

Structures of Solvated Ferrous Ion Clusters in ammonia and Spin-crossover at various Temperatures

(Supporting information)

Ousman Boukar^a, Jean Jules Fifen^{*,b}, Alhadji Malloum^b, Zoubeida Dhaouadi^c,
Hassen Ghalila^c and Jeanet Conradie^d

^aDepartment of Physics, Faculty of Science, University of Maroua, P. O. Box 46, Maroua
Cameroon

^bDepartment of Physics, Faculty of Science, University of Ngaoundere, P.O.BOX 454, Ngaoundere,
Cameroon.

^cLaboratoire de Spectroscopie Atomique Moléculaire et Applications, Faculté des Sciences de
Tunis, Université de Tunis El Manar, Campus
Universitaire 1060, Tunis, Tunisie.

^dDepartment of Chemistry, University of the Free State, PO Box 339, Bloemfontein, 9300, South
Africa

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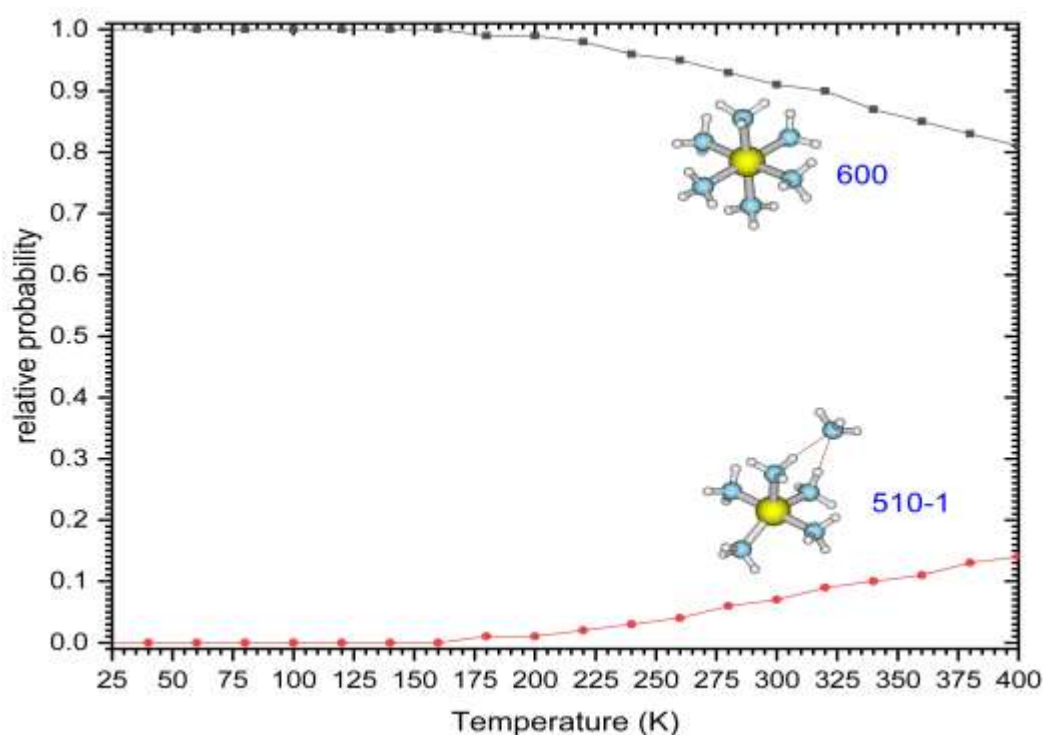


Figure 1s: Temperature dependence of the relative stability of different $\text{Fe}^{2+}(\text{NH}_3)_{n=6}$ isomers at MP2/6-31++G(d,p) level of theory at triplet spin-state

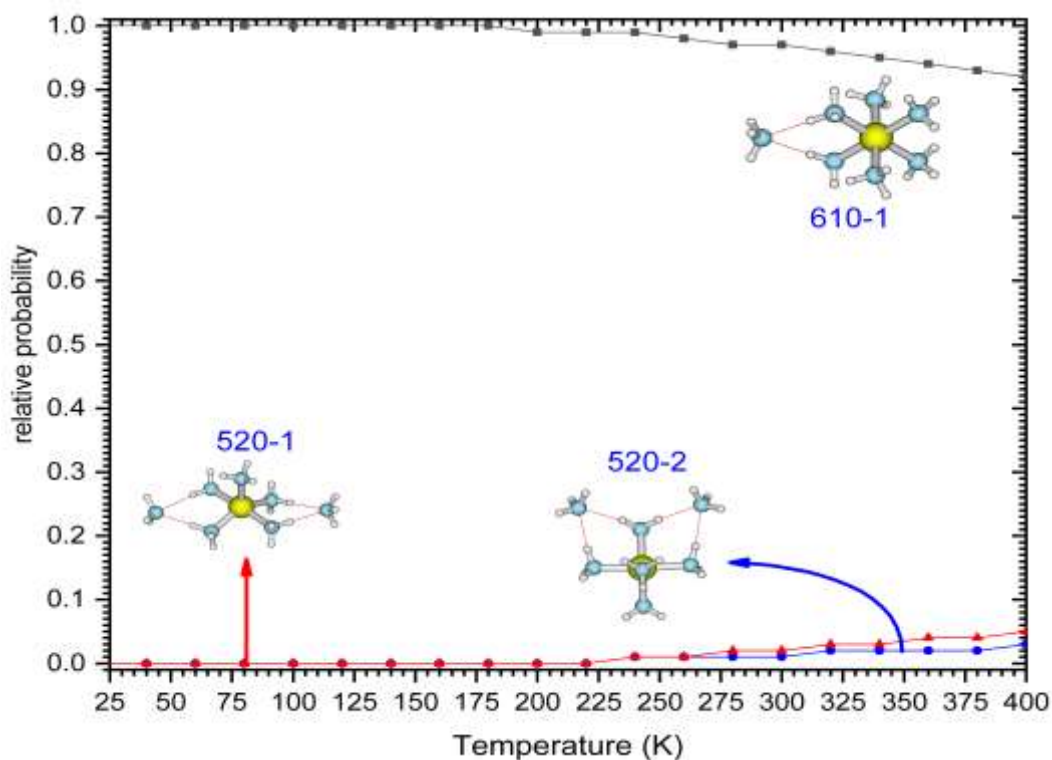


Figure 2s: Temperature dependence of the relative stability of different $\text{Fe}^{2+}(\text{NH}_3)_{n=7}$ isomers at MP2/6-31++G(d,p) level of theory at triplet spin-state

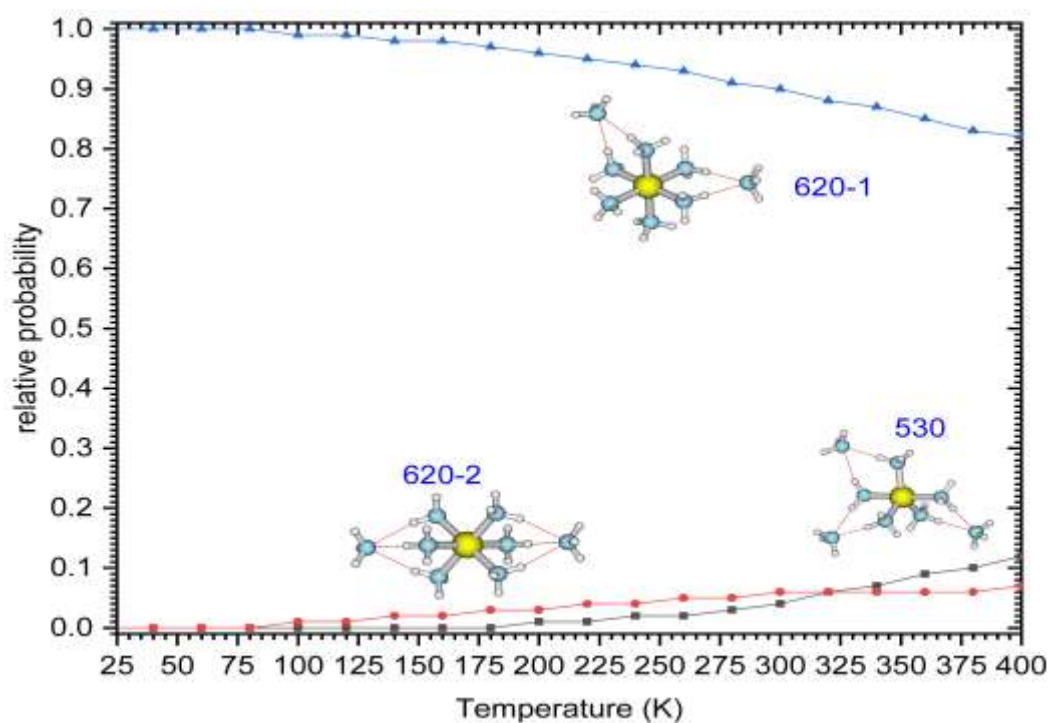


Figure 3s: Temperature dependence of the relative stability of different $\text{Fe}^{2+}(\text{NH}_3)_{n=8}$ isomers at MP2/6-31++G(d,p) level of theory at triplet spin-state

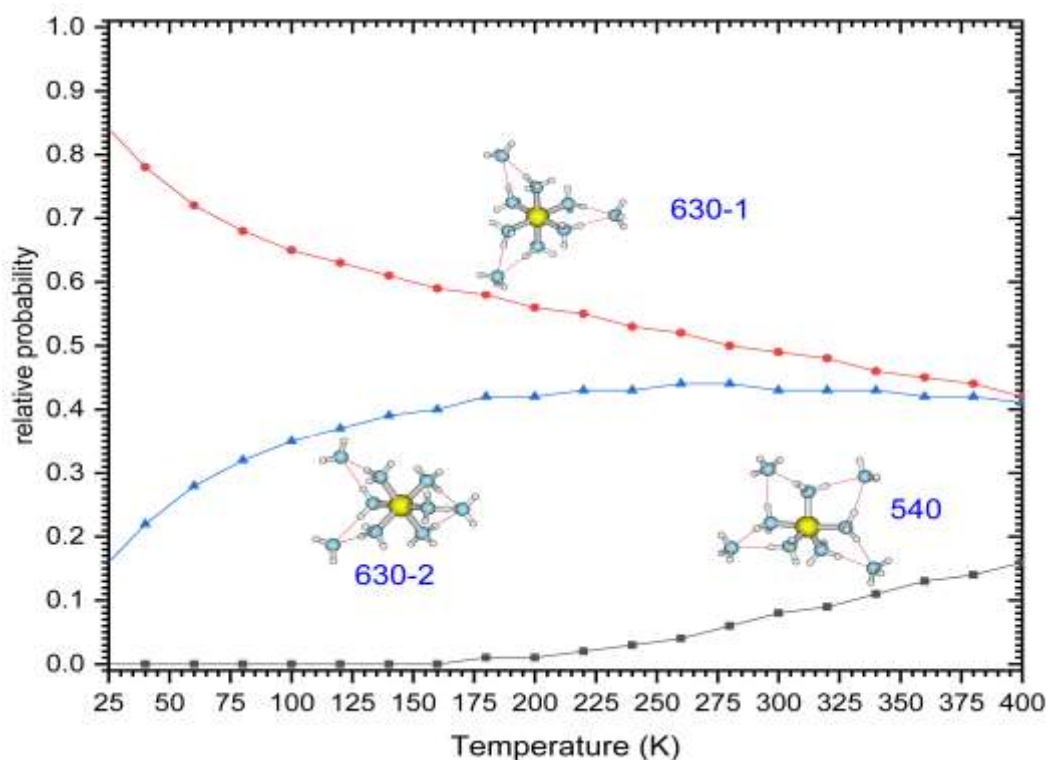


Figure 4s: Temperature dependence of the relative stability of different $\text{Fe}^{2+}(\text{NH}_3)_{n=9}$ isomers at MP2/6-31++G(d,p) level of theory theory at triplet spin-state

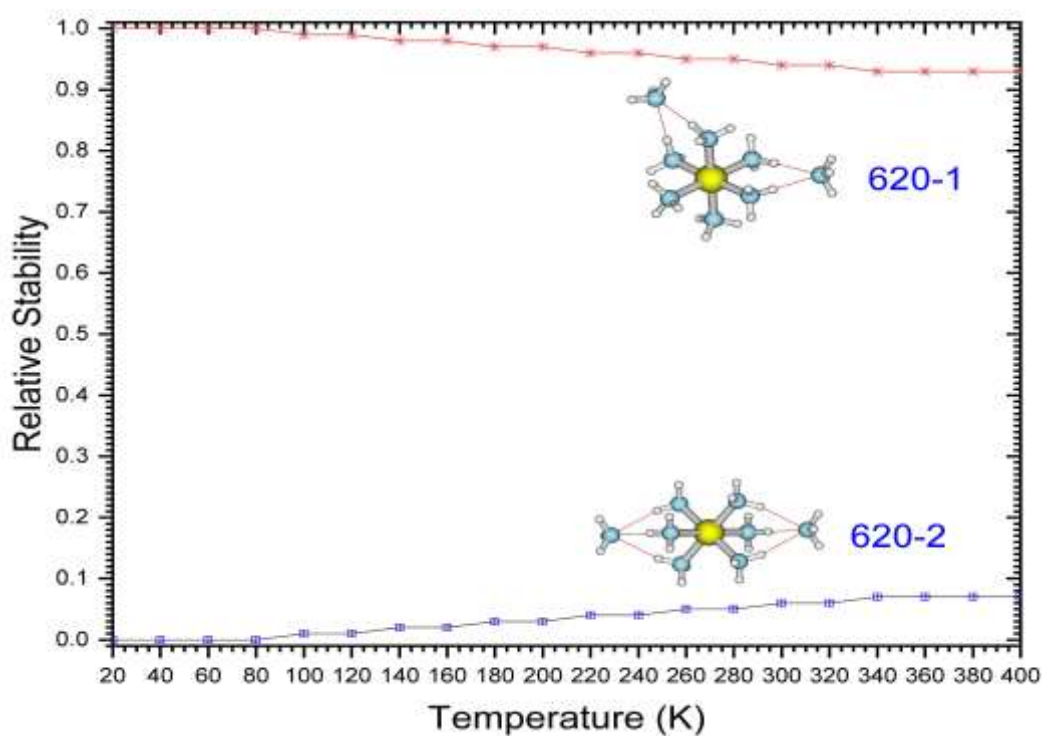


Figure 5s: Temperature dependence of the relative stability of different $\text{Fe}^{2+}(\text{NH}_3)_{n=8}$ isomers at MP2/6-31++G(d,p) level of theory at singlet spin-state

