.48	7.96
aug-cc-PVQZ	8.84	8.65	9.13	9.19	9.21	9.08	9.58	7.61

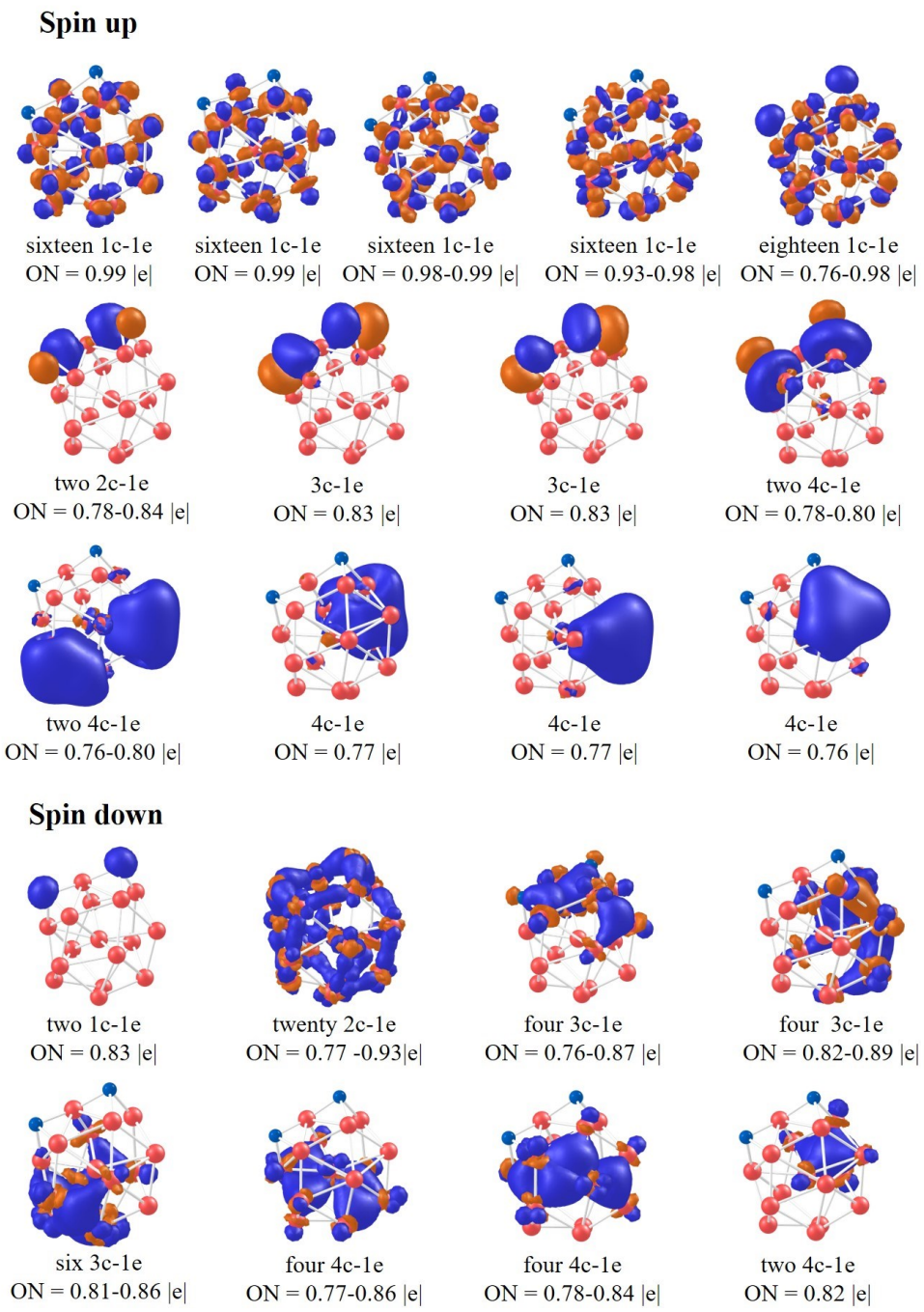


Figure S4. The results of our AdNDP analysis for the ground-state $Fe_{16}N_2^-$ cluster in both spin-up and spin-down representations. ON denotes the occupation number**.**

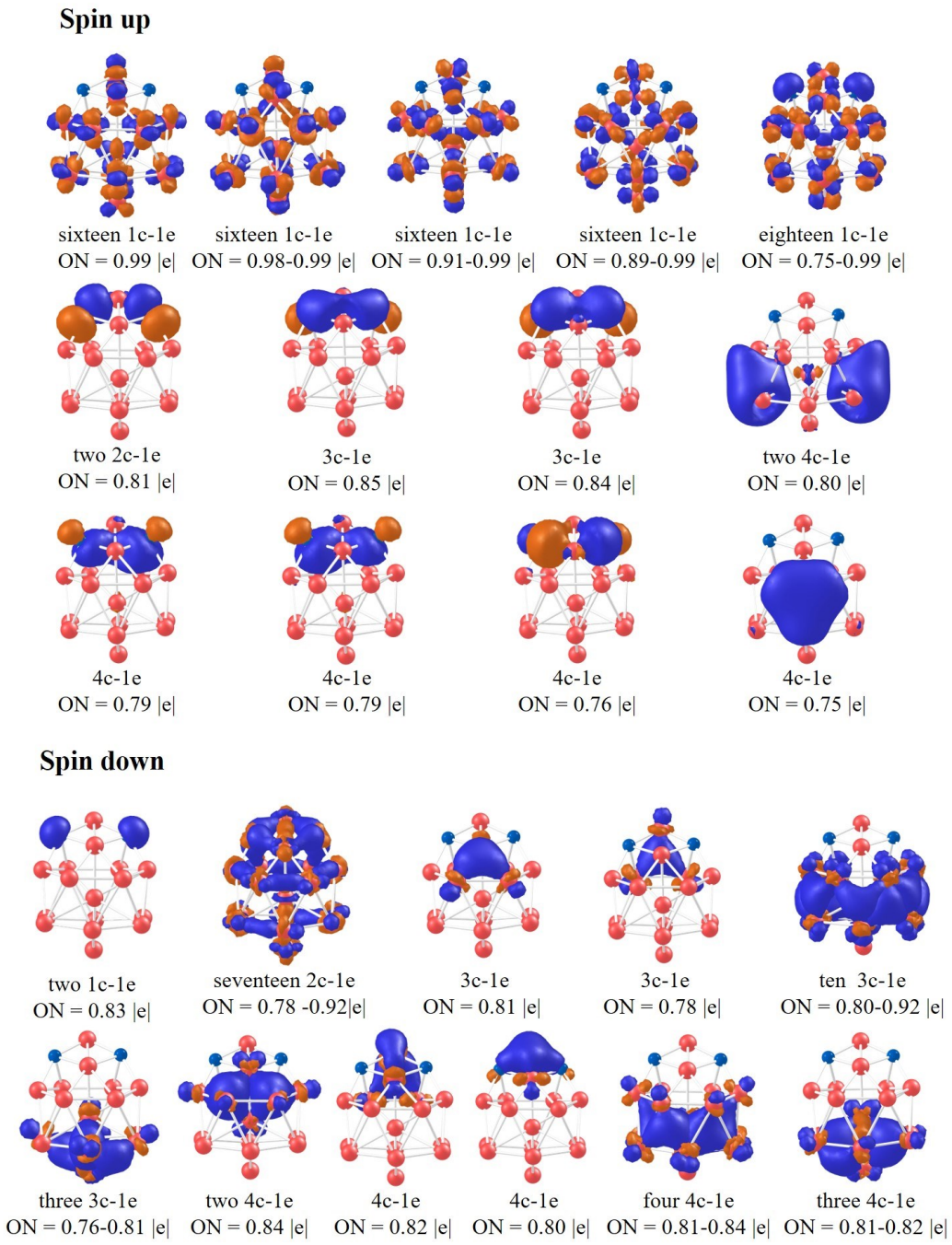


Figure S5. The results of our AdNDP analysis for the ground-state $Fe_{16}N_2^+$ cluster in both spin-up and spin-down representations. ON denotes the occupation number**.**

