

Mn(N₁₃) calculation by B3PW91/TZVP method

Dipole moment: 1.6588 Debye

 $\Delta E(\text{multipl.}=1) = 23.3 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=3) = 0.0 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=5) = 155.1 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=7) = 243.1 \text{ kJ/mol}$

Alpha occupied eigenvalues (highest) = -8.0612346 eV

Alpha virtual eigenvalues (lowest) = -3.9035466 eV

Beta occupied eigenvalues (highest) = -8.4721056 eV

Beta virtual eigenvalues (lowest) = -6.4759800 eV

<S**2> = 2.0016

APT charges:

```

N1      0.261301
N2     -0.118753
N3     -0.117810
N4      0.261117
N5     -0.117804
N6     -0.118758
N7      0.261301
N8     -0.118743
N9     -0.117809
N10     0.261105
N11    -0.117803
N12    -0.118749
Mn1     0.274568
N13    -0.373162

```

Sum of APT charges = 0.00000

Cartesian Coordinates (Standard orientation)

Number in structure	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
N1	7	0	-0.000013	1.646223	-0.075011
N2	7	0	1.160603	2.059815	-0.624183
N3	7	0	2.060054	1.160556	-0.624442
N4	7	0	1.646336	0.000001	-0.075331
N5	7	0	2.060059	-1.160551	-0.624443
N6	7	0	1.160609	-2.059809	-0.624182
N7	7	0	-0.000010	-1.646223	-0.075011
N8	7	0	-1.160785	-2.059825	-0.623840
N9	7	0	-2.060232	-1.160563	-0.623818
N10	7	0	-1.646358	-0.000001	-0.074835
N11	7	0	-2.060237	1.160558	-0.623818
N12	7	0	-1.160790	2.059820	-0.623839
Mn1	25	0	0.000124	0.000000	0.841849
N13	7	0	0.000349	-0.000000	2.351543

Summary of Natural Population Analysis:

		Natural Population				
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
N	1	-0.06717	1.99922	5.02850	0.03945	7.06717
N	2	0.02707	1.99957	4.94373	0.02963	6.97293
N	3	0.02713	1.99957	4.94366	0.02963	6.97287
N	4	-0.06720	1.99922	5.02852	0.03946	7.06720
N	5	0.02714	1.99957	4.94366	0.02963	6.97286
N	6	0.02707	1.99957	4.94373	0.02963	6.97293
N	7	-0.06717	1.99922	5.02850	0.03945	7.06717
N	8	0.02707	1.99957	4.94373	0.02963	6.97293
N	9	0.02713	1.99957	4.94366	0.02963	6.97287
N	10	-0.06720	1.99922	5.02853	0.03946	7.06720
N	11	0.02713	1.99957	4.94366	0.02963	6.97287
N	12	0.02707	1.99957	4.94373	0.02963	6.97293
Mn	1	-0.15431	17.96001	7.16302	0.03128	25.15431
N	13	0.20624	1.99976	4.78623	0.00777	6.79376
=====						
* Total *		-0.00000	43.95320	71.61286	0.43394	116.00000

Mn(N₁₃) calculation by M06/TZVP method

Dipole moment: 1.7663 Debye

 $\Delta E(\text{multipl.}=1) = 39.6 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=3) = 0.0 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=5) = 128.7 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=7) = 197.7 \text{ kJ/mol}$

Alpha occupied eigenvalues (highest) = -8.1170151 eV

Alpha virtual eigenvalues (lowest) = -4.0738812 eV

Beta occupied eigenvalues (highest) = -8.6307399 eV

Beta virtual eigenvalues (lowest) = -6.2008869 eV

<S**2> = 2.0209

APT charges:

```

N1      0.228791
N2     -0.234800
N3      0.082099
N4      0.076062
N5     -0.018556
N6     -0.018399
N7      0.076419
N8      0.083119
N9     -0.237330
N10     0.230569
N11    -0.107800
N12    -0.104463
Mn1     0.296273
N13    -0.351983

```

Sum of APT charges = 0.00000

Cartesian Coordinates (Standard orientation)