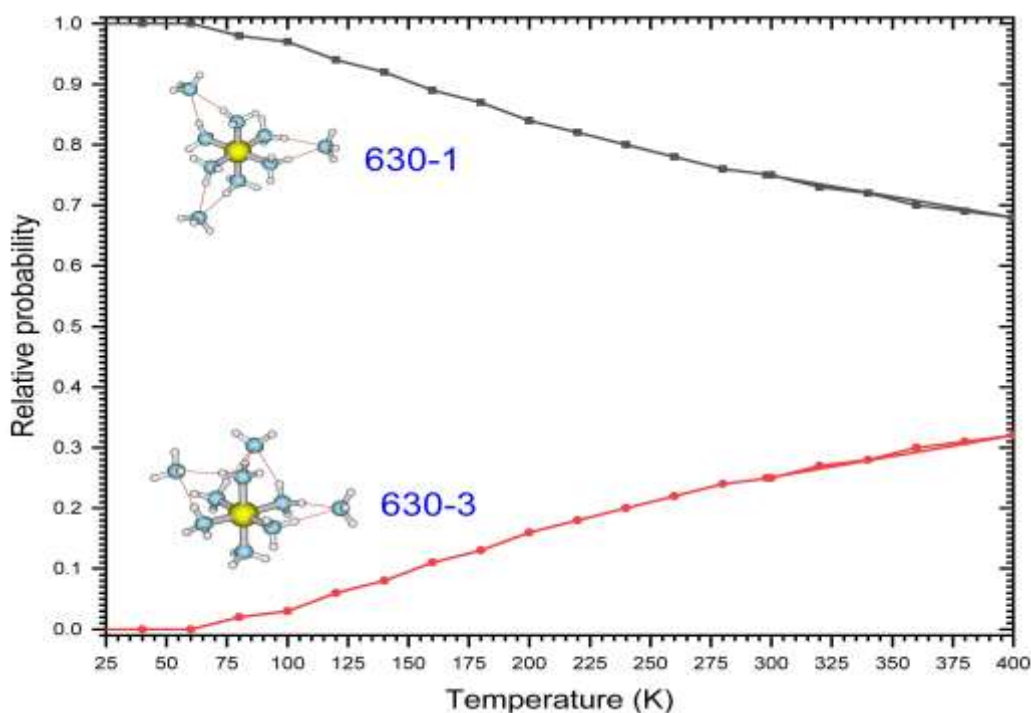


Figure 6s: Temperature dependence of the relative stability of different $\text{Fe}^{2+}(\text{NH}_3)_{n=9}$ isomers at MP2/6-31++G(d,p) level of theory at singlet spin-state

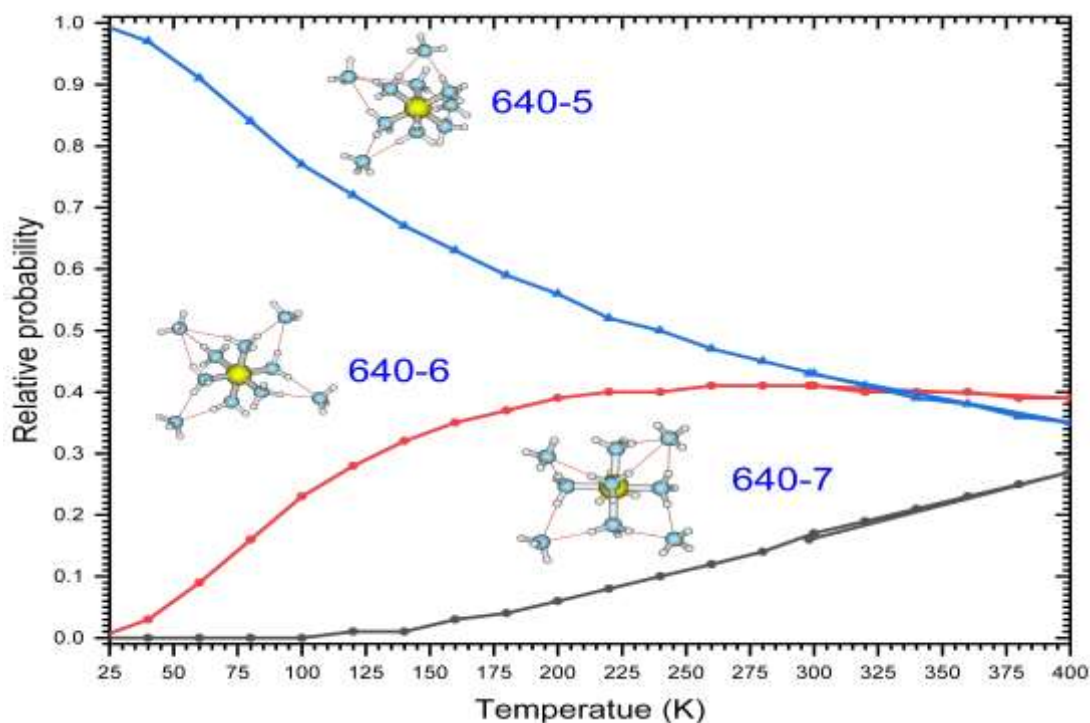


Figure 7s: Temperature dependence of the relative stability of different $\text{Fe}^{2+}(\text{NH}_3)_{n=10}$ isomers at MP2/6-31++G(d,p) level of theory at singlet spin-state

Table 1s : Relative zero-point electronic energies of all isomers presented in this work (in kJ/mol) and calculated at the MP2/6-31++G(d,p) level of theory.

Structures	Relative energies at HS	Relative energies at IS	Relative energies at LS
The monomer (n=1)			
100	0.0	0.0	0.0
The dimer (n=2)			
200-1	0.0	-	-
200-2	-	0.0	0.0
The trimer (n=3)			
300-1	0.0	-	317.0
300-2	-	0.0	12.1
300-3	-	-	0.0
210-1	-	180.3	197.5
210-2	-	185.5	194.8
The tetramer (n=4)			
400-1	0.0	-	-
400-2	-	0.0	17.1
400-3	-	-	0.0
310-1	96.8	-	-
310-2	-	132.1	147.2
310-3	-	156.7	147.7
310-4	-	-	133.0
310-5	-	-	136.9
220-1	-	293.9	306.6
220-2	250.6	312.7	-
220-3	269.0	327.6	350.7
The pentamer (n=5)			
500-1	0.0	0.0	-
500-2	-	-	0.0
410-1	27.7	-	-

410-2	-	35.6	113.4
410-3	-	-	100.2
320-1	111.7	-	-
320-2	130.6	-	-
320-3	176.2	-	-
320-4	178.0	-	-
320-5	-	194.9	244.7
320-6	-	-	241.9
320-7	-	-	226.2
230-1	274.2	-	-
230-2	-	343.5	411.6
500-3	-	-	541.5
The hexamer (n=6)			
600	0.0	0.0	0.0
510-1	25.0	10.2	-
510-2	-	-	73.1
420-1	50.7	-	-
420-2	-	34.4	184.4
420-3	-	-	172.7
330-1	138.5	-	-
330-2	193.6	-	-
330-3	-	213.9	314.2
321	-	-	348.1
240	293.4	-	501.9
The heptamer (n=7)			
610-1	0.0	0.0	0.0
610-2	1.5	-	-
520-1	24.3	9.8	-
520-2	28.3	11.3	-
520-3	-	-	73.4
430-1	49.8	-	-
430-2	52.0	-	-
430-3	-	-	174.0

340-1	129.1	-	-
340-2	-	-	304.1
331	-	-	342.3
The octamer (n=8)			
620-1	0.0	0.0	0.0
620-2	1.7	3.2	0.0
530-1	26.7	11.6	-
530-2	-	-	75.2
530-3	-	-	75.2
521	49.9	-	-
440-1	49.1	-	-
440-2	-	-	190.3
350	129.9	-	-
341	-	-	344.4
242	339.3	-	560.4
The nanomer (n=9)			
630-1	0.0	0.0	0.0
630-2	2.5	0.4	-
630-3	-	-	2.4
540-1	29.6	10.2	-
540-2	-	-	79.0
450-1	57.4	-	-
450-2	61.5	-	-
450-3	-	-	183.0
450-4	-	-	183.3
360-1	201.3	-	-
351	219.2	-	-
360-2	-	-	309.1
The decamer (n=10)			
640-1	0.0	-	-
640-2	-	0.0	-
640-3	0.7	-	-
640-4	5.0	-	-

640-5	-	-	0.0
640-6	-	-	1.3
640-7	-	-	5.5
550	-	-	86.4
460-1	62.6	-	-
451	72.5	-	-
442	85.0	-	-
460-2	-	-	187.3
370-1	205.2	-	-
361	-	-	328.9
370-2	-	-	335.2

Table 2s : Temperature dependence of the relative free energies between the Intermediate spin state (IS) and the Low spin state (LS) of $\text{Fe}^{2+}(\text{NH}_3)_{n=1}$. Calculations are performed at MP2-6-31++G(d,p) level of theory

Temperature (K)	100_IS	100_LS
1	0	143.09
20	0	143.51
40	0	143.51
60	0	143.51
80	0	143.93
100	0	143.93
120	0	144.35
140	0	144.35
160	0	144.77
180	0	144.77
200	0	145.18
220	0	145.18
240	0	145.18
260	0	145.6
280	0	145.6
300	0	146.02
320	0	146.02
340	0	146.44
360	0	146.44
380	0	146.44
400	0	146.86

Table 3s : Temperature dependence of the relative free energies between the Intermediate spin state (IS) and the Low spin state (LS) of $\text{Fe}^{2+}(\text{NH}_3)_n$. Calculations are performed at MP2-6-31++G(d,p) level of theory

Temperature (K)	200-2_IS	200-2_LS
1	0	134.31
20	0	134.31
40	0	134.31
60	0	134.31
80	0	134.72
100	0	134.72
120	0	134.72
140	0	134.72
160	0	134.72
180	0	134.72
200	0	134.72
220	0	134.72
240	0	134.72
260	0	134.72
280	0	134.72
300	0	134.72
320	0	135.14
340	0	135.14
360	0	135.14
380	0	135.14
400	0	135.14

Table 4s : Temperature dependence of the relative free energies between the Intermediate spin state (IS) and the Low spin state (LS) of $\text{Fe}^{2+}(\text{NH}_3)_n$. Calculations are performed at MP2-6-31++G(d,p) level of theory

Temperature (K)	300-2_IS	300-2_LS	300-3_LS
1	0	135.14	123.01
20	0	135.56	123.43
40	0	135.56	123.43
60	0	135.56	123.43
80	0	135.56	123.43
100	0	135.98	123.43
120	0	135.98	123.43
140	0	135.98	123.43
160	0	135.98	123.85
180	0	136.40	123.85
200	0	136.40	123.85
220	0	136.40	123.85
240	0	136.40	123.85
260	0	136.82	123.85
280	0	136.82	123.85
300	0	136.82	123.85
320	0	136.82	123.85
340	0	137.24	123.85
360	0	137.24	124.26
380	0	137.24	124.26
400	0	137.65	124.26

Table 5s : Temperature dependence of the relative free energies between the Intermediate spin state (IS) and the Low spin state (LS) of $\text{Fe}^{2+}(\text{NH}_3)_n$. Calculations are performed at MP2-6-31++G(d,p) level of theory

Temperature (K)	400-2_IS	400-2_LS	400-3_LS
1	0	144.35	127.19
20	0	144.77	127.61
40	0	144.77	127.61
60	0	145.18	128.03
80	0	145.18	128.03
100	0	145.60	128.45
120	0	145.60	128.45
140	0	146.02	128.45
160	0	146.02	128.87
180	0	146.44	128.87
200	0	146.44	128.87
220	0	146.86	128.87
240	0	146.86	129.29
260	0	147.28	129.29
280	0	147.28	129.29
300	0	147.70	129.70
320	0	147.70	129.70
340	0	148.11	129.70
360	0	148.11	129.70
380	0	148.53	129.70
400	0	148.95	130.12

Table 6s : Temperature dependence of the relative free energies between the Intermediate spin state (IS) and the Low spin state (LS) of $\text{Fe}^{2+}(\text{NH}_3)_n$. Calculations are performed at MP2-6-31++G(d,p) level of theory

Temperature (K)	500-1_IS	500-1_LS
1	0	68.62
20	0	69.04
40	0	69.04
60	0	69.45
80	0	69.87
100	0	70.71
120	0	71.13
140	0	71.55
160	0	71.96
180	0	72.80
200	0	73.22
220	0	74.06
240	0	74.48
260	0	75.31
280	0	75.73
300	0	76.57
320	0	76.99
340	0	77.82
360	0	78.66
380	0	79.08
400	0	79.91

Table 7s : Temperature dependence of the relative free energies between the Intermediate spin state (IS) and the Low spin state (LS) of $\text{Fe}^{2+}(\text{NH}_3)_n=6$. Calculations are performed at MP2-6-31++G(d,p) level of theory

Temperature (K)	600_IS	600_LS
1	0.42	0.00
20	0	0.00
40	0	0.00
60	0	0.00
80	0	0.42
100	0	0.84
120	0	1.67
140	0	2.09
160	0	2.93
180	0	3.35
200	0	4.18
220	0	5.02
240	0	5.86
260	0	6.69
280	0	7.53
300	0	8.37
320	0	9.20
340	0	10.04
360	0	10.88
380	0	12.13
400	0	12.97

Table 8s : Temperature dependence of the relative free energies between the Intermediate spin state (IS) and the Low spin state (LS) of $\text{Fe}^{2+}(\text{NH}_3)_n=7$. Calculations are performed at MP2-6-31++G(d,p) level of theory

Temperature (K)	610-1_IS	610-1_LS
1	2.09	0
20	1.67	0
40	1.26	0
60	0.84	0
80	0.42	0
100	0	0.42
120	0	1.67
140	0	2.51
160	0	3.77
180	0	4.60
200	0	5.86
220	0	7.11
240	0	8.37
260	0	9.62
280	0	10.88
300	0	12.13
320	0	13.39
340	0	14.64
360	0	16.32
380	0	17.57
400	0	18.83

Table 9s : Temperature dependence of the relative free energies between the Intermediate spin state (IS) and the Low spin state (LS) of $\text{Fe}^{2+}(\text{NH}_3)_n$. Calculations are performed at MP2-6-31++G(d,p) level of theory

Temperature (K)	530-1_IS	620-1_IS	620-1_LS	620-2_IS	620-2_LS
1	16.32	4.60	0	7.95	0.00
20	16.32	4.60	0	7.95	0.42
40	15.90	4.60	0	7.95	0.84
60	15.06	4.18	0	7.95	1.26
80	14.64	3.77	0	7.53	1.67
100	13.39	3.35	0	7.53	2.09
120	12.55	2.51	0	7.11	2.93
140	11.72	2.09	0	6.69	3.35
160	10.46	1.26	0	6.28	3.77
180	9.20	0.42	0	5.44	4.18
200	8.79	0.00	0.42	5.44	5.02
220	8.37	0.00	1.26	5.86	6.28
240	8.37	0.00	2.09	6.28	7.53
260	7.95	0.00	3.35	6.28	8.79
280	7.53	0.00	4.18	6.69	10.46
300	7.53	0.00	5.02	7.11	11.72
320	7.11	0.00	6.28	7.11	12.97
340	7.11	0.00	7.11	7.53	14.64
360	6.69	0.00	8.37	7.95	15.90
380	6.69	0.00	9.20	7.95	17.57
400	6.28	0.00	10.46	8.37	18.83