EXCERPTS from the OUTPUTS for the GROUND STATES of $Fe_{16}N_2$, $Fe_{16}N_2^-$, and $Fe_{16}N_2^+$,

FREQ=RAMAN

NEUTRAL

$$$$$$$$$$$$$ Fe16N2 NEUTRAL S = 47

 # UBPW91/6-311+G* scf=(VSHIFT=5,NoIncFock,MAXCYC=200,Tight,NoVarAcc) NOSYMM OPT=(RFO,MaxCyc=100) IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GU ESS=READ GEOM=CHECKPOINT

Charge = 0 Multiplicity = 47

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.276518	-0.356750	-0.131151
2	26	0	-2.661476	-0.425341	-1.136041
3	26	0	-2.555406	-0.003658	1.090930
4	26	0	2.299896	-0.406861	-0.388035
5	26	0	1.057249	-0.270742	-2.377467
6	26	0	0.817101	1.617991	-0.711528
7	26	0	1.149040	-2.094256	1.232279
8	26	0	1.390829	0.275956	1.760656
9	26	0	1.059411	-2.428673	-1.005040
10	26	0	1.418653	2.663772	1.289012
11	26	0	-0.596413	1.385986	1.766314
12	26	0	-1.690532	1.837310	-0.346967
13	26	0	-1.357179	-2.325574	0.285775
14	26	0	-0.916610	-1.724470	-2.087900
15	26	0	-0.742168	-1.052300	2.276804
16	26	0	-0.988794	0.855393	-2.344862
17	7	0	2.353204	1.343342	0.462563
18	7	0	-0.213050	2.778597	0.481463

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.588925	0.000000			
3	Fe	2.609882	2.269024	0.000000		
4	Fe	2.589674	5.017477	5.091549	0.000000	
5	Fe	2.613860	3.923513	5.015215	2.349583	0.000000
6	Fe	2.330760	4.056589	4.153601	2.530486	2.529888
7	Fe	2.628704	4.786883	4.255996	2.607142	4.045231

```
 8  Fe   2.599865   5.030293   4.012416   2.430950   4.187388
 9  Fe   2.615580   4.227944   4.831221   2.450963   2.557387
10  Fe   3.743531   5.663123   4.790362   3.608028   4.710101
11  Fe   2.596120   3.996130   2.494976   4.030400   4.759229
12  Fe   2.619143   2.585529   2.490927   4.578374   4.014612
13  Fe   2.284277   2.708070   2.734103   4.184456   4.140610
14  Fe   2.471688   2.374517   3.968855   3.869308   2.468460
15  Fe   2.549288   3.965392   2.407027   4.095377   5.050838
16  Fe   2.622431   2.428867   3.872585   4.029633   2.335708
17  N    3.187201   5.552548   5.128714   1.946682   3.514333
18  N    3.195266   4.344690   3.687685   4.149466   4.368707
           6          7          8          9         10
 6  Fe   0.000000
 7  Fe   4.203493   0.000000
 8  Fe   2.870874   2.440400   0.000000
 9  Fe   4.064524   2.263949   3.882517   0.000000
10  Fe   2.336169   4.765999   2.434110   5.596850   0.000000
11  Fe   2.862089   3.929871   2.276253   4.997378   2.433321
12  Fe   2.543468   5.100431   4.046565   5.117994   3.609225
13  Fe   4.612354   2.688960   4.061376   2.741668   5.797009
14  Fe   4.009015   3.927753   4.912979   2.360752   6.009465
15  Fe   4.300221   2.398619   2.565219   3.988809   4.410678
16  Fe   2.551586   5.105556   4.780547   4.095773   4.719225
17  N    1.952827   3.722843   1.936628   4.249219   1.816573
18  N    1.957407   5.115047   3.236043   5.562779   1.824219
           11         12         13         14         15
11  Fe   0.000000
12  Fe   2.422137   0.000000
13  Fe   4.067731   4.223872   0.000000
14  Fe   4.963107   4.039317   2.487923   0.000000
15  Fe   2.495412   4.016642   2.442061   4.419602   0.000000
16  Fe   4.163804   2.334134   4.144214   2.593633   5.005988
17  N    3.225186   4.153450   5.221029   5.158296   4.314151
18  N    1.933178   1.937852   5.234490   5.232039   4.263682
           16         17         18
16  Fe   0.000000
17  N    4.391888   0.000000
18  N    3.505511   2.940403   0.000000
 Alpha  occ. eigenvalues --   -0.17272  -0.17100  -0.17079  -0.16893  -0.16446
 Alpha  occ. eigenvalues --   -0.15915  -0.15215  -0.14606
 Alpha virt. eigenvalues --   -0.12415  -0.12243  -0.11668  -0.10629  -0.09566
  Beta  occ. eigenvalues --   -0.16398  -0.15821  -0.15144  -0.14499  -0.14421
  Beta  occ. eigenvalues --   -0.14289  -0.14149
  Beta virt. eigenvalues --   -0.12734  -0.12656  -0.12458  -0.12366  -0.12315
Mulliken charges and spin densities:
           1          2
 1  Fe  12.062233  -6.300986   central atom
 2  Fe  -0.778954   3.739005
 3  Fe  -0.809404   3.743566
```

4	Fe	-0.376567	3.391619
5	Fe	-0.793799	3.730595
6	Fe	-1.134690	2.983292
7	Fe	-0.778748	3.722573
8	Fe	-0.716490	3.137268
9	Fe	-0.761071	3.699880
10	Fe	0.199548	2.101952
11	Fe	-0.685076	3.130998
12	Fe	-0.338907	3.329713
13	Fe	-1.053737	4.350468
14	Fe	-0.944671	3.738462
15	Fe	-1.039807	3.736648
16	Fe	-0.776468	3.715070
17	N	-0.636638	0.026341
18	N	-0.636753	0.023537

Sum of Mulliken charges = 0.00000 46.00000
Dipole moment (field-independent basis, Debye):
X= -0.8708 Y= -1.5518 Z= -0.2155 Tot= 1.7924

Isotropic polarizability for W= 0.000000 506.77 Bohr**3.