Number in structure	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
N1	7	0	0.882043	1.423939	-0.059860
N2	7	0	2.112801	1.142281	-0.626507
N3	7	0	2.332529	-0.097436	-0.648977
N4	7	0	1.390814	-0.858308	-0.075581
N5	7	0	1.119495	-2.079925	-0.647255
N6	7	0	-0.094920	-2.360211	-0.646714
N7	7	0	-0.873365	-1.380433	-0.074644
N8	7	0	-2.053275	-1.108707	-0.647307
N9	7	0	-2.398560	0.102307	-0.624829
N10	7	0	-1.415322	0.894312	-0.058941
N11	7	0	-1.131282	2.028744	-0.672348
N12	7	0	0.129653	2.319166	-0.672927
Mn1	25	0	-0.001343	0.010285	0.867250
N13	7	0	0.010721	-0.038787	2.375715

Summary of Natural Population Analysis:

		Natural Population				
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
N	1	-0.05721	1.99925	5.02000	0.03795	7.05721
N	2	-0.00513	1.99957	4.97622	0.02934	7.00513
N	3	0.06338	1.99956	4.90734	0.02973	6.93662
N	4	-0.12247	1.99922	5.08629	0.03696	7.12247
N	5	0.03121	1.99956	4.93957	0.02967	6.96879
N	6	0.03103	1.99956	4.93975	0.02966	6.96897
N	7	-0.12229	1.99922	5.08610	0.03696	7.12229
N	8	0.06341	1.99956	4.90731	0.02972	6.93659
N	9	-0.00526	1.99957	4.97635	0.02934	7.00526
N	10	-0.05688	1.99925	5.01967	0.03796	7.05688
N	11	0.03013	1.99957	4.94092	0.02938	6.96987
N	12	0.03052	1.99957	4.94053	0.02938	6.96948
Mn	1	-0.08079	17.96161	7.08910	0.03008	25.08079
N	13	0.20035	1.99979	4.79192	0.00794	6.79965
=====						
* Total *		-0.00000	43.95486	71.62108	0.42406	116.00000

Mn(N₁₃) calculation by OPBE/TZVP method

Dipole moment: 1.2685 Debye

 $\Delta E(\text{multipl.}=1) = 12.8 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=1) = 27.8 \text{ kJ/mol (by-radical)}$ $\Delta E(\text{multipl.}=3) = 0.0 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=5) = 213.7 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=7) = 302.1 \text{ kJ/mol}$

Alpha occupied eigenvalues (highest) = -6.9799092 eV

Alpha virtual eigenvalues (lowest) = -4.4145504 eV

Beta occupied eigenvalues (highest) = -7.4832942 eV

Beta virtual eigenvalues (lowest) = -6.6327096 eV

<S**2> = 2.0009

APT charges:

```

N1      0.151015
N2     -0.072746
N3     -0.072887
N4      0.151010
N5     -0.072889
N6     -0.072743
N7      0.151015
N8     -0.072753
N9     -0.072881
N10     0.151010
N11    -0.072883
N12    -0.072750
Mn1     0.380386
N13    -0.401903

```

Sum of APT charges = 0.00000

Cartesian Coordinates (Standard orientation)

Number in structure	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
N1	7	0	-0.000013	1.640774	-0.083763
N2	7	0	1.161292	2.067748	-0.622454
N3	7	0	2.067568	1.161428	-0.622568
N4	7	0	1.640712	0.000003	-0.084028
N5	7	0	2.067569	-1.161421	-0.622569
N6	7	0	1.161299	-2.067746	-0.622453
N7	7	0	-0.000007	-1.640774	-0.083763
N8	7	0	-1.161476	-2.067746	-0.622103
N9	7	0	-2.067751	-1.161426	-0.621948
N10	7	0	-1.640730	-0.000003	-0.083537
N11	7	0	-2.067752	1.161420	-0.621949
N12	7	0	-1.161482	2.067745	-0.622102
Mn1	25	0	0.000129	0.000000	0.844430
N13	7	0	0.000349	0.000000	2.369448