Table 10s : Temperature dependence of the relative free energies between the Intermediate spin state (IS) and the Low spin state (LS) of $\text{Fe}^{2+}(\text{NH}_3)_n$. Calculations are performed at MP2-6-31++G(d,p) level of theory

Temperature (K)	540-1_IS	630-1_IS	630-1_LS	630-2_IS	630-3_LS
1	21.76	11.30	0	11.72	2.51
20	21.34	11.30	0	11.72	2.51
40	20.92	10.88	0	11.30	2.51
60	20.08	10.46	0	10.88	2.51
80	18.83	10.04	0	10.46	2.93
100	17.99	9.20	0	9.62	2.93
120	16.74	8.37	0	8.79	2.93
140	15.06	7.53	0	7.95	2.93
160	13.81	6.69	0	7.11	2.93
180	12.55	5.44	0	6.28	2.93
200	10.88	4.60	0	5.02	2.93
220	9.62	3.35	0	3.77	2.93
240	7.95	2.51	0	2.93	2.93
260	6.28	1.26	0	1.67	2.93
280	5.02	0.00	0	0.42	2.93
300	4.60	0.00	1.26	0.42	4.18
320	4.18	0.00	2.51	0.42	5.02
340	4.18	0.00	3.77	0.42	6.28
360	3.77	0.00	5.02	0.00	7.53
380	3.35	0.00	6.28	0.00	9.20
400	3.35	0.00	7.95	0.00	10.46

Table 11s : Temperature dependence of the relative free energies between the Intermediate spin state (IS) and the Low spin state (LS) of $\text{Fe}^{2+}(\text{NH}_3)_{n=10}$. Calculations are performed at MP2-6-31++G(d,p) level of theory

Temperature (K)	640-2_Is	640-5_LS	640-6_LS
1	9.20	0.00	1.26
20	8.79	0.00	1.26
40	8.37	0.00	1.26
60	7.53	0.00	1.26
80	6.69	0.00	1.26
100	5.44	0.00	0.84
120	4.18	0.00	0.84
140	2.93	0.00	0.84
160	1.26	0.00	0.84
180	0.00	0.00	0.84
200	0.00	1.67	2.09
220	0.00	3.35	3.77
240	0.00	5.02	5.44
260	0.00	6.69	6.69
280	0.00	8.37	8.37
300	0.00	10.04	10.04
320	0.00	11.72	11.72
340	0.00	13.39	13.39
360	0.00	15.06	15.06
380	0.00	17.15	16.74
400	0.00	18.83	18.41

**Cartesian coordinates of all the proposed isomers of
[Fe²(NH₃)_{n=1-10}] at MP2-6-31++G(d,p) level of theory
quintet spin-state**

Cartesian coordinates of the monomer : [Fe(NH₃)₂]²⁺

Cartesian coordinates of : 100_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.443949	0.000157	-0.001551
1	-1.854304	-0.033494	0.942314
1	-1.861179	-0.800907	-0.493806
1	-1.861674	0.833228	-0.436770
26	0.603262	0.000003	-0.000034

Cartesian coordinates of the dimer : [Fe(NH₃)₂]₂²⁺

Cartesian coordinates of : 200-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.058719	0.000145	-0.019044
1	-2.473318	0.817178	-0.480714
1	-2.484530	-0.006687	0.915483
1	-2.473228	-0.810200	-0.492454
26	0.000004	-0.000100	0.014692
7	2.058708	0.000144	-0.019043
1	2.473217	-0.810188	-0.492479
1	2.484527	-0.006707	0.915481
1	2.473305	0.817192	-0.480694

Cartesian coordinates of the trimer : [Fe(NH₃)₃]₂²⁺

Cartesian coordinates of : 300-1HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
26	0.000000	-0.000000	0.000000
7	1.984922	-0.675981	0.000000
1	2.525885	-0.364738	-0.812084
1	2.525843	-0.364868	0.812162
1	2.084250	-1.694942	-0.000080
7	-0.407044	2.056983	0.000000

1	0.425738	2.652484	-0.000146
1	-0.947127	2.369839	-0.812050
1	-0.946879	2.369888	0.812197
7	-1.577879	-1.381001	-0.000000
1	-1.578991	-2.004914	-0.812235
1	-2.509988	-0.957540	0.000226
1	-1.578733	-2.005205	0.812011

Cartesian coordinates of the tetramer : [Fe(NH3)4]2+

Cartesian coordinates of : 220-2_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.113488	0.416148	0.000006
1	4.301407	1.003154	0.810673
1	4.301393	1.003204	-0.810627
1	4.856044	-0.281847	-0.000022
7	1.747632	-0.999496	-0.000003
1	1.866787	-1.613419	-0.810573
1	2.653917	-0.374221	0.000000
1	1.866784	-1.613423	0.810564
7	-1.747632	0.999496	-0.000003
1	-1.866787	1.613419	-0.810573
1	-1.866783	1.613424	0.810564
1	-2.653916	0.374222	0.000002
7	-4.113488	-0.416148	0.000006
1	-4.301400	-1.003185	-0.810639
1	-4.856044	0.281847	0.000001
1	-4.301401	-1.003172	0.810661
26	0.000000	0.000000	-0.000003

Cartesian coordinates of : 220-3_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.393308	2.224706	0.276168
1	2.583972	2.284811	1.274167
1	2.089143	3.157309	0.004260
1	3.306052	2.110472	-0.160834
7	0.861812	0.000001	-0.625200
1	1.026012	-0.000014	-1.635352
1	1.397405	0.851046	-0.255803
1	1.397428	-0.851029	-0.255790
26	-1.055474	-0.000045	-0.135490
7	2.393360	-2.224644	0.276191
1	3.305969	-2.110610	-0.161145
1	2.089042	-3.157311	0.004673
1	2.584344	-2.284451	1.274147
7	-3.066832	0.000050	0.362937

1	-3.354377	-0.809201	0.922281
1	-3.700132	0.000718	-0.441946
1	-3.354057	0.808632	0.923407

 Cartesian coordinates of : 310-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
26	0.021776	0.010559	-0.068978
7	0.140619	-0.054996	1.993673
1	1.091081	-0.173298	2.350969
1	-0.417951	-0.836292	2.452378
1	-0.198542	0.795692	2.448203
7	0.675237	1.741629	-1.070688
1	0.636130	1.674799	-2.090716
1	1.645192	1.994839	-0.863646
1	0.134857	2.580870	-0.844072
7	-0.727659	-1.686534	-1.061744
1	-0.192900	-2.539739	-0.880080
1	-0.740147	-1.599800	-2.080902
1	-1.690396	-1.922668	-0.808780
7	-1.302348	-2.075060	3.426284
1	-0.970175	-3.035107	3.365414
1	-2.313173	-2.132555	3.323549
1	-1.154661	-1.810001	4.398665

 Cartesian coordinates of : 400-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.289967	1.280607	-1.138396
1	1.922258	0.771451	-1.759052
1	1.901613	1.887829	-0.589739
1	0.785427	1.916576	-1.759063
7	-1.289967	-1.280607	-1.138395
1	-1.922258	-0.771451	-1.759052
1	-0.785427	-1.916576	-1.759063
1	-1.901614	-1.887829	-0.589739
7	-1.280616	1.289958	1.138396
1	-0.771462	1.922240	1.759063
1	-1.916594	0.785416	1.759052
1	-1.887828	1.901614	0.589739
26	0.000000	0.000000	-0.000000
7	1.280616	-1.289958	1.138396
1	1.887828	-1.901614	0.589739
1	0.771462	-1.922240	1.759063
1	1.916595	-0.785416	1.759052

Cartesian coordinates of the pentamer : [Fe(NH3)5]2+

Cartesian coordinates of : 230-1_HS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

7 -4.353537 0.753858 0.043587
1 -4.376977 1.561591 0.662755
1 -5.186952 0.216539 0.277304
1 -4.528694 1.121506 -0.889436
7 -2.213612 -1.008462 0.351445
1 -2.527853 -1.817226 -0.191523
1 -2.301128 -1.300700 1.327976
1 -3.002378 -0.273235 0.213076
7 1.501876 0.128503 -0.641841
1 2.226000 -0.556770 -0.267115
1 1.668890 0.164954 -1.650086
1 1.797435 1.080350 -0.272823
26 -0.357906 -0.382241 -0.151641
7 3.532583 -1.671024 0.298537
1 3.773617 -1.599942 1.284629
1 4.377719 -1.401953 -0.201404
1 3.428496 -2.667228 0.118635
7 2.414033 2.694173 0.286866
1 2.476200 2.843784 1.291364
1 1.940672 3.517283 -0.079072
1 3.371103 2.769981 -0.051785

Cartesian coordinates of : 320-1_HS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

7 -0.239385 -2.534736 -0.152149
1 -0.272338 -3.006848 0.754427
1 0.516376 -2.995732 -0.664437
1 -1.095191 -2.825647 -0.629671
7 1.588155 0.272848 1.085776
1 2.013220 -0.414225 1.711945
1 2.395027 0.640316 0.488950
1 1.332892 1.050027 1.699392
7 -1.360798 0.764033 -0.954778
1 -1.663909 0.412512 -1.865667
1 -2.260891 0.925314 -0.401938
1 -0.999717 1.699818 -1.152873
26 0.002459 -0.442573 -0.005002
7 -3.805051 1.291644 0.408864
1 -3.897225 2.295536 0.551084
1 -4.010135 0.875183 1.314113
1 -4.590545 1.036110 -0.186298
7 3.816048 1.280063 -0.373285
1 3.983388 2.251236 -0.117779
1 3.837501 1.264368 -1.390271
1 4.654837 0.781957 -0.081914

 Cartesian coordinates of : 410-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.821679	-0.747338	1.396022
1	0.792195	-0.319807	2.322014
1	1.762061	-0.553605	1.023654
1	0.793246	-1.752347	1.570559
7	-1.948450	1.536515	0.663093
1	-2.611232	1.232838	1.378552
1	-1.460408	2.327267	1.087367
1	-2.527299	1.951917	-0.068746
7	0.819134	0.797632	-1.368292
1	0.771109	0.422429	-2.315885
1	1.759649	0.566941	-1.017822
1	0.808969	1.811168	-1.486720
7	-1.875206	-1.584415	-0.688070
1	-1.348597	-2.355403	-1.102502
1	-2.534253	-1.305449	-1.416916
1	-2.452834	-2.022446	0.031436
26	-0.605208	0.000764	0.001492
7	3.600353	-0.004928	-0.006676
1	4.029287	-0.799275	0.466218
1	4.003167	0.812486	0.449184
1	4.027777	-0.018860	-0.931742

 Cartesian coordinates of : 500-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.026950	-2.227286	-0.014097
1	0.842304	-2.642450	0.437639
1	0.023443	-2.625999	-0.954683
1	-0.771677	-2.659264	0.451565
7	2.273084	-0.075367	-0.034441
1	2.707718	-0.459014	0.805180
1	2.672525	-0.617905	-0.800805
1	2.697514	0.847229	-0.133774
7	-0.058240	1.269261	-1.768446
1	-0.430047	2.203994	-1.593615
1	-0.648834	0.897808	-2.513585
1	0.843738	1.432684	-2.215438
7	0.020922	1.237509	1.788149
1	-0.819135	1.798306	1.931380
1	0.788615	1.908165	1.832092
1	0.111616	0.693140	2.647666
26	0.003121	-0.035947	0.000178
7	-2.267859	-0.123989	0.029084
1	-2.667911	-0.450740	0.909020
1	-2.679636	-0.731483	-0.679854
1	-2.715380	0.779260	-0.129164

Cartesian coordinates of the hexamer : [Fe(NH₃)₆]²⁺

Cartesian coordinates of : 240_HS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

7	-3.475410	2.266772	-0.170839
1	-3.170894	3.191579	0.124351
1	-4.380323	2.133119	0.275627
1	-3.679588	2.354473	-1.163638
7	-1.884544	0.000035	0.661582
1	-2.437074	-0.842614	0.333317
1	-1.971466	0.000073	1.679878
1	-2.437127	0.842620	0.333243
7	1.884541	0.000023	-0.661574
1	2.437106	-0.842601	-0.333303
1	1.971458	0.000057	-1.679870
1	2.437093	0.842634	-0.333247
26	-0.000001	0.000030	0.000005
7	-3.475227	-2.266915	-0.170622
1	-4.380718	-2.132362	0.274399
1	-3.171395	-3.191396	0.126290
1	-3.678063	-2.355950	-1.163577
7	3.475351	-2.266832	0.170621
1	3.678310	-2.355747	1.163561
1	4.380784	-2.132314	-0.274529
1	3.171499	-3.191353	-0.126146
7	3.475293	2.266850	0.170822
1	3.679138	2.354862	1.163662
1	3.170916	3.191574	-0.124770
1	4.380353	2.133015	-0.275292

Cartesian coordinates of : 330-1_HS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

7	-3.964978	1.392170	0.654209
1	-4.029206	2.255622	1.189518
1	-4.745376	0.823900	0.976418
1	-4.200293	1.655247	-0.299744
7	-1.259297	-1.944651	-1.486580
1	-2.246023	-2.098372	-1.271714
1	-1.241909	-1.663581	-2.469155
1	-0.836107	-2.875057	-1.468161
7	-1.427112	0.209859	1.319471
1	-1.663457	-0.478104	2.037606
1	-2.353220	0.629266	1.016387
1	-0.948728	0.956553	1.827182
26	-0.285520	-0.568235	-0.208909

7	1.665410	-0.142528	-0.532995
1	2.266281	-0.385099	0.296062
1	1.839719	0.874145	-0.739830
1	2.083605	-0.645827	-1.317229
7	3.430971	-0.827439	1.703375
1	3.082686	-1.202374	2.582168
1	3.984175	-0.013561	1.961341
1	4.105737	-1.513199	1.371876
7	2.277714	2.654467	-1.156898
1	3.049496	2.624254	-1.819457
1	2.632796	3.175596	-0.358827
1	1.584383	3.261550	-1.586881