Frequencies --	46.7073	60.1268	90.7130
Frequencies --	97.2905	105.3613	108.5591
Frequencies --	112.0586	119.0071	121.6650
Frequencies --	127.8349	130.5781	136.1528
Frequencies --	140.6685	150.1279	157.0332
Frequencies --	161.2617	167.7847	169.8518
Frequencies --	174.8961	182.2319	188.9921
Frequencies --	191.1971	197.7397	202.1621
Frequencies --	203.7746	210.1538	216.6002
Frequencies --	218.5802	236.6436	246.8283
Frequencies --	248.4966	250.8244	256.2954
Frequencies --	259.0904	259.5437	272.7784
Frequencies --	282.7379	284.0892	293.7785
Frequencies --	297.1534	310.3538	335.4606
Frequencies --	354.9961	362.1050	461.3561
Frequencies --	476.4115	569.5918	589.8861

Zero-point vibrational energy 64822.8 (Joules/Mol)
15.49303 (Kcal/Mol) 0.672 eV

IR Intensities

IR Inten --	0.0085	0.0048	0.0123
IR Inten --	0.2092	0.2391	0.0539
IR Inten --	0.1321	0.7571	0.1177
IR Inten --	0.2744	0.0542	0.1301
IR Inten --	0.0933	0.0829	0.2028
IR Inten --	0.2707	0.0784	0.1203
IR Inten --	0.1889	0.3563	1.2976
IR Inten --	1.0931	0.8320	0.1243

IR Inten	--	0.5161	0.6725	0.8302
IR Inten	--	0.6924	0.5184	0.6585
IR Inten	--	0.4513	0.1018	0.0924
IR Inten	--	0.1672	0.0693	0.2737
IR Inten	--	0.6071	0.4382	0.3940
IR Inten	--	0.1177	0.9535	0.4615
IR Inten	--	4.5235	1.7532	22.4289
IR Inten	--	3.5339	4.7422	7.3316

Raman Activities

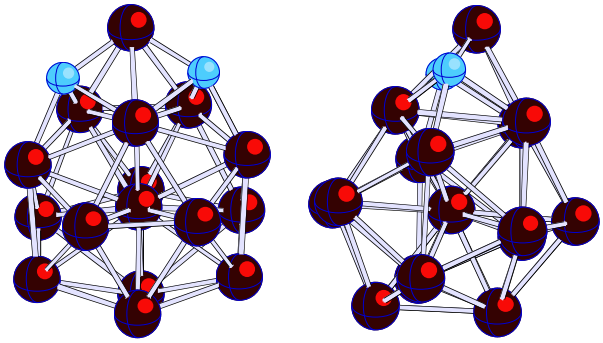
Raman Activ --	0.4442	3.6080	9.6426
Raman Activ --	15.3020	7.7457	2.4052
Raman Activ --	8.3678	4.1329	6.6967
Raman Activ --	7.5945	3.7016	0.7381
Raman Activ --	2.1469	6.4427	2.3070
Raman Activ --	14.6738	3.0050	3.5321
Raman Activ --	0.6136	2.1857	0.7302
Raman Activ --	2.6198	14.5023	2.3455
Raman Activ --	0.7762	3.3429	2.3339
Raman Activ --	3.1471	1.6147	4.7457
Raman Activ --	29.6009	23.4453	9.1802
Raman Activ --	30.9243	26.5101	4.5785
Raman Activ --	6.5295	4.0796	1.4964
Raman Activ --	6.8968	3.7685	6.8934
Raman Activ --	12.4889	5.4171	3.5274
Raman Activ --	0.3360	1.7964	4.9155

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.43)3d(7.42)4p(1.68)4d(0.05)5p(0.01)
Fe	2	[core]4S(0.50)3d(6.96)4p(0.42)4d(0.01)
Fe	3	[core]4S(0.47)3d(6.95)4p(0.37)4d(0.01)5p(0.01)
Fe	4	[core]4S(0.33)3d(6.92)4p(0.51)4d(0.02)5p(0.01)
Fe	5	[core]4S(0.46)3d(6.93)4p(0.35)4d(0.01)5p(0.01)
Fe	6	[core]4S(0.24)3d(7.02)4p(0.65)4d(0.04)5p(0.01)
Fe	7	[core]4S(0.47)3d(6.95)4p(0.37)4d(0.01)5p(0.01)
Fe	8	[core]4S(0.35)3d(6.94)4p(0.56)4d(0.02)5p(0.01)
Fe	9	[core]4S(0.51)3d(6.97)4p(0.41)4d(0.01)
Fe	10	[core]4S(0.26)3d(6.93)4p(0.28)4d(0.02)
Fe	11	[core]4S(0.35)3d(6.94)4p(0.56)4d(0.02)5p(0.01)
Fe	12	[core]4S(0.33)3d(6.92)4p(0.50)4d(0.02)5p(0.01)
Fe	13	[core]4S(0.37)3d(6.96)4p(0.39)4d(0.01)5p(0.01)
Fe	14	[core]4S(0.43)3d(7.03)4p(0.45)4d(0.01)
Fe	15	[core]4S(0.48)3d(6.99)4p(0.37)4d(0.01)5p(0.01)
Fe	16	[core]4S(0.46)3d(6.93)4p(0.35)4d(0.01)5p(0.01)
N	17	[core]2S(1.56)2p(4.13)3S(0.01)3p(0.02)
N	18	[core]2S(1.56)2p(4.14)3S(0.01)3p(0.02)

```
************************************************
*******        Alpha spin orbitals        *******
************************************************
  Atom  No         Natural Electron Configuration
--------------------------------------------------------------------------
   Fe    1     [core]4S( 0.21)3d( 4.90)4p( 0.84)4d( 0.03)
   Fe    2     [core]4S( 0.33)3d( 4.93)4p( 0.26)4d( 0.01)   5.53
   Fe    3     [core]4S( 0.29)3d( 4.93)4p( 0.23)4d( 0.01)   5.46
   Fe    4     [core]4S( 0.21)3d( 4.81)4p( 0.29)4d( 0.01)   5.32
   Fe    5     [core]4S( 0.29)3d( 4.93)4p( 0.21)4d( 0.01)
   Fe    6     [core]3d( 4.61)4p( 0.35)5S( 0.13)4d( 0.03)  5.12
   Fe    7     [core]4S( 0.29)3d( 4.93)4p( 0.22)4d( 0.01)
   Fe    8     [core]3d( 4.76)4p( 0.31)5S( 0.22)4d( 0.02)
   Fe    9     [core]4S( 0.34)3d( 4.92)4p( 0.25)4d( 0.01)
   Fe   10      [core]3d( 4.45)4p( 0.17)5S( 0.16)4d( 0.01)  4.79
   Fe   11      [core]3d( 4.75)4p( 0.31)5S( 0.22)4d( 0.02)
   Fe   12      [core]4S( 0.21)3d( 4.81)4p( 0.29)4d( 0.01)
   Fe   13      [core]4S( 0.23)3d( 4.94)4p( 0.21)4d( 0.01)
   Fe   14      [core]4S( 0.27)3d( 4.92)4p( 0.27)4d( 0.01)  3.0
   Fe   15      [core]4S( 0.31)3d( 4.92)4p( 0.21)4d( 0.01)
   Fe   16      [core]4S( 0.29)3d( 4.93)4p( 0.21)4d( 0.01)
    N   17     [core]2S( 0.79)2p( 2.08)4p( 0.01)
    N   18     [core]2S( 0.79)2p( 2.07)4p( 0.01)


************************************************
*******        Beta  spin orbitals        *******
************************************************
  Atom  No         Natural Electron Configuration
--------------------------------------------------------------------------
   Fe    1     [core]4S( 0.22)3d( 2.52)4p( 0.84)4d( 0.02)
   Fe    2     [core]4S( 0.18)3d( 2.04)4p( 0.16)   2.38 diff
   Fe    3     [core]4S( 0.17)3d( 2.03)4p( 0.14)    2,34   difference  3.12 MuB
   Fe    4     [core]4S( 0.12)3d( 2.11)4p( 0.21)4d( 0.01)   2.45   difference   2.87 MuB
   Fe    5     [core]4S( 0.17)3d( 2.00)4p( 0.14)
   Fe    6     [core]3d( 2.41)4p( 0.30)5S( 0.11)4d( 0.01)  2.83  difference 2.29 MuB
   Fe    7     [core]4S( 0.18)3d( 2.02)4p( 0.14)
   Fe    8     [core]3d( 2.18)4p( 0.25)5S( 0.14)4d( 0.01)
   Fe    9     [core]4S( 0.18)3d( 2.04)4p( 0.16)
   Fe   10      [core]3d( 2.48)4p( 0.11)5S( 0.10)4d( 0.01)   2.70 difference  2.1
   Fe   11      [core]3d( 2.19)4p( 0.25)5S( 0.13)4d( 0.01)
   Fe   12      [core]4S( 0.12)3d( 2.11)4p( 0.21)4d( 0.01)
   Fe   13      [core]4S( 0.14)3d( 2.02)4p( 0.18)
   Fe   14      [core]4S( 0.16)3d( 2.11)4p( 0.18)
   Fe   15      [core]4S( 0.17)3d( 2.07)4p( 0.16)
   Fe   16      [core]4S( 0.17)3d( 2.00)4p( 0.14)
    N   17     [core]2S( 0.77)2p( 2.06)4p( 0.01)
    N   18     [core]2S( 0.77)2p( 2.06)
```