Summary of Natural Population Analysis:

		Natural Population				
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
N	1	-0.05069	1.99924	5.01379	0.03766	7.05069
N	2	0.02657	1.99958	4.94587	0.02798	6.97343
N	3	0.02656	1.99958	4.94588	0.02798	6.97344
N	4	-0.05069	1.99924	5.01379	0.03766	7.05069
N	5	0.02656	1.99958	4.94588	0.02798	6.97344
N	6	0.02657	1.99958	4.94587	0.02798	6.97343
N	7	-0.05070	1.99924	5.01379	0.03766	7.05070
N	8	0.02657	1.99958	4.94587	0.02798	6.97343
N	9	0.02656	1.99958	4.94588	0.02798	6.97344
N	10	-0.05069	1.99924	5.01379	0.03766	7.05069
N	11	0.02656	1.99958	4.94588	0.02798	6.97344
N	12	0.02657	1.99958	4.94587	0.02798	6.97343
Mn	1	-0.19174	17.96237	7.20107	0.02830	25.19174
N	13	0.18199	1.99976	4.81057	0.00768	6.81801
=====						
* Total *		-0.00000	43.95573	71.63379	0.41048	116.00000

Mn(N₁₃) calculation by M062X/Def2TZVP method

Dipole moment: 1.2685 Debye

$\Delta E(\text{multipl.}=3) = 0.0 \text{ kJ/mol}$

Alpha occupied eigenvalues (highest)= -9.352077 eV
Alpha virtual eigenvalues (lowest) = -2.100612 eV
Beta occupied eigenvalues (highest)= -10.279938 eV
Beta virtual eigenvalues (lowest) = -4.792225 eV

$\langle S^2 \rangle = 2.0264$

APT charges:

N1 -0.151221
N2 0.079003
N3 0.079289
N4 -0.151530
N5 0.024653
N6 0.023780
N7 -0.151221
N8 0.079003
N9 0.079291
N10 -0.151532
N11 0.024653
N12 0.023781
Mn1 0.377347
N13 -0.185296

Sum of APT charges = 0.00000

Cartesian Coordinates (Standard orientation)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
N1	7	0	-0.788859	-1.445347	-0.096834
N2	7	0	-2.120684	-1.279526	-0.562646
N3	7	0	-2.474995	-0.097930	-0.561605
N4	7	0	-1.453660	0.772668	-0.094778
N5	7	0	-1.226698	1.790042	-0.870105
N6	7	0	0.040450	2.170397	-0.869182
N7	7	0	0.788912	1.445553	-0.092543
N8	7	0	2.121083	1.280924	-0.557792
N9	7	0	2.475394	0.099328	-0.559520
N10	7	0	1.453713	-0.772460	-0.095682
N11	7	0	1.227326	-1.787846	-0.873779
N12	7	0	-0.039823	-2.168198	-0.874774
Mn1	25	0	-0.000331	-0.001139	0.875082
N13	7	0	-0.000868	-0.003021	2.348354

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
N	1	-0.11295	1.99919	5.05781	0.05595	7.11295
N	2	0.05719	1.99956	4.90327	0.03998	6.94281
N	3	0.05718	1.99956	4.90329	0.03996	6.94282
N	4	-0.11299	1.99919	5.05784	0.05597	7.11299
N	5	0.01249	1.99955	4.94945	0.03851	6.98751
N	6	0.01226	1.99955	4.94970	0.03849	6.98774
N	7	-0.11295	1.99919	5.05781	0.05595	7.11295
N	8	0.05719	1.99956	4.90327	0.03998	6.94281
N	9	0.05718	1.99956	4.90329	0.03996	6.94282
N	10	-0.11299	1.99919	5.05783	0.05597	7.11299
N	11	0.01249	1.99955	4.94945	0.03851	6.98751
N	12	0.01226	1.99955	4.94970	0.03849	6.98774
Mn	1	-0.06540	17.95755	7.06138	0.04646	25.06540
N	13	0.23904	1.99981	4.74232	0.01883	6.76096
=====						
* Total *		0.00000	43.95054	71.44644	0.60301	116.00000