 Cartesian coordinates of : 330-2_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	2.625113	-3.271547	-0.276618
1	2.315306	-4.178426	0.066476
1	3.607478	-3.212500	-0.016653
1	2.623216	-3.356420	-1.290238
7	1.193320	1.322436	-0.963300
1	0.891462	1.667004	-1.874854
1	1.296562	2.184204	-0.368081
1	2.145926	0.988559	-1.110816
7	1.178480	-1.203162	1.124661
1	1.904993	-0.646296	1.576787
1	1.698356	-1.941347	0.570424
1	0.726661	-1.713715	1.885086
26	-0.103003	-0.078538	-0.065468
7	-1.991634	0.361069	-0.836582
1	-2.101623	0.063921	-1.808509
1	-2.189863	1.362883	-0.855667
1	-2.803781	-0.078560	-0.322374
7	-4.299608	-0.783615	0.474643
1	-5.102501	-0.463497	-0.062913
1	-4.486481	-0.489231	1.430243
1	-4.375792	-1.797913	0.485051
7	1.532168	3.759342	0.624134
1	2.530981	3.930934	0.717935
1	1.154092	3.879931	1.560576
1	1.178211	4.550788	0.091122

 Cartesian coordinates of : 420-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	0.877727	1.966375	1.045114
1	1.314534	2.672493	0.451149
1	1.602612	1.701014	1.712721
1	0.189219	2.482618	1.594128
7	1.615363	-0.416463	-1.236914

1	1.940584	0.218338	-1.967405
1	2.473651	-0.663289	-0.684955
1	1.368985	-1.273448	-1.734098
7	-1.016332	-0.927157	1.304322
1	-1.083887	-0.591396	2.265125
1	-0.650124	-1.876025	1.381113
1	-1.986704	-1.020040	0.971030
7	-1.665074	0.798383	-1.267731
1	-1.949672	1.777603	-1.261952
1	-2.468769	0.266099	-0.911627
1	-1.583675	0.553389	-2.254720
26	0.040977	0.322048	-0.064157
7	-3.965457	-1.011933	0.114975
1	-4.587841	-0.383555	0.620485
1	-4.104630	-1.919759	0.556211
1	-4.396571	-1.121254	-0.801644
7	4.083753	-1.166937	0.164115
1	4.148093	-1.291938	1.171234
1	4.844155	-0.534637	-0.075716
1	4.354785	-2.065329	-0.230172

 Cartesian coordinates of : 510-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.003406	1.435312	-0.551859
1	-0.986174	1.724257	-1.530537
1	-0.963354	2.307639	-0.024957
1	-1.948406	1.055587	-0.392619
7	-1.126734	-1.560790	-0.008175
1	-2.026640	-1.073767	0.052914
1	-1.202938	-2.140432	-0.843537
1	-1.119402	-2.223710	0.765964
7	0.839775	-0.168743	2.128241
1	1.457321	0.534896	2.531641
1	1.239470	-1.060403	2.422977
1	-0.025966	-0.090462	2.662338
26	0.516820	-0.022353	-0.045243
7	2.130745	1.562761	-0.283049
1	2.360486	1.783182	-1.252176
1	3.026413	1.328943	0.145252
1	1.883075	2.462081	0.129253
7	1.814311	-1.446723	-1.102157
1	2.815387	-1.275527	-1.008669
1	1.647252	-1.454792	-2.109489
1	1.687324	-2.416432	-0.811844
7	-3.861602	0.231774	-0.086366
1	-4.299297	-0.472418	0.505112
1	-4.293240	0.105101	-1.000272
1	-4.240256	1.112320	0.258510

 Cartesian coordinates of : 600_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.977243	1.602700	1.296221
1	1.935187	1.370454	1.558190
1	0.504194	1.759293	2.185746
1	1.052030	2.530689	0.880130
7	1.874480	0.054630	-1.298818
1	2.146431	1.001714	-1.562061
1	2.718417	-0.339277	-0.883488
1	1.775210	-0.434784	-2.187734
7	-1.874762	0.043910	1.298817
1	-1.772696	-0.444927	2.187733
1	-2.716432	-0.354816	0.883487
1	-2.152125	0.989424	1.562059
26	-0.000000	0.000005	-0.000000
7	0.901203	-1.646591	1.296314
1	1.666824	-2.175750	0.879535
1	0.221424	-2.359811	1.559825
1	1.274658	-1.314535	2.185032
7	-0.891767	-1.651727	-1.296305
1	-1.654347	-2.185258	-0.879523
1	-0.207918	-2.361048	-1.559813
1	-1.267116	-1.321819	-2.185025
7	-0.986397	1.597076	-1.296229
1	-1.066496	2.524623	-0.880140
1	-1.942995	1.359349	-1.558200
1	-0.514249	1.756372	-2.185752

Cartesian coordinates of the heptamer : [Fe(NH3)7]2+

Cartesian coordinates of : 340_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.511858	-0.959987	-0.103506
1	1.439961	-1.976485	-0.168922
1	2.134776	-0.784626	0.719825
1	2.053568	-0.668130	-0.953474
7	-1.957674	-0.797028	-0.916628
1	-2.370143	-1.637886	-0.422705
1	-2.727413	-0.132561	-1.008962
1	-1.767810	-1.108391	-1.870832
7	-0.518931	1.705216	1.133033
1	-1.131305	1.590051	1.942636
1	-0.921449	2.516726	0.588398
1	0.361498	2.048279	1.520331
26	-0.289164	-0.029411	0.032015
7	3.344612	-0.580492	2.186445
1	2.983879	-0.600625	3.136994

1	3.949150	0.236202	2.144026
1	3.972328	-1.379058	2.125816
7	3.097550	-0.238349	-2.478304
1	4.003016	0.115342	-2.178858
1	2.763010	0.431988	-3.165627
1	3.302472	-1.083215	-3.006690
7	-1.606375	4.012052	-0.233865
1	-0.992787	4.800414	-0.039671
1	-2.508331	4.275205	0.156868
1	-1.737571	4.019513	-1.242236
7	-3.176337	-3.092914	0.337141
1	-2.812472	-3.466959	1.209966
1	-3.182014	-3.878308	-0.309888
1	-4.157024	-2.892267	0.520389

 Cartesian coordinates of : 430-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	1.631829	-0.516480	-1.273801
1	2.473140	-0.831076	-0.739398
1	1.918150	0.337138	-1.753446
1	1.521076	-1.204863	-2.018726
7	0.337872	1.266618	1.296680
1	1.153945	1.115528	1.889949
1	0.518475	2.172358	0.804186
1	-0.423653	1.466906	1.945385
7	-1.780659	-0.125887	-1.298356
1	-1.846894	-0.822445	-2.040939
1	-1.838206	0.771897	-1.779216
1	-2.673415	-0.209501	-0.762905
7	-0.545878	-2.023713	1.150733
1	-0.322061	-2.905305	0.688897
1	-1.531730	-2.096222	1.402699
1	-0.041727	-2.058706	2.036937
26	-0.080338	-0.291737	-0.057822
7	4.093537	-1.436227	0.095183
1	4.337163	-2.357906	-0.260360
1	4.200945	-1.503419	1.103901
1	4.848403	-0.826901	-0.211866
7	-4.391352	-0.363091	0.102169
1	-4.970802	0.323634	-0.376006
1	-4.536083	-0.182555	1.092356
1	-4.843897	-1.256756	-0.076401
7	0.850640	3.888712	0.036088
1	0.806712	4.054211	-0.966106
1	1.771032	4.216626	0.320041
1	0.196296	4.552985	0.443528

 Cartesian coordinates of : 430-2_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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7	1.736439	-1.739161	0.055633
1	2.630952	-1.199455	0.008216
1	1.787270	-2.400475	-0.719931
1	1.816481	-2.318912	0.891722
7	-0.191244	0.916104	-1.574937
1	-0.181074	1.857525	-1.163431
1	-1.058062	0.851422	-2.107972
1	0.553498	0.900155	-2.270845
7	-1.662945	-1.792949	-0.051681
1	-2.574019	-1.281501	-0.003915
1	-1.726303	-2.377548	-0.885828
1	-1.691443	-2.453233	0.725905
26	0.017128	-0.521695	-0.001506
7	0.177089	0.927801	1.566861
1	1.071055	0.938399	2.057206
1	0.066942	1.864770	1.159804
1	-0.529206	0.848133	2.297549
7	-0.133270	3.731026	0.001559
1	0.786048	4.162195	-0.076624
1	-0.674866	4.140316	-0.757853
1	-0.540775	4.141247	0.840155
7	-4.327351	-0.518820	0.089904
1	-4.810427	-0.945367	0.877430
1	-4.862771	-0.795927	-0.729797
1	-4.488580	0.479951	0.188907
7	4.361700	-0.384212	-0.083794
1	4.902118	-0.643557	0.738440
1	4.496692	0.618077	-0.186433
1	4.858207	-0.800675	-0.868363

Cartesian coordinates of : 520-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.584902	1.591330	-0.104760
1	1.630897	2.263768	0.659323
1	1.540182	2.161094	-0.948777
1	2.505355	1.142641	-0.135370
7	-1.496123	1.337335	-0.785961
1	-1.485640	2.284003	-0.407935
1	-1.418905	1.460197	-1.795913
1	-2.446029	0.973252	-0.625762
7	-1.581229	-1.609201	-0.063854
1	-1.603823	-2.284627	0.698552
1	-1.558604	-2.176554	-0.910428
1	-2.502257	-1.161172	-0.069460
7	-0.035329	0.098393	2.236049
1	0.879276	-0.059716	2.659086
1	-0.655472	-0.565753	2.697116
1	-0.325568	1.010432	2.588903
26	-0.001025	-0.006855	0.033391
7	1.518259	-1.408668	-0.630296
1	2.464022	-1.016209	-0.522972

1	1.436841	-1.656651	-1.616588
1	1.522332	-2.301483	-0.137950
7	-4.366196	0.112691	-0.364007
1	-4.745322	-0.156401	-1.270117
1	-4.783226	1.021194	-0.169145
1	-4.814800	-0.513369	0.302017
7	4.377427	-0.109696	-0.379608
1	4.811370	-0.995182	-0.124808
1	4.834348	0.572245	0.222909
1	4.729696	0.091241	-1.313801

 Cartesian coordinates of : 520-2_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-0.000020	-2.776555	-0.830908
1	0.809778	-3.328739	-0.549230
1	-0.000026	-2.816310	-1.850876
1	-0.809819	-3.328731	-0.549221
7	2.242552	-0.634801	-0.169661
1	2.762590	-1.134830	0.549927
1	2.655542	-0.943199	-1.049123
1	2.512404	0.350672	-0.078289
7	0.000009	1.307178	-0.792000
1	-0.833084	1.818683	-0.481765
1	0.000009	1.382383	-1.809201
1	0.833107	1.818674	-0.481765
7	-0.000002	-0.725568	2.136677
1	-0.808389	-0.261562	2.549228
1	0.808382	-0.261552	2.549224
1	0.000005	-1.658802	2.549521
26	-0.000005	-0.718938	-0.069294
7	-2.242560	-0.634773	-0.169659
1	-2.762604	-1.134795	0.549930
1	-2.655555	-0.943166	-1.049120
1	-2.512399	0.350703	-0.078287
7	2.870606	2.556940	-0.017584
1	3.151056	2.934679	-0.920773
1	3.747685	2.326240	0.445493
1	2.518043	3.357632	0.503145
7	-2.870575	2.556973	-0.017583
1	-3.151022	2.934715	-0.920772
1	-2.518001	3.357661	0.503145
1	-3.747656	2.326285	0.445495

 Cartesian coordinates of : 610-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	1.143481	0.014831	1.553807
1	1.147431	0.827935	2.167895
1	2.066434	0.007415	1.104977

1	1.143033	-0.784689	2.185479
7	-2.129534	-0.016500	1.572796
1	-1.751694	-0.007080	2.519606
1	-2.765425	0.779724	1.542059
1	-2.742722	-0.830563	1.548830
7	3.978695	0.001210	0.000017
1	4.376045	0.938801	-0.000370
1	4.403971	-0.459093	-0.802776
1	4.404005	-0.458434	0.803170
26	-0.490895	-0.000145	-0.000000
7	1.143495	0.014946	-1.553814
1	1.147460	0.828093	-2.167844
1	1.143052	-0.784528	-2.185544
1	2.066442	0.007494	-1.104974
7	-2.129515	-0.016357	-1.572800
1	-1.751679	-0.006615	-2.519607
1	-2.765541	0.779752	-1.541841
1	-2.742565	-0.830530	-1.549051
7	-0.417311	-2.295185	-0.000089
1	-0.846525	-2.747097	-0.806691
1	-0.846657	-2.747175	0.806399
1	0.542625	-2.639016	-0.000030
7	-0.466175	2.295881	0.000087
1	0.485275	2.662382	0.000069
1	-0.905804	2.737570	0.806749
1	-0.905854	2.737628	-0.806517

 Cartesian coordinates of : 610-2_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	0.946350	-1.364481	1.095634
1	1.891804	-1.047230	0.866785
1	0.925073	-2.354078	0.853493
1	0.893622	-1.347962	2.112950
7	-1.764696	-1.805571	-0.580330
1	-1.280313	-2.449852	-1.204269
1	-2.061133	-2.386195	0.203482
1	-2.626808	-1.579821	-1.075319
7	-1.849953	1.380651	-1.196185
1	-1.869799	1.139754	-2.186437
1	-1.591486	2.366398	-1.173668
1	-2.829511	1.370934	-0.913245
7	0.923032	-0.244737	-1.750493
1	0.878099	0.502974	-2.441459
1	0.854159	-1.102058	-2.296710
1	1.879528	-0.222343	-1.390142
26	-0.494701	-0.004429	0.000753
7	0.895055	1.694235	0.612749
1	1.847270	1.339444	0.501376
1	0.832320	1.993225	1.584743
1	0.867180	2.559179	0.074890
7	-1.831458	0.349758	1.797311
1	-2.776195	-0.027995	1.732199

1	-1.965170	1.338322	2.008564
1	-1.456487	-0.047554	2.657811
7	3.796072	-0.001782	0.020757
1	4.208900	0.722097	-0.565552
1	4.231250	-0.864022	-0.304044
1	4.209101	0.155425	0.938888

Cartesian coordinates of the octamer : [Fe(NH₃)₈]²⁺

Cartesian coordinates of : 242_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.715695	-1.913947	-0.091466
1	4.516803	-1.300336	0.071188
1	3.987290	-2.547285	-0.839612
1	3.627342	-2.496816	0.736792
7	3.715686	1.913947	-0.091459
1	4.516796	1.300338	0.071195
1	3.987282	2.547289	-0.839601
1	3.627328	2.496813	0.736801
26	-0.000001	-0.000003	0.000008
7	1.784689	-0.000004	-0.873092
1	2.404711	-0.820647	-0.593082
1	2.404708	0.820642	-0.593084
1	1.759654	-0.000006	-1.894175
7	6.395095	0.000005	0.333817
1	6.750884	-0.804449	0.844526
1	6.750833	0.804345	0.844741
1	6.899752	0.000136	-0.549353
7	-1.784695	0.000002	0.873101
1	-2.404714	0.820645	0.593084
1	-1.759665	0.000007	1.894185
1	-2.404712	-0.820645	0.593092
7	-3.715688	1.913949	0.091455
1	-4.516796	1.300339	-0.071204
1	-3.627327	2.496816	-0.736805
1	-3.987288	2.547290	0.839596
7	-3.715690	-1.913948	0.091466
1	-3.627329	-2.496819	-0.736791
1	-4.516797	-1.300338	-0.071197
1	-3.987292	-2.547285	0.839609
7	-6.395090	0.000002	-0.333839
1	-6.899753	0.000016	0.549327
1	-6.750851	-0.804401	-0.844647
1	-6.750847	0.804393	-0.844670