HF= -20331.365856\S2=552.55072\S2-1=0.\S2A=552.012983



TITLE coordinates
Fe -0.2765183796,-0.3567500138,-0.1311512724
Fe -2.6614764779,-0.4253410333,-1.1360409941
Fe -2.5554059005,-0.0036579323,1.0909303339
Fe 2.2998960966,-0.4068614195,-0.3880345514
Fe 1.0572486016,-0.2707418894,-2.3774666022
Fe 0.8171007545,1.6179909243,-0.7115280446
Fe 1.1490397248,-2.0942562258,1.2322793019
Fe 1.3908288256,0.2759559522,1.7606564497
Fe 1.0594113694,-2.4286733044,-1.0050401688
Fe 1.4186534641,2.6637724064,1.2890123725
Fe -0.5964131378,1.3859859552,1.7663143662
Fe -1.6905322584,1.8373097599,-0.3469668424
Fe -1.3571786446,-2.3255742482,0.2857754042
Fe -0.9166101366,-1.7244700166,-2.0879001105
Fe -0.7421681693,-1.0522999718,2.2768039681
Fe -0.9887937351,0.8553928591,-2.3448621367
N 2.3532038368,1.3433423838,0.4625627425
N -0.2130498335,2.7785968141,0.4814627843
END

FREQ=RAMAN
ANION
$$$$$$$$$$$$$ Fe16N2 ANION S = 48

UBPW91/6-311+G* scf=(VSHIFT=5,NoIncFock,MAXCYC=200,Tight,NoVarAcc) NOSYMM OPT=(RFO,MaxCyc=100) IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine
---
Charge = -1 Multiplicity = 48
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	26	0	0.138121	-0.025486	0.062913
2	26	0	2.466884	1.215678	-0.539363
3	26	0	0.564305	2.081217	-1.402635
4	26	0	-1.052980	-1.765588	1.186600
5	26	0	1.289809	-1.685502	1.796014
6	26	0	0.162546	0.135427	2.745733
7	26	0	-1.027996	-1.782419	-1.587050
8	26	0	-2.546052	-0.455326	-0.361214
9	26	0	0.693306	-2.592194	-0.391978
10	26	0	-1.820094	0.602778	1.704564
11	26	0	-1.624110	1.914019	-0.216206
12	26	0	0.489605	2.051394	1.168880
13	26	0	1.159060	-0.486154	-2.036164
14	26	0	2.571947	-1.133210	-0.189986
15	26	0	-1.116596	0.523904	-2.240629
16	26	0	2.296024	0.546473	1.672595
17	7	0	-2.681243	1.061811	-1.407731
18	7	0	-0.262538	3.093198	-0.164343

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.706725	0.000000			
3	Fe	2.601473	2.261461	0.000000		
4	Fe	2.389424	4.925072	4.910973	0.000000	
5	Fe	2.661894	3.905936	4.994585	2.422077	0.000000
6	Fe	2.687753	4.155571	4.599615	2.742673	2.342749
7	Fe	2.677503	4.722333	4.182956	2.773814	4.102040
8	Fe	2.751260	5.287109	4.146436	2.518289	4.569551
9	Fe	2.665172	4.203235	4.783183	2.494935	2.442378
10	Fe	2.631415	4.877401	4.186386	2.542814	3.862135
11	Fe	2.635345	4.162733	2.494940	3.979140	5.049406
12	Fe	2.379104	2.743383	2.572772	4.116944	3.872728
13	Fe	2.379213	2.616687	2.710441	4.112941	4.017601
14	Fe	2.685986	2.377052	3.979157	3.928739	2.427571
15	Fe	2.680009	4.026685	2.439854	4.122101	5.192951
16	Fe	2.752228	2.317280	3.848549	4.098493	2.451411
17	N	3.360628	5.223117	3.401881	4.168450	5.794908
18	N	3.152517	3.333987	1.800317	5.104669	5.393399