Fe(N₁₃) calculation by B3PW91/TZVP method

Dipole moment: 1.6973 Debye

 $\Delta E(\text{multipl.}=2) = 0.0 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=4) = 160.6 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=6) = 318.2 \text{ kJ/mol}$

Alpha occupied eigenvalues (highest) = -8.2677585 eV

Alpha virtual eigenvalues (lowest) = -3.8698062 eV

Beta occupied eigenvalues (highest) = -8.4399978 eV

Beta virtual eigenvalues (lowest) = -6.5276790 eV

<S**2> = 0.7508

APT charges:

```

N1      0.338713
N2     -0.139156
N3     -0.138945
N4      0.338664
N5     -0.138946
N6     -0.139155
N7      0.338712
N8     -0.139162
N9     -0.138933
N10     0.338656
N11    -0.138933
N12    -0.139162
Fe1    -0.054800
N13    -0.187554

```

Sum of APT charges = 0.00000

Cartesian Coordinates (Standard orientation)

Number in structure	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
N1	7	0	-0.000013	1.624464	-0.085685
N2	7	0	1.163777	2.065465	-0.596785
N3	7	0	2.065447	1.163840	-0.596958
N4	7	0	1.624484	0.000002	-0.085957
N5	7	0	2.065451	-1.163834	-0.596958
N6	7	0	1.163783	-2.065462	-0.596785
N7	7	0	-0.000008	-1.624464	-0.085686
N8	7	0	-1.163954	-2.065466	-0.596436
N9	7	0	-2.065622	-1.163841	-0.596340
N10	7	0	-1.624505	-0.000002	-0.085471
N11	7	0	-2.065625	1.163835	-0.596340
N12	7	0	-1.163960	2.065463	-0.596436
Fe1	26	0	0.000115	0.000000	0.757857
N13	7	0	0.000340	0.000000	2.258618

Summary of Natural Population Analysis:

		Natural Population				
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
N	1	-0.01579	1.99916	4.97709	0.03954	7.01579
N	2	0.02580	1.99957	4.94500	0.02962	6.97420
N	3	0.02582	1.99957	4.94499	0.02962	6.97418
N	4	-0.01580	1.99916	4.97710	0.03954	7.01580
N	5	0.02582	1.99957	4.94499	0.02962	6.97418
N	6	0.02580	1.99957	4.94500	0.02962	6.97420
N	7	-0.01579	1.99916	4.97709	0.03954	7.01579
N	8	0.02580	1.99957	4.94500	0.02962	6.97420
N	9	0.02582	1.99957	4.94499	0.02962	6.97418
N	10	-0.01581	1.99916	4.97710	0.03954	7.01581
N	11	0.02582	1.99957	4.94499	0.02962	6.97418
N	12	0.02580	1.99957	4.94500	0.02962	6.97420
Fe	1	-0.42714	17.96755	8.43364	0.02595	26.42714
N	13	0.28386	1.99975	4.70842	0.00796	6.71614
=====						
* Total *		-0.00000	43.96053	72.61041	0.42906	117.00000

Fe(N₁₃) calculation by M06/TZVP method

Dipole moment: 1.7903 Debye

 $\Delta E(\text{multipl.}=2) = 0.0 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=4) = 174.0 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=6) = 205.2 \text{ kJ/mol}$

Alpha occupied eigenvalues (highest) = -8.4065295 eV

Alpha virtual eigenvalues (lowest) = -3.5770266 eV

Beta occupied eigenvalues (highest) = -8.4993156 eV

Beta virtual eigenvalues (lowest) = -6.2003427 eV

<S**2> = 0.7537

APT charges:

```

N1      0.254992
N2     -0.258311
N3      0.120123
N4      0.070184
N5     -0.001914
N6     -0.001913
N7      0.070195
N8      0.120138
N9     -0.258355
N10     0.255025
N11    -0.102104
N12    -0.102046
Fe1    -0.007252
N13    -0.158763

```

Sum of APT charges = 0.00000

Cartesian Coordinates (Standard orientation)