 Cartesian coordinates of : 350_HS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

 7 2.775351 -0.866099 2.852865
 1 2.229818 -0.558612 3.653708
 1 3.709012 -0.492816 3.007163
 1 2.868944 -1.872990 2.959308
 7 -0.688996 1.785436 -1.316177
 1 -0.384326 2.723415 -0.944771
 1 -0.380164 1.765520 -2.289475
 1 -1.707571 1.828789 -1.365926
 7 2.015230 0.017089 0.127930
 1 2.478585 -0.658843 -0.523911
 1 2.241742 -0.305020 1.096921
 1 2.524338 0.893795 0.011333
 26 0.013487 0.171310 -0.218880
 7 -1.340581 -1.214956 0.412005
 1 -1.870620 -1.647744 -0.378993
 1 -2.055022 -0.822543 1.067147
 1 -0.916864 -1.997079 0.912205
 7 -2.876838 -2.519489 -1.763553
 1 -3.870847 -2.328292 -1.665177
 1 -2.784142 -3.524353 -1.635240
 1 -2.667651 -2.355663 -2.744821
 7 -3.404814 -0.210044 2.290438
 1 -3.501095 -0.915422 3.017062
 1 -4.320803 -0.151044 1.852691
 1 -3.286005 0.669332 2.786443
 7 3.420663 -1.847482 -1.687453
 1 2.912795 -2.438890 -2.339858
 1 3.982177 -2.484957 -1.128268
 1 4.087778 -1.331619 -2.256177
 7 0.083425 4.437610 -0.406648
 1 0.767235 4.861580 -1.029233
 1 0.446798 4.581270 0.531999
 1 -0.738857 5.033663 -0.469103

 Cartesian coordinates of : 440-1_HS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

 7 0.895023 -1.558872 -1.115960
 1 1.777123 -1.263944 -1.588155
 1 0.296908 -1.911932 -1.862541
 1 1.141042 -2.381629 -0.566062
 7 -1.558863 -0.894983 1.115995
 1 -1.911915 -0.296847 1.862563
 1 -1.263929 -1.777070 1.588212
 1 -2.381625 -1.141020 0.566112
 7 1.558855 0.895027 1.115972
 1 1.263916 1.777129 1.588159

1	1.911906	0.296918	1.862563
1	2.381620	1.141048	0.566086
26	0.000000	0.000001	-0.000004
7	-0.895013	1.558831	-1.116026
1	-0.296892	1.911862	-1.862616
1	-1.777110	1.263885	-1.588217
1	-1.141037	2.381610	-0.566161
7	-3.418735	0.845463	-2.527756
1	-3.360251	1.332077	-3.419428
1	-3.678399	-0.108536	-2.764213
1	-4.234265	1.239010	-2.064392
7	0.845508	3.418765	2.527684
1	1.239058	4.234286	2.064308
1	1.332126	3.360289	3.419354
1	-0.108488	3.678438	2.764143
7	-0.845532	-3.418676	2.527796
1	-1.332161	-3.360172	3.419457
1	0.108462	-3.678340	2.764276
1	-1.239074	-4.234213	2.064441
7	3.418756	-0.845557	-2.527697
1	3.360279	-1.332203	-3.419351
1	4.234282	-1.239086	-2.064312
1	3.678422	0.108433	-2.764187

 Cartesian coordinates of : 521_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-3.291860	0.055170	1.089300
1	-3.810313	-0.822246	1.061675
1	-3.967645	0.769017	0.818473
1	-3.130802	0.222090	2.081974
7	-0.587283	1.750786	0.970344
1	0.435791	1.808992	0.842027
1	-0.746347	1.756550	1.976912
1	-0.956910	2.643943	0.644432
7	-2.564853	-0.192211	-1.933694
1	-3.488608	-0.601057	-1.797006
1	-2.737703	0.692588	-2.412117
1	-2.114867	-0.783327	-2.632319
26	-1.355215	0.042191	-0.111608
7	0.496717	0.119839	-1.379752
1	1.209665	0.595181	-0.818747
1	0.892956	-0.791250	-1.603062
1	0.462572	0.628478	-2.261836
7	-0.606585	-1.732706	0.863897
1	-0.858997	-1.844376	1.844940
1	-0.920614	-2.597960	0.423719
1	0.430305	-1.772744	0.830838
7	2.463003	1.876518	0.509398
1	2.667463	2.764131	0.054067
1	3.169903	1.221698	0.164356
1	2.701207	2.026612	1.487959
7	2.398953	-1.918187	0.775432

1	2.656429	-2.820141	0.380653
1	2.665593	-1.976959	1.755713
1	3.038564	-1.241356	0.359296
7	4.833032	-0.055318	-0.615966
1	4.888609	-0.442602	-1.554775
1	5.399299	-0.672113	-0.038053
1	5.362181	0.812631	-0.660029

 Cartesian coordinates of : 530-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.556066	0.347206	-1.504935
1	-1.516898	-0.242518	-2.336058
1	-1.395217	1.293275	-1.848174
1	-2.534227	0.317094	-1.189690
7	-1.988699	-1.108223	1.165989
1	-2.834397	-0.713349	0.744711
1	-2.115174	-2.118168	1.117613
1	-2.040384	-0.886286	2.158797
7	0.026133	1.399353	1.414597
1	0.673113	2.097865	1.026474
1	0.413646	1.143794	2.322574
1	-0.834850	1.898724	1.633217
26	-0.190481	-0.299003	0.062184
7	1.600327	0.431284	-1.070340
1	1.533279	0.469703	-2.085605
1	2.408239	-0.162961	-0.873513
1	1.849878	1.374490	-0.765672
7	0.901082	-2.131452	0.451843
1	1.898699	-2.035362	0.211046
1	0.565319	-2.929057	-0.088076
1	0.872346	-2.441417	1.422615
7	-4.548930	0.127645	-0.482194
1	-5.041165	0.239546	0.401931
1	-4.994485	-0.670819	-0.930166
1	-4.841825	0.931752	-1.033952
7	2.091173	3.479704	0.221253
1	1.551664	4.289797	0.520096
1	2.447126	3.740655	-0.695955
1	2.909266	3.473907	0.827033
7	3.912860	-1.874682	-0.340013
1	4.146692	-2.163311	-1.287869
1	4.170139	-2.670115	0.241413
1	4.596565	-1.159001	-0.102972

 Cartesian coordinates of : 620-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.860872	0.408377	1.237444
1	-2.501055	-0.304127	0.867389

1	-2.395347	1.275632	1.254302
1	-1.722087	0.168134	2.217811
7	-0.926275	2.071072	-1.334707
1	-1.834465	1.808290	-1.714712
1	-1.089848	2.963381	-0.870454
1	-0.365001	2.308594	-2.151819
7	1.860860	0.408240	-1.237447
1	1.722074	0.167893	-2.217789
1	2.501044	-0.304223	-0.867317
1	2.395333	1.275495	-1.254401
7	-0.915380	-1.158537	-1.315588
1	-0.381711	-2.023235	-1.386383
1	-1.109673	-0.894617	-2.280124
1	-1.822219	-1.424332	-0.919626
26	-0.000004	0.445906	0.000000
7	0.915482	-1.158220	1.315897
1	0.381792	-2.022881	1.386992
1	1.109906	-0.894045	2.280337
1	1.822264	-1.424150	0.919896
7	0.926182	2.071367	1.334407
1	1.089390	2.963720	0.870112
1	1.834545	1.808821	1.714163
1	0.365070	2.308735	2.151675
7	-3.819641	-1.829312	0.040508
1	-3.791877	-2.701874	-0.483475
1	-4.598653	-1.312251	-0.362509
1	-4.140233	-2.104107	0.967069
7	3.819654	-1.829302	-0.040492
1	4.599710	-1.310712	0.358525
1	4.137824	-2.107699	-0.966811
1	3.793257	-2.699807	0.486972

 Cartesian coordinates of : 620-2_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	1.251301	-1.608457	0.971080
1	1.246646	-1.616813	1.989780
1	2.237007	-1.616797	0.713873
1	0.883839	-2.518585	0.685849
7	0.140210	-1.290691	-1.857224
1	1.031914	-1.306744	-2.349510
1	-0.026993	-2.255403	-1.563562
1	-0.554566	-1.101613	-2.577621
7	-1.251301	1.608457	-0.971080
1	-1.246646	1.616813	-1.989780
1	-0.883839	2.518585	-0.685849
1	-2.237007	1.616797	-0.713873
7	1.764402	1.290783	-0.596556
1	1.521329	2.255457	-0.361652
1	2.020025	1.306940	-1.582524
1	2.634690	1.101764	-0.102282
26	0.000000	0.000000	0.000000
7	-0.140210	1.290691	1.857224

1	0.554566	1.101613	2.577621
1	-1.031914	1.306744	2.349510
1	0.026993	2.255403	1.563562
7	-1.764402	-1.290783	0.596556
1	-2.634690	-1.101764	0.102282
1	-2.020025	-1.306940	1.582524
1	-1.521329	-2.255457	0.361652
7	-0.412099	-4.257145	-0.320190
1	-0.583714	-4.732101	0.564588
1	0.402456	-4.732062	-0.705963
1	-1.181907	-4.554184	-0.917705
7	0.412099	4.257145	0.320190
1	-0.402456	4.732062	0.705963
1	0.583714	4.732101	-0.564588
1	1.181907	4.554184	0.917705

Cartesian coordinates of the nanomer : [Fe(NH₃)₉]²⁺

Cartesian coordinates of : 360-HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.732149	-0.036360	2.401518
1	-4.439090	0.674452	2.230628
1	-3.279272	0.239203	3.268864
1	-4.250629	-0.881848	2.626992
7	0.900541	-4.057409	-1.172691
1	0.631424	-4.914989	-0.696601
1	0.386365	-4.065897	-2.049453
1	1.874876	-4.189479	-1.431840
26	-0.240004	-0.088050	0.049567
7	-2.243763	-0.521948	-0.137014
1	-2.749555	-0.339067	0.757423
1	-2.418263	-1.504921	-0.344397
1	-2.746517	0.019174	-0.871692
7	-3.769499	0.960057	-2.231406
1	-4.661863	0.478095	-2.307032
1	-3.398898	0.986461	-3.177535
1	-4.001842	1.923358	-2.004636
7	1.449240	1.076529	-0.004679
1	1.349641	2.005237	0.452195
1	1.787165	1.269295	-0.969639
1	2.204341	0.583318	0.478697
7	0.659918	-1.835013	0.830854
1	1.610253	-1.615842	1.148537
1	0.744425	-2.589256	0.118958
1	0.179789	-2.267998	1.618623
7	3.603756	-0.846256	1.671422
1	4.347800	-0.926447	0.981936
1	3.710960	-1.666999	2.263940
1	3.872950	-0.066870	2.267708

7	2.460036	1.677767	-2.770606
1	2.162426	1.145614	-3.583836
1	3.473798	1.599996	-2.756349
1	2.267768	2.649570	-2.999761
7	1.221841	3.771446	1.310218
1	1.254309	3.771863	2.326295
1	0.432305	4.362664	1.064710
1	2.046002	4.288905	1.015201

 Cartesian coordinates of : 361-HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	2.696629	-2.444406	-0.224528
1	3.573309	-1.939701	-0.079050
1	2.896787	-3.175899	-0.902250
1	2.499800	-2.931613	0.645430
7	3.266936	1.457668	-0.130966
1	3.859521	0.628663	-0.056411
1	3.593617	1.960285	-0.953644
1	3.537594	2.050377	0.650929
26	-0.674612	-0.010815	-0.226400
7	1.003678	-0.408621	-1.362498
1	1.546933	-1.217821	-0.960588
1	1.657114	0.376686	-1.287149
1	0.877367	-0.614120	-2.352684
7	5.593711	-0.944953	0.174360
1	5.875644	-0.873734	1.148910
1	6.147472	-0.248427	-0.317922
1	5.961776	-1.838284	-0.143487
7	-2.637684	-0.204820	0.345963
1	-2.794830	-1.037667	0.957635
1	-3.291426	-0.314264	-0.460274
1	-2.979909	0.592395	0.881409
7	0.248605	1.458474	0.973228
1	-0.167955	2.401007	0.821856
1	1.242337	1.527693	0.726330
1	0.204842	1.307697	1.980333
7	-0.921709	4.182832	0.558259
1	-1.788071	4.339935	0.050315
1	-0.233285	4.775989	0.101698
1	-1.069442	4.599809	1.474163
7	-4.539788	-0.522938	-1.920922
1	-4.360572	-0.083645	-2.820022
1	-5.428137	-0.138422	-1.608728
1	-4.728694	-1.499591	-2.131627
7	-3.166278	-2.548024	2.092788
1	-2.610362	-2.680503	2.933576
1	-3.171314	-3.451182	1.625827
1	-4.118904	-2.410973	2.422038

 Cartesian coordinates of : 450-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.689193	0.625138	0.918468
1	-1.982570	1.450768	0.388732
1	-1.512005	0.948554	1.867981
1	-2.518526	0.003330	0.982733
7	1.948843	-0.136251	0.727546
1	2.379647	0.736045	0.412703
1	2.022412	-0.154519	1.765119
1	2.566045	-0.876137	0.394714
7	0.200722	1.258375	-1.570140
1	1.078082	1.774322	-1.422188
1	-0.569082	1.933581	-1.495131
1	0.211567	0.934460	-2.535089
26	-0.010577	-0.213146	-0.054381
7	-0.490946	-2.231501	-0.442919
1	-1.422124	-2.337009	-0.844522
1	-0.493898	-2.825793	0.385724
1	0.157014	-2.690476	-1.118423
7	-4.152152	-1.093024	1.190363
1	-4.074037	-2.029412	1.578351
1	-4.742138	-1.189254	0.367881
1	-4.714514	-0.575772	1.861933
7	2.942221	2.706190	-0.919557
1	2.968706	3.382136	-0.159442
1	2.881412	3.270036	-1.764928
1	3.876265	2.303655	-0.952884
7	2.290805	-0.234269	3.695292
1	2.511246	0.675633	4.091824
1	3.109150	-0.810612	3.875535
1	1.558572	-0.616356	4.287536
7	-2.298267	3.216892	-1.093152
1	-3.294278	3.016429	-1.034115
1	-2.173592	3.593957	-2.030475
1	-2.148434	4.009750	-0.472915
7	1.274946	-3.644320	-2.378298
1	0.695090	-3.967388	-3.149000
1	1.638969	-4.489726	-1.945489
1	2.077162	-3.199017	-2.815464