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	4.885543	0.000000			
8	Fe	4.163967	2.359734	0.000000		
9	Fe	4.191282	2.246511	3.880798	0.000000	
10	Fe	2.287644	4.141414	2.431880	4.573895	0.000000
11	Fe	3.889552	3.987257	2.546527	5.070233	2.333907
12	Fe	2.502871	4.959475	4.223748	4.903129	2.778517
13	Fe	4.924017	2.581709	4.066234	2.712135	4.904506
14	Fe	4.004135	3.915718	5.165536	2.387200	5.088517

```
   15  Fe   5.162453   2.398780   2.556254   4.050102   4.008201
   16  Fe   2.423285   5.205587   5.346558   4.084409   4.116628
   17  N    5.118260   3.294697   1.848020   5.076523   3.261698
   18  N    4.171049   5.136309   4.224361   5.769674   3.481521
              11         12         13         14         15
   11  Fe   0.000000
   12  Fe   2.530835   0.000000
   13  Fe   4.101111   4.142418   0.000000
   14  Fe   5.185864   4.040343   2.413153   0.000000
   15  Fe   2.507643   4.066676   2.498126   4.533929   0.000000
   16  Fe   4.561272   2.404510   4.014213   2.523228   5.192284
   17  N    1.806521   4.203864   4.187965   5.822115   1.852344
   18  N    1.801952   1.851636   4.282104   5.088958   3.411986
              16         17         18
   16  Fe   0.000000
   17  N    5.875983   0.000000
   18  N    4.050480   3.394508   0.000000
 Alpha  occ. eigenvalues --   -0.06055  -0.05820  -0.05413  -0.05265  -0.04830
 Alpha  occ. eigenvalues --   -0.04506  -0.03643  -0.03156  -0.02758
 Alpha virt. eigenvalues --   -0.01216  -0.00900   0.00546   0.01499   0.01975
  Beta  occ. eigenvalues --   -0.04985  -0.04735  -0.03506  -0.03274  -0.03169
  Beta  occ. eigenvalues --   -0.02513  -0.02254
  Beta virt. eigenvalues --   -0.01600  -0.01540  -0.01198  -0.01062  -0.00875
Mulliken charges and spin densities:
              1          2
    1  Fe  12.684874  -4.900354
    2  Fe  -0.807165   3.610450
    3  Fe  -0.860207   2.958916
    4  Fe  -1.179847   4.053721
    5  Fe  -0.791393   3.538007
    6  Fe  -0.844009   3.576155
    7  Fe  -0.848476   3.778111
    8  Fe  -0.506123   3.215669
    9  Fe  -0.839420   3.564251
   10  Fe  -1.091854   3.698709
   11  Fe  -0.349922   2.156221
   12  Fe  -0.897294   3.307105
   13  Fe  -1.230492   4.015316
   14  Fe  -0.819690   3.516258
   15  Fe  -0.567225   3.210597
   16  Fe  -0.678024   3.536759
   17  N   -0.660338   0.202038
   18  N   -0.713395  -0.037928
 Sum of Mulliken charges =  -1.00000  47.00000

Isotropic polarizability for W=    0.000000      582.13 Bohr**3.


Frequencies --     47.9329              70.2628              85.5054
```

Frequencies --	90.6831	96.0100	108.1230
Frequencies --	113.1766	118.5622	119.0892
Frequencies --	129.2366	131.0966	136.7786
Frequencies --	142.1057	144.8388	147.8629
Frequencies --	148.4558	155.6278	167.4948
Frequencies --	170.9160	175.1981	178.5960
Frequencies --	185.3350	189.8674	191.8844
Frequencies --	200.2400	209.0132	220.2454
Frequencies --	224.6336	227.3294	229.9864
Frequencies --	236.4185	242.8981	247.1231
Frequencies --	249.2572	268.0715	269.3027
Frequencies --	274.4776	278.5029	285.2213
Frequencies --	290.4914	295.2028	297.2996
Frequencies --	436.5404	443.9635	480.0715
Frequencies --	501.9584	616.4697	635.8137

Zero-point vibrational energy 65227.4 (Joules/Mol)
15.58972 (Kcal/Mol) 0.676 eV

IR intensities

IR Inten --	0.3549	0.4918	0.1466
IR Inten --	0.0378	0.2737	1.1183
IR Inten --	0.1123	1.1590	1.4100
IR Inten --	0.4825	0.2965	0.3593
IR Inten --	2.0449	0.4734	0.1055
IR Inten --	0.9080	0.3841	0.4498
IR Inten --	1.5950	0.6109	0.2407
IR Inten --	0.0102	0.2599	0.1630
IR Inten --	1.0543	0.6296	0.6201
IR Inten --	0.4209	0.6428	0.6955
IR Inten --	1.6545	1.1687	0.9583
IR Inten --	0.8142	0.0176	0.4379
IR Inten --	0.8468	0.2363	0.6082
IR Inten --	0.0086	0.0616	0.3393
IR Inten --	0.4183	8.4234	2.8260
IR Inten --	5.9198	75.9748	12.9937

Raman Activities

Raman Activ --	15.3115	17.1999	10.6652
Raman Activ --	22.9634	6.6535	12.0167
Raman Activ --	3.8229	26.7031	27.9208
Raman Activ --	12.7968	4.4704	14.5816
Raman Activ --	5.8062	11.4989	7.8258
Raman Activ --	5.3520	2.5914	2.6855
Raman Activ --	5.8128	6.2147	3.6793
Raman Activ --	2.4238	2.7574	13.0477
Raman Activ --	1.4304	4.8164	4.3656
Raman Activ --	10.9741	23.4631	13.7121
Raman Activ --	4.4191	48.3939	50.8817
Raman Activ --	82.2336	3.1106	7.0268

Raman Activ --	2.5389	18.7329	8.0184
Raman Activ --	8.0421	34.3314	4.2021
Raman Activ --	3.3307	21.1749	22.3979
Raman Activ --	20.6365	28.4829	29.3611

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.42)3d(7.38)4p(1.62)4d(0.06)
Fe	2	[core]4S(0.47)3d(6.93)4p(0.45)4d(0.01)5p(0.01)
Fe	3	[core]4S(0.32)3d(6.97)4p(0.49)4d(0.02)5p(0.01)
Fe	4	[core]4S(0.46)3d(6.94)4p(0.55)4d(0.01)
Fe	5	[core]4S(0.46)3d(6.99)4p(0.53)4d(0.01)
Fe	6	[core]4S(0.49)3d(6.98)4p(0.45)4d(0.01)
Fe	7	[core]4S(0.49)3d(6.92)4p(0.44)4d(0.02)5p(0.01)
Fe	8	[core]4S(0.36)3d(6.90)4p(0.54)4d(0.02)5p(0.01)
Fe	9	[core]4S(0.45)3d(7.00)4p(0.46)4d(0.01)
Fe	10	[core]4S(0.43)3d(6.89)4p(0.38)4d(0.02)5p(0.01)
Fe	11	[core]4S(0.26)3d(7.06)4p(0.60)4d(0.04)5p(0.01)
Fe	12	[core]4S(0.33)3d(6.95)4p(0.59)4d(0.03)5p(0.01)
Fe	13	[core]4S(0.46)3d(6.94)4p(0.51)4d(0.01)5p(0.01)
Fe	14	[core]4S(0.51)3d(6.99)4p(0.51)4d(0.01)
Fe	15	[core]4S(0.35)3d(6.88)4p(0.50)4d(0.02)5p(0.01)
Fe	16	[core]4S(0.51)3d(6.95)4p(0.51)4d(0.01)
N	17	[core]2S(1.61)2p(4.05)3p(0.01)
N	18	[core]2S(1.59)2p(3.97)3p(0.01)