Number in structure	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
N1	7	0	0.005439	-1.647224	-0.055490
N2	7	0	-1.198170	-2.096577	-0.580473
N3	7	0	-2.040774	-1.162734	-0.606547
N4	7	0	-1.605953	-0.007710	-0.084669
N5	7	0	-2.055139	1.173767	-0.627891
N6	7	0	-1.173907	2.055103	-0.627762
N7	7	0	0.007547	1.605969	-0.084432
N8	7	0	1.162592	2.040990	-0.606082
N9	7	0	2.096529	1.198485	-0.579995
N10	7	0	1.647235	-0.005246	-0.055252
N11	7	0	2.035136	-1.116114	-0.639844
N12	7	0	1.116433	-2.034915	-0.639980
Fe1	26	0	0.004946	-0.005058	0.785012
N13	7	0	-0.001594	0.001263	2.285079

Summary of Natural Population Analysis:

		Natural Population				
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
N	1	0.01141	1.99918	4.95179	0.03763	6.98859
N	2	-0.00954	1.99958	4.98061	0.02935	7.00954
N	3	0.06669	1.99956	4.90410	0.02965	6.93331
N	4	-0.07352	1.99915	5.03738	0.03700	7.07352
N	5	0.02752	1.99956	4.94321	0.02970	6.97248
N	6	0.02752	1.99956	4.94322	0.02970	6.97248
N	7	-0.07352	1.99915	5.03738	0.03700	7.07352
N	8	0.06669	1.99956	4.90410	0.02965	6.93331
N	9	-0.00954	1.99958	4.98062	0.02935	7.00954
N	10	0.01141	1.99918	4.95178	0.03763	6.98859
N	11	0.03095	1.99957	4.94013	0.02936	6.96905
N	12	0.03095	1.99957	4.94012	0.02936	6.96905
Fe	1	-0.39455	17.96853	8.40198	0.02404	26.39455
N	13	0.28754	1.99978	4.70460	0.00808	6.71246
=====						
* Total *		-0.00000	43.96151	72.62101	0.41748	117.00000

Fe(N₁₃) calculation by OPBE/TZVP method

Dipole moment: 1.2704 Debye

 $\Delta E(\text{multipl.}=2) = 0.0 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=4) = 190.1 \text{ kJ/mol}$ $\Delta E(\text{multipl.}=6) = 286.5 \text{ kJ/mol}$

Alpha occupied eigenvalues (highest) = -7.1896983 eV

Alpha virtual eigenvalues (lowest) = -4.3579536 eV

Beta occupied eigenvalues (highest) = -7.5148578 eV

Beta virtual eigenvalues (lowest) = -6.7660386 eV

 $\langle S^2 \rangle = 0.7501$

APT charges:

```

N1      0.224064
N2     -0.083568
N3     -0.084074
N4      0.224215
N5     -0.084079
N6     -0.083563
N7      0.224064
N8     -0.083585
N9     -0.084064
N10     0.224217
N11    -0.084068
N12    -0.083580
Fe1     0.012470
N13    -0.238448

```

Sum of APT charges = 0.00000

Cartesian Coordinates (Standard orientation)

Number in structure	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
N1	7	0	-0.000012	1.620744	-0.087854
N2	7	0	1.164809	2.071912	-0.596629
N3	7	0	2.071545	1.165020	-0.596640
N4	7	0	1.620602	0.000004	-0.088031
N5	7	0	2.071546	-1.165013	-0.596639
N6	7	0	1.164815	-2.071911	-0.596631
N7	7	0	-0.000005	-1.620743	-0.087854
N8	7	0	-1.164986	-2.071902	-0.596274
N9	7	0	-2.071726	-1.165013	-0.596027
N10	7	0	-1.620622	-0.000003	-0.087548
N11	7	0	-2.071727	1.165007	-0.596026
N12	7	0	-1.164992	2.071901	-0.596275
Fe1	26	0	0.000118	0.000000	0.753843
N13	7	0	0.000344	0.000000	2.269227

Summary of Natural Population Analysis:

		Natural Population				
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
N	1	0.00028	1.99918	4.96302	0.03752	6.99972
N	2	0.02692	1.99958	4.94551	0.02799	6.97308
N	3	0.02687	1.99958	4.94556	0.02799	6.97313
N	4	0.00031	1.99918	4.96299	0.03752	6.99969
N	5	0.02687	1.99958	4.94556	0.02799	6.97313
N	6	0.02692	1.99958	4.94550	0.02799	6.97308
N	7	0.00028	1.99918	4.96302	0.03752	6.99972
N	8	0.02692	1.99958	4.94551	0.02799	6.97308
N	9	0.02687	1.99958	4.94555	0.02799	6.97313
N	10	0.00031	1.99918	4.96299	0.03752	6.99969
N	11	0.02687	1.99958	4.94556	0.02799	6.97313
N	12	0.02692	1.99958	4.94551	0.02799	6.97308
Fe	13	-0.47989	17.96905	8.48809	0.02275	26.47989
N	14	0.26353	1.99975	4.72937	0.00735	6.73647
=====						
* Total *		-0.00000	43.96215	72.63373	0.40412	117.00000

Fe(N₁₃) calculation by M062X/TZVP method

Dipole moment: 3.5299 Debye

 $\Delta E(\text{multipl.}=2) = 0.0 \text{ kJ/mol}$

Alpha occupied eigenvalues (highest)= -9.6320679 eV
 Alpha virtual eigenvalues (lowest) = -1.9422498 eV
 Beta occupied eigenvalues (highest)= -8.9646066 eV
 Beta virtual eigenvalues (lowest) = -4.7144046 eV

<S**2>= 1.4530

APT charges:

```

N1  -0.209333
N2   0.131173
N3  -0.049934
N4  -0.049544
N5  -0.014496
N6  -0.014365
N7  -0.049723
N8  -0.049675
N9   0.131148
N10 -0.209535
N11  0.029422
N12  0.029414
Fe1  0.114770
N13  0.210678

```

Sum of APT charges = -0.00000

Cartesian Coordinates (Standard orientation)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
N1	7	0	1.132786	1.132988	-0.053999
N2	7	0	2.292062	0.659680	-0.588723
N3	7	0	2.392792	-0.574413	-0.606553
N4	7	0	1.192707	-1.171170	-0.110782
N5	7	0	0.664279	-2.073169	-0.883634
N6	7	0	-0.648562	-2.078662	-0.882578
N7	7	0	-1.183225	-1.180969	-0.108957
N8	7	0	-2.388956	-0.594230	-0.602951
N9	7	0	-2.298395	0.640653	-0.585154
N10	7	0	-1.142283	1.123594	-0.052106
N11	7	0	-0.630685	2.276468	-0.608902
N12	7	0	0.610856	2.281629	-0.609913
Fe1	26	0	0.000771	-0.039817	0.818674
N13	7	0	0.004299	-0.294536	2.544370

Summary of Natural Population Analysis:

		Natural Population				
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
N	1	-0.16693	1.99913	5.11202	0.05578	7.16693
N	2	0.07551	1.99955	4.88374	0.04120	6.92449
N	3	0.00437	1.99956	4.95689	0.03918	6.99563
N	4	-0.04042	1.99919	4.98740	0.05383	7.04042
N	5	0.02339	1.99955	4.93804	0.03902	6.97661
N	6	0.02337	1.99955	4.93806	0.03902	6.97663
N	7	-0.04056	1.99919	4.98753	0.05384	7.04056
N	8	0.00441	1.99956	4.95685	0.03918	6.99559
N	9	0.07547	1.99955	4.88377	0.04120	6.92453
N	10	-0.16694	1.99913	5.11203	0.05578	7.16694
N	11	0.02053	1.99955	4.93961	0.04031	6.97947
N	12	0.02058	1.99955	4.93957	0.04030	6.97942
Fe	1	0.05601	17.98122	7.92647	0.03630	25.94399
N	13	0.11122	1.99988	4.86871	0.02019	6.88878
=====						
* Total *		0.00000	43.97419	72.43069	0.59512	117.00000