 Cartesian coordinates of : 450-2_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.384317	-1.314096	1.550345
1	1.304546	-1.241053	1.981652
1	0.325457	-2.253422	1.144876
1	-0.276028	-1.293785	2.326083
7	-0.357337	-1.331023	-1.546085
1	0.279045	-1.275468	-2.339848

1	-0.238548	-2.266185	-1.144088
1	-1.291845	-1.306502	-1.951512
7	1.771631	1.142353	-0.378639
1	2.560073	0.539789	-0.680755
1	2.099424	1.661862	0.459339
1	1.678621	1.848450	-1.108601
26	-0.004951	0.138366	-0.001440
7	-1.803708	1.103370	0.372234
1	-1.724795	1.817456	1.096066
1	-2.576816	0.485249	0.682089
1	-2.146199	1.608272	-0.468865
7	-4.143005	-0.561540	1.338917
1	-4.946509	-0.220260	0.817189
1	-4.339066	-0.331983	2.310086
1	-4.200315	-1.574729	1.285206
7	4.150184	-0.478581	-1.320470
1	4.944515	-0.130121	-0.789546
1	4.353178	-0.242986	-2.288765
1	4.218098	-1.491289	-1.269930
7	0.086644	-4.163263	0.000397
1	0.746106	-4.573092	0.658945
1	0.334075	-4.583668	-0.893230
1	-0.812578	-4.574894	0.241404
7	2.745331	2.720110	2.001541
1	2.901779	3.667711	1.666837
1	3.657470	2.390398	2.306799
1	2.199051	2.823990	2.852310
7	-2.821742	2.639497	-2.015811
1	-3.723542	2.282431	-2.321007
1	-2.277026	2.754599	-2.866138
1	-3.005659	3.583929	-1.686158

 Cartesian coordinates of : 540-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.970465	-0.093423	-1.024597
1	-2.685654	-0.618096	-0.518279
1	-2.010847	-0.426622	-1.985656
1	-2.276306	0.881689	-1.059183
7	-0.830461	-1.748496	1.369752
1	-1.824987	-1.914181	1.169102
1	-0.375613	-2.659217	1.320833
1	-0.783964	-1.490653	2.354558
7	2.015543	-0.147555	1.020971
1	2.696007	-0.716316	0.514211
1	2.075898	-0.439082	1.994390
1	2.356758	0.815754	0.996251
7	-0.250896	1.827678	0.612343
1	0.647562	2.324198	0.615092
1	-0.624105	1.941506	1.554283
1	-0.901789	2.329606	-0.001738
26	0.001011	-0.232605	0.037860
7	0.936936	-1.291930	-1.621371

1	1.038843	-0.707943	-2.450846
1	0.433070	-2.117281	-1.943038
1	1.887083	-1.607968	-1.384803
7	3.877784	-2.171455	-0.904446
1	4.285670	-2.558963	-0.056386
1	4.591381	-1.553035	-1.284196
1	3.846137	-2.957361	-1.550839
7	-2.534869	3.188291	-1.158130
1	-1.979604	3.918043	-1.599673
1	-3.066205	3.661482	-0.430356
1	-3.226986	2.937031	-1.860674
7	2.658196	3.135553	0.858089
1	3.263060	3.060230	1.673209
1	2.245775	4.062919	0.935631
1	3.288627	3.199263	0.061998
7	-3.911405	-2.172667	0.771371
1	-4.560906	-1.535345	1.226992
1	-3.925222	-3.011238	1.348434
1	-4.372508	-2.452673	-0.091543

Cartesian coordinates of : 630-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-0.031171	-1.882096	-1.231881
1	-0.744264	-2.514021	-0.853000
1	0.837831	-2.413468	-1.233670
1	-0.266060	-1.762161	-2.215713
7	1.668737	-0.825671	1.324055
1	1.685900	-0.447384	2.269690
1	1.648216	-1.835986	1.449590
1	2.588758	-0.608657	0.928603
7	-0.039314	1.881792	1.236161
1	-0.282192	1.762000	2.218073
1	-0.748611	2.514701	0.851912
1	0.830569	2.411724	1.244958
7	-1.584831	-0.905276	1.315591
1	-2.435942	-0.359559	1.438331
1	-1.278484	-1.129831	2.260659
1	-1.878895	-1.798230	0.908484
26	0.020514	0.000086	0.002104
7	-1.583319	0.900986	-1.316055
1	-2.434236	0.354901	-1.438499
1	-1.275675	1.123001	-2.261303
1	-1.877976	1.795045	-0.911765
7	1.669045	0.831070	-1.316200
1	2.589178	0.619030	-0.918040
1	1.643931	1.841091	-1.443229
1	1.691010	0.451687	-2.261317
7	-2.334028	-3.790626	0.002656
1	-3.297231	-3.681712	0.313601
1	-1.938414	-4.496973	0.619707
1	-2.412469	-4.250058	-0.902417
7	-2.334821	3.790038	-0.013065

1	-1.932118	4.498077	-0.623553
1	-2.422976	4.246620	0.892559
1	-3.294620	3.682702	-0.334910
7	4.522105	0.001195	-0.004621
1	4.911239	-0.757045	-0.561134
1	4.948308	-0.104115	0.913821
1	4.945052	0.846491	-0.382625

 Cartesian coordinates of : 630-2_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.102519	-1.643235	-1.300280
1	-1.737632	-1.369510	-2.048028
1	-1.702462	-1.961849	-0.531364
1	-0.637222	-2.479720	-1.648708
7	-0.958471	0.000301	1.361420
1	-1.573862	-0.816426	1.380542
1	-0.461800	0.000421	2.249886
1	-1.573770	0.817104	1.380260
7	1.615538	1.570174	0.318289
1	1.163282	2.246497	0.931050
1	2.130177	2.131535	-0.358114
1	2.329697	1.107339	0.889357
7	-1.102526	1.642664	-1.300973
1	-0.637233	2.478943	-1.649899
1	-1.702363	1.961708	-0.532156
1	-1.737745	1.368582	-2.048499
26	0.239289	-0.000151	-0.538684
7	1.401988	-0.000602	-2.516754
1	1.211641	0.804496	-3.111629
1	1.211811	-0.806089	-3.111157
1	2.413066	-0.000465	-2.392337
7	1.615543	-1.570146	0.318982
1	2.329680	-1.107035	0.889850
1	2.130216	-2.131797	-0.357154
1	1.163301	-2.246204	0.932045
7	3.870870	0.000487	2.052737
1	4.483698	-0.803178	1.930442
1	3.635179	0.000522	3.042900
1	4.483545	0.804255	1.930354
7	-2.939294	2.645505	1.136161
1	-3.889229	2.358665	0.909678
1	-2.879536	3.615228	0.832170
1	-2.917547	2.697775	2.152393
7	-2.939579	-2.644808	1.137079
1	-2.879952	-3.614659	0.833471
1	-3.889476	-2.357930	0.910484
1	-2.917837	-2.696681	2.153332

Cartesian coordinates of the decamer : [Fe(NH3)10]2+

Cartesian coordinates of : 370-1_HS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

7	3.235404	-0.076197	-2.688042
1	4.095045	-0.593306	-2.523061
1	3.525368	0.807549	-3.098590
1	2.758918	-0.575679	-3.433780
7	3.533391	-1.068692	2.126050
1	3.674194	-2.067201	1.998022
1	4.454595	-0.653636	2.010316
1	3.310486	-0.948753	3.110672
26	-0.019760	0.169201	0.065378
7	1.987691	0.531019	0.010758
1	2.398846	0.288646	-0.910605
1	2.491856	-0.031087	0.716371
1	2.237838	1.523260	0.176509
7	2.778455	3.423511	0.491613
1	3.679084	3.544316	0.035821
1	2.941847	3.632584	1.472823
1	2.198070	4.182067	0.144710
7	-2.029118	0.582611	-0.087312
1	-2.390314	0.542448	-1.060726
1	-2.303659	1.515107	0.277618
1	-2.549314	-0.114237	0.451730
7	-0.226403	-1.732576	0.968113
1	-1.169981	-1.838838	1.353167
1	0.434913	-1.908990	1.722450
1	-0.093369	-2.516239	0.298746
7	-3.334375	-1.770690	1.880848
1	-3.697107	-1.150887	2.601581
1	-3.175139	-2.655612	2.357619
1	-4.120053	-1.952398	1.260401
7	-2.886138	3.277700	0.966061
1	-2.380428	3.719425	1.728949
1	-3.842378	3.182276	1.298001
1	-2.925204	3.974405	0.226845
7	-3.128073	0.518824	-2.894265
1	-2.608881	0.989392	-3.630531
1	-4.015961	1.010901	-2.835431
1	-3.353991	-0.400009	-3.265493
7	0.131172	-4.067066	-0.898892
1	-0.649764	-4.248626	-1.523663
1	0.192794	-4.887132	-0.300682
1	0.961418	-4.098059	-1.484131

 Cartesian coordinates of : 442_HS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

 7 3.836557 0.154759 -1.828749
 1 4.520786 -0.114938 -1.120398
 1 4.304514 0.841432 -2.415872
 1 3.711219 -0.658709 -2.425446
 7 3.616171 -0.351497 1.921006
 1 4.419202 -0.406501 1.291925
 1 3.661508 0.567113 2.353774
 1 3.806312 -1.007682 2.674781
 26 0.006029 0.287342 -0.093837
 7 1.511990 1.617675 -0.747314
 1 2.321909 1.083804 -1.136420
 1 1.903000 2.206743 -0.013140
 1 1.222776 2.261513 -1.482617
 7 6.377402 -0.586675 0.153392
 1 6.750141 -1.010355 -0.692642
 1 6.690416 -1.193868 0.906788
 1 6.898911 0.278267 0.272990
 7 -1.464143 -0.432731 -1.422634
 1 -2.161022 -1.037148 -0.929867
 1 -1.108346 -0.983548 -2.202946
 1 -2.006257 0.316138 -1.852099
 7 -3.466838 -2.080048 -0.047927
 1 -4.347517 -1.561856 -0.045777
 1 -3.331307 -2.403928 0.905843
 1 -3.636330 -2.921083 -0.594229
 7 -4.010579 1.665742 0.357879
 1 -4.443203 2.132729 1.151719
 1 -4.592280 0.847331 0.174366
 1 -4.155403 2.296150 -0.426899
 7 -6.389111 -0.627624 -0.054610
 1 -6.872308 0.174575 -0.450818
 1 -6.797055 -0.758309 0.867811
 1 -6.709842 -1.421128 -0.603955
 7 -1.219830 1.306309 1.308421
 1 -1.291165 0.836837 2.210026
 1 -2.197903 1.403578 0.957749
 1 -0.916179 2.254135 1.529132
 7 1.191946 -1.328174 0.566428
 1 2.040105 -0.972053 1.063334
 1 1.544782 -1.921271 -0.183694
 1 0.728825 -1.963026 1.215110

 Cartesian coordinates of : 451_HS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

 7 2.471862 0.799711 -2.247002
 1 2.923607 -0.020902 -1.844974

1	3.107442	1.576839	-2.085566
1	2.478530	0.654857	-3.253780
7	2.893030	-0.915246	1.219921
1	3.301111	-1.207370	0.328939
1	3.515539	-0.190613	1.571027
1	3.025175	-1.695891	1.859448
26	-0.836519	0.325429	0.179819
7	-0.296330	1.546920	-1.458173
1	0.677152	1.304491	-1.739326
1	-0.299848	2.547572	-1.265832
1	-0.867066	1.431508	-2.294381
7	4.364269	-1.914787	-1.523739
1	4.005592	-2.521795	-2.256301
1	4.886270	-2.529487	-0.903955
1	5.070382	-1.337126	-1.973284
7	-2.946956	0.316993	0.316907
1	-3.440072	0.119317	-0.578736
1	-3.335429	1.196640	0.655684
1	-3.280911	-0.386833	0.974755
7	-0.102218	-1.650688	0.111166
1	-0.572951	-2.328382	0.739322
1	0.874432	-1.590909	0.415084
1	-0.086843	-2.081400	-0.811205
7	-1.447675	-3.676864	1.904637
1	-1.758216	-3.411302	2.835322
1	-0.754690	-4.406346	2.052154
1	-2.241513	-4.146646	1.477142
7	0.400343	1.015517	1.736436
1	1.276523	0.483227	1.677489
1	0.040956	0.866026	2.677764
1	0.638903	2.022675	1.686452
7	-4.485329	-0.216915	-2.185388
1	-4.096176	-0.765950	-2.947015
1	-4.831204	0.637261	-2.615311
1	-5.317406	-0.721496	-1.889330
7	1.053406	3.976359	1.747088
1	1.457216	4.102577	2.672054
1	0.274558	4.628477	1.706676
1	1.747625	4.342821	1.101430

 Cartesian coordinates of : 460-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-0.388540	-0.935298	1.902435
1	-0.256200	-0.168319	2.577990
1	0.157175	-1.721971	2.247991
1	-1.372180	-1.219844	1.949360
7	1.720778	-0.892141	-1.204292
1	2.496786	-0.268510	-0.958141
1	2.040930	-1.864813	-1.037761
1	1.611383	-0.805104	-2.213793
7	0.675322	1.682145	0.352747
1	1.684778	1.729577	0.188531

1	0.533019	1.894112	1.340512
1	0.249914	2.462566	-0.181556
26	0.046241	-0.285068	-0.076205
7	-1.695037	-1.053495	-0.985416
1	-2.384113	-1.221918	-0.246477
1	-1.552319	-1.959465	-1.430755
1	-2.152640	-0.461537	-1.705294
7	-3.524649	-1.780869	1.668012
1	-3.589220	-2.795230	1.719303
1	-4.349743	-1.489974	1.148181
1	-3.698161	-1.456952	2.616984
7	3.918454	1.355001	-0.365151
1	4.393707	1.208657	0.522456
1	3.965900	2.357672	-0.532149
1	4.540285	0.953751	-1.063892
7	2.700830	-3.716622	-0.834093
1	3.575697	-3.740115	-0.316805
1	2.924484	-4.078244	-1.757811
1	2.113261	-4.424917	-0.403196
7	0.046265	1.428361	3.882820
1	-0.618476	2.197630	3.913445
1	0.956389	1.849110	4.053344
1	-0.146284	0.883929	4.720711
7	-3.093679	0.486978	-3.149922
1	-3.796355	1.143309	-2.820709
1	-3.602929	-0.200344	-3.699727
1	-2.529940	1.002932	-3.819559
7	-0.454674	4.056296	-1.118995
1	-0.275385	4.091421	-2.118625
1	-0.005251	4.883493	-0.734952
1	-1.452246	4.218363	-1.013297