****
******* Alpha spin orbitals *******
****

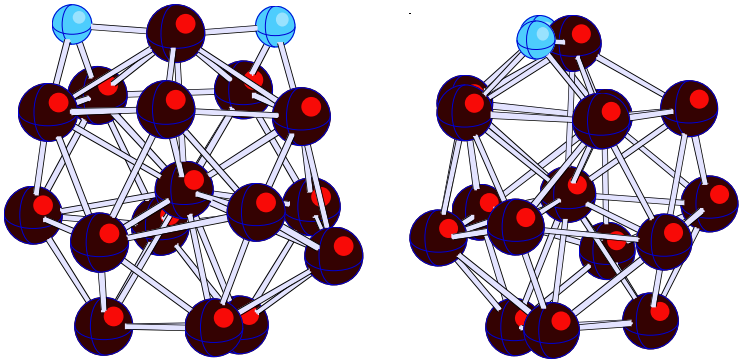
Atom	No	Natural Electron Configuration	
Fe	1	[core]4S(0.21)3d(4.91)4p(0.80)4d(0.03)	
Fe	2	[core]4S(0.30)3d(4.92)4p(0.29)4d(0.01)	
Fe	3	[core]4S(0.20)3d(4.64)4p(0.29)4d(0.02)	
Fe	4	[core]4S(0.30)3d(4.93)4p(0.34)4d(0.01)	
Fe	5	[core]4S(0.30)3d(4.93)4p(0.33)4d(0.01)	
Fe	6	[core]4S(0.31)3d(4.92)4p(0.28)4d(0.01)	
Fe	7	[core]4S(0.32)3d(4.93)4p(0.29)4d(0.01)	
Fe	8	[core]4S(0.23)3d(4.78)4p(0.33)4d(0.02)	
Fe	9	[core]4S(0.28)3d(4.93)4p(0.29)4d(0.01)	
Fe	10	[core]4S(0.27)3d(4.93)4p(0.23)4d(0.01)	
Fe	11	[core]4S(0.15)3d(4.40)4p(0.33)4d(0.03)	1.89
Fe	12	[core]4S(0.19)3d(4.71)4p(0.33)4d(0.02)	
Fe	13	[core]4S(0.30)3d(4.93)4p(0.30)4d(0.01)	
Fe	14	[core]4S(0.32)3d(4.93)4p(0.32)4d(0.01)	3.15
Fe	15	[core]4S(0.22)3d(4.75)4p(0.30)4d(0.02)	
Fe	16	[core]4S(0.33)3d(4.92)4p(0.33)4d(0.01)	3.20

N 17 [core]2S(0.81)2p(2.11)4p(0.01)
N 18 [core]2S(0.80)2p(1.94)4p(0.01)

****
******* Beta spin orbitals *******
****

Fe 1 [core]4S(0.21)3d(2.47)4p(0.82)4d(0.02)
Fe 2 [core]4S(0.17)3d(2.01)4p(0.16)
Fe 3 [core]4S(0.12)3d(2.33)4p(0.20)4d(0.01)
Fe 4 [core]4S(0.16)3d(2.01)4p(0.21)
Fe 5 [core]4S(0.16)3d(2.06)4p(0.20)
Fe 6 [core]4S(0.18)3d(2.06)4p(0.17)
Fe 7 [core]4S(0.16)3d(1.99)4p(0.15)
Fe 8 [core]4S(0.13)3d(2.11)4p(0.22)4d(0.01)
Fe 9 [core]4S(0.17)3d(2.07)4p(0.17)
Fe 10 [core]4S(0.16)3d(1.96)4p(0.15)
Fe 11 [core]4S(0.10)3d(2.66)4p(0.27)4d(0.01)
Fe 12 [core]4S(0.13)3d(2.24)4p(0.26)4d(0.01)
Fe 13 [core]4S(0.16)3d(2.00)4p(0.21)
Fe 14 [core]4S(0.18)3d(2.06)4p(0.19)
Fe 15 [core]4S(0.12)3d(2.13)4p(0.20)4d(0.01)
Fe 16 [core]4S(0.18)3d(2.03)4p(0.18)
N 17 [core]2S(0.80)2p(1.94)
N 18 [core]2S(0.79)2p(2.03)

HF= -20331.4428981\S2=576.284055\S2-1=0.\S2A=575.761904



TITLE coordinates

Fe 0.1381213588,-0.0254860495,0.0629125977
Fe 2.466884469,1.215677954,-0.5393629007
Fe 0.5643049318,2.0812171619,-1.4026345674
Fe -1.0529796832,-1.7655875392,1.1866004445
Fe 1.2898092474,-1.685502201,1.7960135078

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 Fe       0.1625464285,0.1354269598,2.7457329544
 Fe       -1.0279960074,-1.7824193714,-1.5870499184
 Fe       -2.5460520476,-0.4553262909,-0.3612144383
 Fe       0.6933062271,-2.592193506,-0.3919778973
 Fe       -1.8200944196,0.6027776732,1.7045643523
 Fe       -1.6241099143,1.9140187159,-0.2162061811
 Fe       0.489604613,2.051394208,1.1688800757
 Fe       1.1590599529,-0.4861539219,-2.0361643232
 Fe       2.571947168,-1.1332101869,-0.1899862162
 Fe       -1.1165963381,0.5239044317,-2.2406285636
 Fe       2.2960244946,0.5464729532,1.672594988
 N       -2.6812427288,1.0618108246,-1.4077311689
 N       -0.2625377519,3.0931981847,-0.1643427454
END
```

```
FREQ=RAMAN
CATION
$$$$$$$$$$$$$  Fe16N2   CATION    S = 48
---------------------------------------------------------------------
 # UBPW91/6-311+G* scf=(VSHIFT=5,NoIncFock,MAXCYC=200,Tight,NoVarAcc)
 NOSYMM OPT=(RFO,MaxCyc=100) IOP(5/13=1,5/36=1,8/11=1) INT=UltraFine GU
 ESS=READ GEOM=CHECKPOINT
 ---------------------------------------------------------------------
Charge =  +1 Multiplicity = 48
                    Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic          Coordinates (Angstroms)
 Number     Number       Type             X           Y           Z
 ---------------------------------------------------------------------
     1         26          0       -0.295171   -0.366431   -0.122673
     2         26          0       -2.695404   -0.366616   -1.123267
     3         26          0       -2.564447   -0.023519    1.128135
     4         26          0        2.302568   -0.389010   -0.325564
     5         26          0        1.072627   -0.253459   -2.364278
     6         26          0        0.819090    1.610600   -0.676339
     7         26          0        1.175408   -2.057649    1.195259
     8         26          0        1.401204    0.272962    1.844177
     9         26          0        1.005429   -2.419811   -1.061733
    10         26          0        1.418751    2.709518    1.286150
    11         26          0       -0.600360    1.350506    1.808908
    12         26          0       -1.668409    1.827818   -0.324456
    13         26          0       -1.389539   -2.338080    0.277821
    14         26          0       -0.973356   -1.694555   -2.093832
    15         26          0       -0.765473   -1.091586    2.280671
    16         26          0       -0.975984    0.833618   -2.382499
    17          7          0        2.357846    1.344324    0.512436
    18          7          0       -0.233456    2.774793    0.524155
```

Distance matrix (angstroms):

		1	2	3	4	5
1	Fe	0.000000				
2	Fe	2.600443	0.000000			
3	Fe	2.613756	2.281157	0.000000		
4	Fe	2.605748	5.061281	5.092608	0.000000	
5	Fe	2.628388	3.968750	5.047586	2.384845	0.000000
6	Fe	2.335974	4.057191	4.168309	2.514397	2.527476
7	Fe	2.599955	4.818542	4.257782	2.523440	3.991988
8	Fe	2.674886	5.098724	4.040669	2.440991	4.253960
9	Fe	2.605718	4.232678	4.825117	2.519657	2.528679
10	Fe	3.792594	5.673990	4.833252	3.602725	4.714304
11	Fe	2.602311	3.991913	2.491794	4.001110	4.773580
12	Fe	2.596387	2.551149	2.518006	4.547855	4.000733
13	Fe	2.290292	2.748636	2.731416	4.218365	4.169963
14	Fe	2.471703	2.381359	3.962954	3.944984	2.517130
15	Fe	2.554036	3.979574	2.388600	4.086435	5.065236
16	Fe	2.647723	2.445942	3.947461	4.058905	2.319241
17	N	3.220023	5.580159	5.145780	1.926070	3.532730
18	N	3.207723	4.317828	3.691729	4.142836	4.383972

		6	7	8	9	10
6	Fe	0.000000				
7	Fe	4.133509	0.000000			
8	Fe	2.912239	2.429779	0.000000		
9	Fe	4.053081	2.292176	3.981455	0.000000	
10	Fe	2.327784	4.774239	2.499701	5.656272	0.000000
11	Fe	2.873837	3.891714	2.273457	5.003443	2.489377
12	Fe	2.521637	5.049127	4.067317	5.073001	3.591936
13	Fe	4.623909	2.738483	4.130285	2.745352	5.863570
14	Fe	4.018233	3.945522	5.001757	2.346661	6.045024
15	Fe	4.307733	2.424545	2.597500	4.008983	4.495364
16	Fe	2.595568	5.078215	4.881614	4.031777	4.765789
17	N	1.962615	3.665764	1.958702	4.298343	1.828739
18	N	1.975952	5.078167	3.267068	5.570799	1.820628

		11	12	13	14	15
11	Fe	0.000000				
12	Fe	2.433063	0.000000			
13	Fe	4.070958	4.218437	0.000000		
14	Fe	4.964162	4.002612	2.492403	0.000000	
15	Fe	2.492717	4.015582	2.440208	4.420755	0.000000
16	Fe	4.239830	2.388184	4.160288	2.544601	5.049345
17	N	3.229839	4.140638	5.259091	5.208102	4.337676
18	N	1.952895	1.917288	5.247731	5.232244	4.279869

		16	17	18
16	Fe	0.000000		
17	N	4.444760	0.000000	
18	N	3.573254	2.959937	0.000000

Alpha occ. eigenvalues -- -0.30259 -0.30208 -0.29907 -0.29795 -0.29062

Alpha occ. eigenvalues -- -0.28408 -0.28296 -0.27010
Alpha virt. eigenvalues -- -0.25244 -0.24709 -0.23755 -0.23569 -0.22194
Beta occ. eigenvalues -- -0.29071 -0.28177 -0.27761 -0.27352 -0.27142
Beta occ. eigenvalues -- -0.27046
Beta virt. eigenvalues -- -0.26154 -0.25355 -0.25323 -0.25247 -0.25010
Mulliken charges and spin densities:

		1	2
1	Fe	12.150984	-6.225663
2	Fe	-0.699660	3.750411
3	Fe	-0.731538	3.723814
4	Fe	-0.344927	3.412706
5	Fe	-0.690383	3.730025
6	Fe	-1.180566	3.150555
7	Fe	-0.772399	3.760417
8	Fe	-0.585428	3.242426
9	Fe	-0.692142	3.760955
10	Fe	0.355036	2.445967
11	Fe	-0.662420	3.178852
12	Fe	-0.352041	3.410023
13	Fe	-1.002930	4.437884
14	Fe	-0.924615	3.732566
15	Fe	-0.977183	3.720903
16	Fe	-0.663952	3.698312
17	N	-0.603939	0.032827
18	N	-0.621898	0.037021

Sum of Mulliken charges = 1.00000 47.00000

Isotropic polarizability for W= 0.000000 451.87 Bohr**3.

Frequencies --	36.2315	51.5476	60.6280
Frequencies --	75.8035	93.9605	102.6111
Frequencies --	105.2426	114.9775	117.0357
Frequencies --	118.6522	129.8871	134.8391
Frequencies --	138.1905	147.0402	150.8971
Frequencies --	152.8315	157.1101	165.7408
Frequencies --	171.4343	178.1442	183.2431
Frequencies --	190.2588	191.3951	196.8702