 Cartesian coordinates of : 640-1_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	1.950246	-0.000004	-1.064754
1	2.497416	-0.820305	-0.791868
1	2.497399	0.820309	-0.791871
1	1.926319	-0.000005	-2.082237
7	0.802552	1.637985	1.350525
1	1.044724	1.358771	2.299123
1	1.670539	1.995544	0.939811
1	0.191286	2.444594	1.462583
7	-1.950250	-0.000013	1.064740
1	-1.926326	-0.000027	2.082223
1	-2.497419	-0.820311	0.791844
1	-2.497401	0.820305	0.791867
7	0.802577	-1.637986	1.350546
1	0.191333	-2.444614	1.462589
1	1.044721	-1.358767	2.299149
1	1.670581	-1.995518	0.939846
26	-0.000001	-0.000015	-0.000008
7	-0.802560	-1.638012	-1.350540

1	-0.191300	-2.444629	-1.462582
1	-1.044714	-1.358803	-2.299144
1	-1.670557	-1.995558	-0.939836
7	-0.802580	1.637962	-1.350555
1	-1.670549	1.995539	-0.939818
1	-1.044788	1.358731	-2.299139
1	-0.191308	2.444562	-1.462649
7	3.568527	-2.664559	-0.013137
1	3.393861	-3.604174	0.336993
1	4.353817	-2.323257	0.536843
1	3.943910	-2.808229	-0.948143
7	-3.568521	-2.664579	0.013159
1	-4.354247	-2.322674	-0.535823
1	-3.943117	-2.809149	0.948342
1	-3.394230	-3.603858	-0.338058
7	-3.568457	2.664625	0.013224
1	-3.393852	3.604161	-0.337152
1	-3.943631	2.808509	0.948282
1	-4.353875	2.323221	-0.536510
7	3.568471	2.664607	-0.013196
1	3.393868	3.604153	0.337152
1	3.943676	2.808463	-0.948246
1	4.353865	2.323202	0.536570

 Cartesian coordinates of : 640-3_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	1.568176	-0.305342	-1.122897
1	2.415432	-0.685265	-0.694437
1	1.831249	0.592066	-1.536753
1	1.341055	-0.921375	-1.900532
7	-1.568388	0.305134	-1.122557
1	-1.341333	0.920901	-1.900423
1	-1.831752	-0.592329	-1.536105
1	-2.415453	0.685352	-0.693982
7	-1.556053	0.413853	2.019677
1	-1.306928	1.123454	2.706267
1	-1.852610	-0.389603	2.570307
1	-2.402028	0.757976	1.553712
7	0.476072	2.218393	0.361729
1	1.024289	2.589388	1.135489
1	-0.333096	2.832875	0.294081
1	1.036622	2.395879	-0.477583
26	0.000082	-0.000071	0.446614
7	1.556545	-0.413794	2.019397
1	2.402570	-0.757592	1.553280
1	1.307706	-1.123595	2.705884
1	1.852928	0.389647	2.570144
7	-0.475932	-2.218518	0.362026
1	-1.036691	-2.396085	-0.477131
1	-1.023964	-2.589445	1.135949
1	0.333224	-2.833001	0.294247
7	4.204678	-1.472265	0.509023

1	4.409706	-2.118538	1.268216
1	4.902310	-0.736439	0.595770
1	4.462845	-1.981123	-0.333630
7	2.318692	2.700557	-2.260261
1	2.433340	2.314090	-3.194646
1	3.263070	2.908127	-1.942979
1	1.888255	3.610186	-2.412535
7	-4.204347	1.472752	0.510119
1	-4.465069	1.976101	-0.335053
1	-4.406831	2.124055	1.265685
1	-4.901870	0.737674	0.603828
7	-2.319601	-2.700673	-2.259345
1	-2.427229	-2.317465	-3.195904
1	-3.266761	-2.901193	-1.945848
1	-1.894025	-3.613566	-2.405648

 Cartesian coordinates of : 640-4_HS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.040338	-1.871987	-0.230958
1	-0.619407	-2.367329	0.557453
1	-1.077178	-2.551559	-0.987941
1	-2.013655	-1.664635	0.001194
7	0.006279	-0.307822	-2.847054
1	0.685137	-0.986883	-3.187167
1	-0.896366	-0.653793	-3.168115
1	0.178466	0.528388	-3.402523
7	1.374562	1.870542	-0.810257
1	1.561847	2.203095	-1.753983
1	2.291067	1.648420	-0.410179
1	1.034617	2.685812	-0.303742
7	1.940105	-1.173581	-0.252221
1	2.704808	-0.563447	0.045466
1	2.309065	-1.724707	-1.024213
1	1.755147	-1.838240	0.502548
26	0.093439	0.025168	-0.585601
7	0.107676	0.457590	1.655723
1	-0.256577	-0.298965	2.231144
1	-0.486551	1.269999	1.843439
1	1.019413	0.679210	2.050951
7	-1.802226	1.178530	-0.653583
1	-2.031541	1.711568	-1.489747
1	-1.828822	1.842111	0.124414
1	-2.581123	0.530450	-0.501829
7	0.902788	-3.403582	1.995475
1	1.506687	-3.144792	2.772367
1	1.368116	-4.192659	1.551782
1	0.079010	-3.807028	2.436344
7	-1.778930	3.097209	2.026884
1	-2.117477	3.884926	1.478517
1	-1.127212	3.510631	2.690272
1	-2.576152	2.808179	2.589543
7	4.282006	1.034211	0.425858

1	4.667520	0.483178	1.189647
1	4.431242	2.000231	0.709469
1	4.922466	0.889481	-0.351952
7	-4.208424	-0.941897	-0.028642
1	-4.847043	-0.338987	-0.542964
1	-4.519378	-0.888645	0.938671
1	-4.450042	-1.882867	-0.331826

**Cartesian coordinates of all the proposed isomers of
[Fe²⁺ (NH₃)_{n=1-10}] at MP2-6-31++G(d,p) level of theory at
triplet spin-state**

Cartesian coordinates of the monomer : [Fe(NH₃)₂]²⁺

Cartesian coordinates of : 100_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.372151	0.000001	0.000000
1	1.789375	0.887553	-0.315401
1	1.789370	-0.716926	-0.610941
1	1.789378	-0.170633	0.926342
26	-0.575891	0.000000	0.000000

Cartesian coordinates of the dimer : [Fe(NH₃)₂]₂²⁺

Cartesian coordinates of : 200-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.553034	-0.651736	0.000000
1	-1.605172	-1.273417	-0.814722
1	-2.451849	-0.151841	0.000013
1	-1.605159	-1.273435	0.814708
26	-0.000001	0.558526	0.000000
7	1.553036	-0.651733	0.000000
1	1.605177	-1.273411	0.814724
1	2.451854	-0.151843	-0.000020
1	1.605156	-1.273440	-0.814703

Cartesian coordinates of the trimer : [Fe(NH₃)₃]₂²⁺

Cartesian coordinates of : 210-1_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.591252	-0.616800	0.000002
1	3.162100	-0.347082	-0.807808
1	2.620436	-1.641441	-0.002042
1	3.160727	-0.350346	0.809862
7	-1.081394	0.945105	-0.000000
1	-1.268147	1.549492	0.806384
1	-1.268133	1.549528	-0.806361
1	-1.916035	0.231875	-0.000019
26	0.727542	0.172014	-0.000002

7	-3.290282	-0.717710	-0.000003
1	-3.423322	-1.319341	0.811044
1	-3.421818	-1.322239	-0.809135
1	-4.098929	-0.096982	-0.001870

 Cartesian coordinates of : 210-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-0.071373	1.442880	0.000697
1	-1.031834	1.049907	-0.008615
1	-0.003625	2.071225	-0.807818
1	-0.015023	2.058932	0.819496
7	-0.071378	-1.442877	0.000696
1	-1.031840	-1.049903	-0.008614
1	-0.003632	-2.071222	-0.807818
1	-0.015030	-2.058929	0.819496
26	1.243966	-0.000002	-0.000689
7	-2.796614	-0.000000	-0.001418
1	-3.234576	0.798342	-0.462841
1	-3.197402	0.000345	0.937036
1	-3.234612	-0.798667	-0.462246

 Cartesian coordinates of : 300-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-2.001678	-0.534835	0.077492
1	-2.521712	-0.257031	-0.760690
1	-2.449497	-0.028100	0.845374
1	-2.273814	-1.512598	0.225750
7	2.001703	-0.534810	0.077492
1	2.273850	-1.512571	0.225733
1	2.521733	-0.256988	-0.760685
1	2.449515	-0.028084	0.845381
26	-0.000001	-0.276175	-0.074853
7	-0.000022	1.701647	0.017002
1	-0.808012	2.144881	-0.427674
1	0.808042	2.144888	-0.427531
1	-0.000107	2.062130	0.976623

 Cartesian coordinates of the tetramer : [Fe(NH3)4]2+

Cartesian coordinates of : 220-1_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.542300	-0.793202	-0.000101
1	-1.575970	-1.417214	-0.811200

1	-2.516051	-0.273743	-0.000066
1	-1.575991	-1.417352	0.810891
7	1.542312	-0.793186	0.000103
1	1.575980	-1.417222	0.811185
1	1.576007	-1.417317	-0.810906
1	2.516083	-0.273707	0.000085
7	-4.047984	0.358861	0.000029
1	-4.296394	0.921393	0.812064
1	-4.717434	-0.409691	-0.003338
1	-4.294790	0.927068	-0.808532
26	0.000012	0.362297	0.000004
7	4.047937	0.358860	-0.000037
1	4.294702	0.927262	0.808401
1	4.296411	0.921187	-0.812195
1	4.717366	-0.409709	0.003564

 Cartesian coordinates of : 220-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-4.099278	-0.418256	0.002918
1	-4.292592	-1.003102	0.813629
1	-4.293883	-1.005778	-0.805545
1	-4.839002	0.282513	0.002350
7	-1.696709	1.027423	-0.001352
1	-1.807005	1.647551	-0.808650
1	-2.594909	0.423901	0.000352
1	-1.805576	1.649999	0.804252
7	1.696703	-1.027417	-0.001352
1	1.806998	-1.647545	-0.808650
1	1.805563	-1.649996	0.804251
1	2.594909	-0.423904	0.000357
7	4.099286	0.418234	0.002919
1	4.293975	1.005548	-0.805675
1	4.839009	-0.282537	0.002606
1	4.292518	1.003286	0.813499
26	-0.000001	0.000007	-0.001335

 Cartesian coordinates of : 220-3_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-2.334496	-2.289650	0.285915
1	-2.566008	-2.319094	1.276600
1	-1.994011	-3.222756	0.063642
1	-3.231551	-2.220776	-0.191329
7	-0.849811	0.000005	-0.636850
1	-1.016366	0.000010	-1.646898
1	-1.377108	-0.849459	-0.276830
1	-1.377126	0.849456	-0.276820
26	1.030750	0.000010	-0.143731
7	-2.334560	2.289610	0.285922

1	-3.231695	2.220585	-0.191149
1	-1.994191	3.222708	0.063436
1	-2.565897	2.319195	1.276643
7	2.996330	0.000011	0.377499
1	3.285742	0.808828	0.935664
1	3.640751	-0.000036	-0.419109
1	3.285723	-0.808756	0.935745

 Cartesian coordinates of : 310-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-0.853940	1.514588	-0.000741
1	-1.715920	0.948995	-0.008625
1	-0.923572	2.142603	-0.806651
1	-0.931809	2.131574	0.812918
7	-0.301734	-1.309021	-0.001975
1	-1.315232	-1.098038	-0.008511
1	-0.134690	-1.913836	-0.809936
1	-0.144636	-1.908550	0.811958
26	0.774170	0.347129	-0.000273
7	2.603631	-0.503628	0.001284
1	2.793691	-1.100027	0.810789
1	3.369591	0.177455	0.005200
1	2.797432	-1.094888	-0.811116
7	-3.281621	-0.498949	0.000319
1	-3.841383	0.136795	-0.567582
1	-3.696483	-0.447468	0.930332
1	-3.549775	-1.420888	-0.343892

 Cartesian coordinates of : 310-3_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	1.768307	1.420698	0.089540
1	1.490529	2.224375	-0.478318
1	1.839383	1.794104	1.040759
1	2.732801	1.223103	-0.183611
7	1.882796	-1.594684	0.007318
1	2.521179	-1.551004	0.805097
1	2.493031	-1.618390	-0.813386
1	1.494730	-2.541669	0.053574
26	0.474558	-0.126753	-0.033115
7	-1.184774	0.966999	-0.097375
1	-1.303702	1.509529	-0.955987
1	-1.278220	1.654842	0.652886
1	-2.077164	0.382432	-0.030445
7	-3.637555	-0.488443	0.071529
1	-4.365203	0.218523	-0.019966
1	-3.843050	-0.962067	0.948803
1	-3.844240	-1.170189	-0.655516

 Cartesian coordinates of : 400-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.075187	-2.020249	0.157171
1	-0.092467	-2.486922	-0.754291
1	-0.894367	-2.383453	0.648148
1	0.714667	-2.443299	0.648285
7	-2.020253	0.075187	-0.157174
1	-2.443326	-0.714702	-0.648211
1	-2.486918	0.092566	0.754291
1	-2.383438	0.894330	-0.648228
7	0.075184	2.020247	0.157171
1	0.894306	2.383422	0.648269
1	-0.714727	2.443331	0.648165
1	0.092618	2.486916	-0.754290
7	2.020257	-0.075183	-0.157173
1	2.486927	-0.092510	0.754289
1	2.443316	0.714689	-0.648251
1	2.383451	-0.894346	-0.648187
26	-0.000002	-0.000001	0.000002

Cartesian coordinates of the pentamer : [Fe(NH3)5]2+

Cartesian coordinates of : 230-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.446994	0.158549	-0.551806
1	-2.134572	-0.050354	0.249233
1	-1.073549	1.109679	-0.409905
1	-2.024283	0.204044	-1.397233
7	1.446988	0.158562	-0.551804
1	2.134565	-0.050346	0.249233
1	1.073534	1.109689	-0.409897
1	2.024276	0.204067	-1.397232
26	0.000003	-1.096910	-0.702489
7	3.349495	-0.331886	1.482409
1	3.045304	-0.205398	2.445499
1	4.101392	0.342557	1.351334
1	3.808396	-1.240646	1.464223
7	0.000014	2.937199	-0.226749
1	0.800889	3.323799	0.271315
1	-0.800853	3.323791	0.271332
1	0.000003	3.418337	-1.125371
7	-3.349509	-0.331870	1.482402
1	-3.045286	-0.205584	2.445508
1	-3.808547	-1.240557	1.464075
1	-4.101307	0.342708	1.351448