Frequencies --	202.9990	209.5708	211.3187
Frequencies --	216.8850	227.6160	236.6634
Frequencies --	240.1305	243.8576	249.3993
Frequencies --	253.4347	253.8431	270.6809
Frequencies --	277.5066	282.0409	290.0346
Frequencies --	293.5012	304.8895	328.1146
Frequencies --	340.9837	358.0277	477.0277
Frequencies --	485.9742	574.1064	585.9031

Zero-point vibrational energy 63277.0 (Joules/Mol)
15.12356 (Kcal/Mol) 0.656 eV

IR Intensity

IR Inten	--	0.0857	0.1324	0.0289
IR Inten	--	0.3241	0.3288	0.0522
IR Inten	--	0.1717	0.6435	0.1700
IR Inten	--	0.0814	0.2757	0.1708
IR Inten	--	0.0420	0.1541	0.0212
IR Inten	--	0.2198	0.2519	0.1970
IR Inten	--	0.3558	0.0838	1.4280
IR Inten	--	1.9485	2.3292	3.1594
IR Inten	--	0.5967	0.3667	1.8481
IR Inten	--	0.3945	0.8965	0.9732
IR Inten	--	0.5903	0.2133	0.1874
IR Inten	--	0.0396	0.0795	0.1415
IR Inten	--	1.1522	1.3725	2.2776
IR Inten	--	1.0151	6.3802	1.5676
IR Inten	--	6.8764	1.0788	14.7566
IR Inten	--	21.5884	4.2397	3.6215

Raman Activities

Raman Activ	--	0.6204	0.6556	7.8774
Raman Activ	--	6.7700	4.8681	5.1552
Raman Activ	--	9.4737	4.0003	5.8265
Raman Activ	--	4.2691	4.9466	5.1823
Raman Activ	--	2.5419	3.2697	4.2736
Raman Activ	--	10.1226	3.8079	1.2703
Raman Activ	--	0.7295	4.2639	1.2536
Raman Activ	--	3.5726	5.9694	0.1785
Raman Activ	--	2.1519	0.9507	2.0296
Raman Activ	--	1.0476	0.6645	0.8145
Raman Activ	--	2.5619	9.9971	25.2109
Raman Activ	--	25.9044	38.9371	3.6710
Raman Activ	--	2.1760	0.8295	1.2796
Raman Activ	--	5.1158	4.1926	7.3347
Raman Activ	--	2.8925	0.9773	1.2584
Raman Activ	--	2.3481	1.2223	0.5536

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.45)3d(7.43)4p(1.73)4d(0.05)5p(0.01)
Fe	2	[core]4S(0.49)3d(6.92)4p(0.38)4d(0.01)
Fe	3	[core]4S(0.44)3d(6.94)4p(0.34)4d(0.01)
Fe	4	[core]4S(0.33)3d(6.88)4p(0.50)4d(0.02)5p(0.01)
Fe	5	[core]4S(0.45)3d(6.91)4p(0.32)4d(0.01)5p(0.01)
Fe	6	[core]4S(0.24)3d(6.96)4p(0.64)4d(0.04)5p(0.01)
Fe	7	[core]4S(0.44)3d(6.93)4p(0.35)4d(0.01)
Fe	8	[core]4S(0.37)3d(6.88)4p(0.50)4d(0.02)5p(0.01)
Fe	9	[core]4S(0.49)3d(6.92)4p(0.36)4d(0.01)
Fe	10	[core]4S(0.25)3d(6.83)4p(0.25)4d(0.02)
Fe	11	[core]4S(0.36)3d(6.91)4p(0.54)4d(0.02)5p(0.01)

Fe	12	[core]4S(0.33)3d(6.89)4p(0.49)4d(0.02)5p(0.01)	
Fe	13	[core]4S(0.37)3d(6.93)4p(0.35)4d(0.01)5p(0.01)	
Fe	14	[core]4S(0.43)3d(7.01)4p(0.41)4d(0.01)	
Fe	15	[core]4S(0.48)3d(6.97)4p(0.33)4d(0.01)5p(0.01)	
Fe	16	[core]4S(0.45)3d(6.90)4p(0.32)4d(0.01)5p(0.01)	
N	17	[core]2S(1.58)2p(4.15)3S(0.01)3p(0.02)	
N	18	[core]2S(1.57)2p(4.14)3S(0.01)3p(0.02)	

****
******* Alpha spin orbitals *******
****

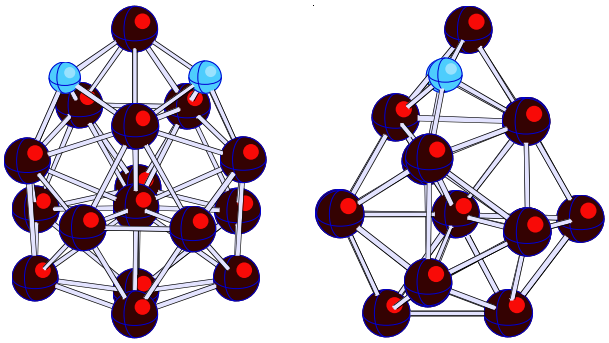
Atom	No	Natural Electron Configuration	
Fe	1	[core]4S(0.22)3d(4.91)4p(0.87)4d(0.03)	
Fe	2	[core]4S(0.32)3d(4.93)4p(0.23)4d(0.01)	
Fe	3	[core]4S(0.27)3d(4.93)4p(0.20)4d(0.01)	
Fe	4	[core]4S(0.21)3d(4.82)4p(0.29)4d(0.01)	
Fe	5	[core]4S(0.28)3d(4.94)4p(0.19)4d(0.01)	
Fe	6	[core]3d(4.66)4p(0.35)5S(0.13)4d(0.03)	
Fe	7	[core]4S(0.28)3d(4.94)4p(0.21)4d(0.01)	
Fe	8	[core]4S(0.23)3d(4.79)4p(0.29)4d(0.02)	
Fe	9	[core]4S(0.32)3d(4.93)4p(0.22)4d(0.01)	3.16
Fe	10	[core]3d(4.55)4p(0.15)5S(0.16)4d(0.01)	2.4
Fe	11	[core]4S(0.22)3d(4.77)4p(0.30)4d(0.02)	
Fe	12	[core]4S(0.21)3d(4.81)4p(0.28)4d(0.01)	
Fe	13	[core]4S(0.23)3d(4.94)4p(0.18)4d(0.01)	
Fe	14	[core]4S(0.26)3d(4.93)4p(0.24)4d(0.01)	3.13
Fe	15	[core]4S(0.31)3d(4.93)4p(0.18)4d(0.01)	
Fe	16	[core]4S(0.28)3d(4.94)4p(0.19)4d(0.01)	
N	17	[core]2S(0.80)2p(2.10)4p(0.01)	
N	18	[core]2S(0.80)2p(2.09)4p(0.01)	

****
******* Beta spin orbitals *******
****

Atom	No	Natural Electron Configuration
Fe	1	[core]4S(0.23)3d(2.53)4p(0.86)4d(0.02)
Fe	2	[core]4S(0.18)3d(1.99)4p(0.15)
Fe	3	[core]4S(0.17)3d(2.00)4p(0.14)
Fe	4	[core]4S(0.12)3d(2.06)4p(0.21)4d(0.01)
Fe	5	[core]4S(0.17)3d(1.97)4p(0.13)
Fe	6	[core]3d(2.30)4p(0.30)5S(0.11)4d(0.01)
Fe	7	[core]4S(0.17)3d(1.99)4p(0.14)
Fe	8	[core]4S(0.13)3d(2.09)4p(0.22)4d(0.01)
Fe	9	[core]4S(0.18)3d(1.99)4p(0.15)
Fe	10	[core]3d(2.27)4p(0.10)5S(0.09)4d(0.01)
Fe	11	[core]4S(0.13)3d(2.14)4p(0.24)4d(0.01)
Fe	12	[core]4S(0.12)3d(2.08)4p(0.21)4d(0.01)

Fe 13 [core]4S(0.14)3d(2.00)4p(0.17)
Fe 14 [core]4S(0.16)3d(2.08)4p(0.17)
Fe 15 [core]4S(0.17)3d(2.04)4p(0.14)
Fe 16 [core]4S(0.17)3d(1.96)4p(0.13)
N 17 [core]2S(0.78)2p(2.05)4p(0.01)
N 18 [core]2S(0.78)2p(2.05)

HF= -20331.1646186\S2=576.305859\S2-1=0.\S2A=575.762941



TITLE. coordinates
Fe -0.2951710431,-0.3664307087,-0.1226733278
Fe -2.6954041435,-0.3666162086,-1.1232666651
Fe -2.5644467013,-0.023519279,1.128135211
Fe 2.3025684146,-0.3890096233,-0.3255635055
Fe 1.0726272616,-0.2534590981,-2.3642775225
Fe 0.8190902418,1.6106003651,-0.6763391897
Fe 1.1754084842,-2.0576488148,1.1952589758
Fe 1.4012044865,0.2729619252,1.8441772106
Fe 1.0054291965,-2.4198113509,-1.061733366
Fe 1.4187509762,2.7095178039,1.286150385
Fe -0.6003598346,1.3505063979,1.8089081407
Fe -1.6684085745,1.8278178805,-0.3244559129
Fe -1.3895386928,-2.338079558,0.2778209294
Fe -0.9733557852,-1.694554591,-2.093832388
Fe -0.7654729466,-1.0915857036,2.2806714576
Fe -0.9759842759,0.833618177,-2.3824986529
N 2.3578460948,1.3443241564,0.5124357623
N -0.2334561613,2.7747932376,0.5241554596
END