Cartesian coordinates of : 320-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.000004	-2.591598	0.115050
1	0.000012	-2.905686	1.089495
1	0.812228	-3.048668	-0.303122
1	-0.812250	-3.048665	-0.303097
7	1.988256	-0.355073	-0.058706
1	2.445309	-0.729920	-0.892602
1	2.310371	0.656173	-0.017762
1	2.472994	-0.804280	0.720559
7	-1.988249	-0.355069	-0.058809
1	-2.473031	-0.804335	0.720397
1	-2.310364	0.656172	-0.017797
1	-2.445257	-0.729853	-0.892759
26	0.000002	-0.575996	-0.041460
7	-3.009480	2.336784	0.045893
1	-2.816891	2.887814	0.879319
1	-4.021630	2.225603	0.033370
1	-2.804115	2.952626	-0.737631
7	3.009472	2.336790	0.045827
1	2.816627	2.888024	0.879058
1	2.804361	2.952445	-0.737911
1	4.021625	2.225596	0.033651

Cartesian coordinates of : 410-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.868245	-1.410459	0.002778
1	1.814119	-1.002219	-0.007947
1	0.839470	-2.043345	-0.798958
1	0.851331	-2.026072	0.818295
7	0.860747	1.420779	0.000739
1	1.809850	1.020887	-0.006948
1	0.826431	2.048270	-0.805272
1	0.835493	2.038364	0.814770
7	-1.999117	-1.454710	-0.002142
1	-1.941212	-2.071614	-0.815570
1	-2.970775	-1.143227	0.006772
1	-1.930701	-2.085011	0.800067
26	-0.574559	0.003425	0.000109
7	-2.033676	1.437239	-0.000153
1	-1.702995	2.402881	0.001368
1	-2.657363	1.385158	0.808071
1	-2.655366	1.386827	-0.810037
7	3.669084	0.005067	-0.003292
1	4.097776	-0.760176	-0.522448
1	4.066236	-0.063280	0.932752
1	4.099278	0.838082	-0.403258

 Cartesian coordinates of : 500-1_IS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

7	-0.024541	-2.137745	0.140030
1	0.747216	-2.548987	0.666129
1	0.022610	-2.594546	-0.772784
1	-0.859772	-2.530268	0.574669
7	2.065476	0.000245	-0.000232
1	2.486793	-0.290564	0.883641
1	2.486675	-0.619368	-0.694479
1	2.485582	0.911685	-0.190163
7	-0.028659	0.950076	-1.919068
1	0.014825	1.969035	-1.856414
1	-0.863507	0.767919	-2.476252
1	0.743666	0.704028	-2.539129
7	-0.027746	1.193893	1.777842
1	-0.863719	1.766013	1.897947
1	0.743226	1.856194	1.869831
1	0.019121	0.634361	2.631563
26	0.021945	-0.001264	0.000239
7	-2.036273	-0.003650	0.000880
1	-2.456368	-0.302339	0.882227
1	-2.456560	-0.618135	-0.697855
1	-2.458142	0.908095	-0.181301

 Cartesian coordinates of the hexamer : [Fe(NH3)6]2+

Cartesian coordinates of : 330-3_IS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

7	3.733781	-1.258958	-0.088773
1	4.087704	-2.145548	0.268873
1	4.274190	-0.556273	0.412840
1	4.073947	-1.224891	-1.048368
7	1.097416	0.734625	-0.698542
1	1.036495	0.939626	-1.697496
1	1.134282	1.668987	-0.207372
1	2.013609	0.294870	-0.565165
7	0.877167	-1.908355	0.586854
1	0.854739	-2.066276	1.596375
1	1.871215	-1.691777	0.359305
1	0.694440	-2.821810	0.165679
26	-0.307510	-0.443993	-0.060331
7	-1.888797	0.642517	-0.510918
1	-2.013554	0.814217	-1.510007
1	-1.894321	1.566221	-0.075647
1	-2.802822	0.187087	-0.200448
7	-4.404135	-0.494987	0.258197
1	-5.097526	0.232888	0.096624

1	-4.539556	-0.777435	1.226253
1	-4.717105	-1.286125	-0.300172
7	1.288195	3.328862	0.577462
1	2.279140	3.531360	0.693017
1	0.879253	3.491382	1.494724
1	0.935751	4.081380	-0.010358

Cartesian coordinates of : 420-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	1.438069	1.419560	0.062350
1	2.385992	1.022031	0.014548
1	1.423255	1.981290	0.915639
1	1.388093	2.100639	-0.696840
7	1.437924	-1.419701	0.062343
1	1.423064	-1.981426	0.915634
1	2.385876	-1.022248	0.014539
1	1.387888	-2.100776	-0.696845
7	-1.437924	1.419701	-0.062343
1	-2.385876	1.022248	-0.014539
1	-1.387888	2.100776	0.696845
1	-1.423064	1.981427	-0.915634
26	0.000000	0.000000	0.000000
7	-1.438069	-1.419560	-0.062350
1	-1.423255	-1.981289	-0.915639
1	-1.388093	-2.100639	0.696841
1	-2.385992	-1.022031	-0.014548
7	4.253854	-0.000004	-0.043550
1	4.667641	-0.802121	-0.516606
1	4.667548	0.801367	-0.517952
1	4.678519	0.000780	0.882617
7	-4.253854	0.000003	0.043550
1	-4.667547	-0.801362	0.517962
1	-4.678519	-0.000791	-0.882617
1	-4.667642	0.802126	0.516596

Cartesian coordinates of : 510-1_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-0.925010	1.342274	-0.802897
1	-0.954134	1.410377	-1.821594
1	-0.844577	2.308239	-0.487277
1	-1.865251	1.031384	-0.529554
7	-0.923218	-1.441131	-0.218669
1	-1.856830	-1.044600	-0.052568
1	-0.995414	-1.888324	-1.133653
1	-0.830179	-2.217000	0.436691
7	0.456362	-0.066332	2.081335
1	1.041043	0.605956	2.576995
1	0.721876	-0.969983	2.474157

1	-0.484205	0.099152	2.441009
26	0.517624	-0.002006	-0.103033
7	1.932185	1.486714	-0.094264
1	2.161536	1.848252	-1.021539
1	2.834168	1.225403	0.305104
1	1.654535	2.314002	0.434604
7	1.990232	-1.373866	-0.756813
1	2.771882	-1.474509	-0.107901
1	2.429182	-1.108862	-1.640147
1	1.663875	-2.327153	-0.912760
7	-3.737151	0.057479	0.014732
1	-4.120939	-0.631437	0.659641
1	-4.231662	-0.108717	-0.860451
1	-4.106930	0.944002	0.354140

 Cartesian coordinates of : 600_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	0.291235	-2.209659	-0.129892
1	0.646116	-2.650882	0.718168
1	0.957578	-2.484943	-0.851313
1	-0.549332	-2.741811	-0.355083
7	2.243016	0.281877	0.002950
1	2.775238	-0.554488	0.245701
1	2.660964	0.595266	-0.873433
1	2.551672	0.977906	0.682519
7	-0.194675	2.218449	0.073834
1	0.021445	2.660545	0.967237
1	-1.123989	2.569625	-0.159030
1	0.422846	2.688957	-0.588055
7	0.010791	-0.140459	2.055744
1	-0.369118	0.674812	2.537073
1	0.934784	-0.267751	2.468938
1	-0.537135	-0.919572	2.421195
26	-0.009363	-0.009725	-0.001276
7	-2.254035	-0.199866	0.058419
1	-2.686916	0.391956	0.767561
1	-2.597581	-1.134990	0.277674
1	-2.740490	0.048261	-0.802905
7	-0.074414	0.071993	-2.058869
1	-0.428654	0.947319	-2.444676
1	-0.672816	-0.643205	-2.472960
1	0.825391	-0.060495	-2.520724

 Cartesian coordinates of the heptamer : [Fe(NH3)7]2+

Cartesian coordinates of : 520-1_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.433512	-1.444812	-0.216130
1	-1.328848	-2.195161	0.466122
1	-1.489897	-1.925137	-1.114903
1	-2.373792	-1.060423	-0.065007
7	1.464396	-1.334411	-0.772268
1	1.364254	-2.291715	-0.437369
1	1.522322	-1.424370	-1.787748
1	2.397068	-1.020187	-0.478413
7	1.431027	1.464488	-0.224064
1	1.314975	2.232403	0.436189
1	1.510639	1.922390	-1.132804
1	2.364160	1.076056	-0.043506
7	0.054542	-0.061520	2.057770
1	-0.870688	0.007449	2.481568
1	0.602513	0.666194	2.514584
1	0.438226	-0.933923	2.421361
26	-0.001285	0.011202	-0.146026
7	-1.488303	1.391321	-0.629644
1	-2.422367	1.036783	-0.392925
1	-1.529210	1.609978	-1.626088
1	-1.403729	2.298891	-0.173416
7	4.262601	-0.037292	0.059974
1	4.772313	0.084967	-0.813451
1	4.626713	-0.903535	0.452925
1	4.630225	0.686389	0.675138
7	-4.288207	0.000164	0.038783
1	-4.681999	0.860553	0.415793
1	-4.658665	-0.728202	0.646722
1	-4.768610	-0.136215	-0.849036

 Cartesian coordinates of : 520-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-0.000015	-2.739399	-0.566181
1	0.808436	-3.251468	-0.214022
1	-0.000052	-2.925118	-1.570701
1	-0.808438	-3.251469	-0.213962
7	2.038974	-0.638273	-0.191416
1	2.516264	-1.192905	0.518783
1	2.442102	-0.954701	-1.074140
1	2.385015	0.323539	-0.074739
7	0.000010	1.263359	-0.845535
1	-0.829202	1.781810	-0.543290
1	0.000009	1.328784	-1.864023
1	0.829231	1.781798	-0.543294
7	-0.000008	-0.472669	2.062447
1	-0.807037	0.032264	2.427110
1	0.806998	0.032309	2.427101
1	0.000020	-1.358044	2.569797
26	-0.000005	-0.679795	-0.127452
7	-2.038981	-0.638247	-0.191440
1	-2.516285	-1.192881	0.518748
1	-2.442105	-0.954662	-1.074171

1	-2.385011	0.323568	-0.074757
7	2.955783	2.393656	0.002628
1	3.260660	2.757058	-0.898706
1	3.819844	2.143738	0.480547
1	2.616864	3.207671	0.511786
7	-2.955752	2.393687	0.002641
1	-3.260622	2.757107	-0.898689
1	-2.616822	3.207689	0.511811
1	-3.819818	2.143776	0.480554

 Cartesian coordinates of : 610-1_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.042780	0.016236	1.501457
1	-1.978664	0.012630	1.081831
1	-1.024815	0.829641	2.115784
1	-1.026847	-0.783413	2.133606
7	0.453402	2.366596	0.013887
1	-0.500077	2.728079	0.007544
1	0.885590	2.820786	0.818022
1	0.892479	2.812723	-0.791193
7	2.000470	-0.017979	-1.497225
1	1.658958	0.007967	-2.457358
1	2.602184	-0.840960	-1.462933
1	2.647788	0.767991	-1.436027
7	-0.971985	0.015595	-1.442993
1	-0.943731	-0.783251	-2.075807
1	-0.945319	0.829592	-2.056284
1	-1.919536	0.009808	-1.045258
26	0.478998	-0.001361	0.009332
7	0.391125	-2.367564	0.012989
1	-0.573235	-2.699124	0.013989
1	0.815473	-2.834916	0.813743
1	0.810062	-2.827048	-0.795294
7	1.935351	-0.020376	1.467955
1	2.569286	0.778156	1.435296
1	2.551371	-0.832647	1.431193
1	1.575346	-0.018636	2.421866
7	-3.865987	0.009083	-0.075703
1	-4.273163	-0.469171	-0.877562
1	-4.261780	0.946889	-0.107480
1	-4.312490	-0.430842	0.727130

 Cartesian coordinates of the octamer : [Fe(NH3)8]2+

Cartesian coordinates of : 530-1_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	1.495672	0.505711	1.406543

1	1.523161	0.072802	2.330153
1	1.284690	1.486559	1.585468
1	2.461235	0.476444	1.061676
7	1.765287	-1.369759	-0.773760
1	2.643986	-0.874824	-0.582882
1	1.920266	-2.317840	-0.430522
1	1.715593	-1.468854	-1.787113
7	0.016299	1.000874	-1.573404
1	-0.452734	1.850857	-1.246008
1	-0.536024	0.672216	-2.365058
1	0.899573	1.303929	-1.980843
26	0.164573	-0.414591	0.068237
7	-1.416783	0.506765	0.958357
1	-1.395991	0.532311	1.977217
1	-2.304989	0.055024	0.722433
1	-1.501306	1.482544	0.654393
7	-1.034624	-2.098656	-0.232149
1	-2.034394	-1.871969	-0.155886
1	-0.874013	-2.834662	0.456465
1	-0.913323	-2.559392	-1.133163
7	4.436180	0.158878	0.158698
1	4.878249	0.021367	-0.748289
1	4.941172	-0.461309	0.789181
1	4.719883	1.097220	0.434196
7	-1.582330	3.506450	-0.272175
1	-0.916328	4.191743	-0.623582
1	-1.877188	3.882017	0.627085
1	-2.398532	3.605406	-0.872777
7	-4.059222	-1.285559	0.179090
1	-4.444435	-1.383553	1.116553
1	-4.370623	-2.121588	-0.312218
1	-4.590179	-0.530013	-0.249057

Cartesian coordinates of : 620-1_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.715802	0.436879	1.109774
1	-2.393663	-0.266572	0.789133
1	-2.226841	1.318783	1.115411
1	-1.564333	0.226723	2.095685
7	-0.887143	2.006336	-1.317679
1	-1.808285	1.747514	-1.670097
1	-1.037474	2.900958	-0.852006
1	-0.350448	2.242088	-2.151720
7	1.720118	0.394206	-1.124421
1	1.566153	0.156115	-2.103566
1	2.394488	-0.302653	-0.784123
1	2.235169	1.273359	-1.155078
7	-0.906333	-1.154224	-1.300846
1	-0.355371	-2.008221	-1.375429
1	-1.090715	-0.887304	-2.267075
1	-1.812905	-1.440217	-0.921513
26	0.002744	0.432880	-0.007371

7	0.877441	-1.128856	1.285617
1	0.316066	-1.976413	1.356658
1	1.046356	-0.855235	2.252800
1	1.787878	-1.427797	0.924984
7	0.923871	2.034055	1.306468
1	1.103051	2.917289	0.829360
1	1.832953	1.761484	1.679195
1	0.378844	2.296979	2.126894
7	-3.793767	-1.772270	0.139549
1	-4.097461	-2.178398	-0.743373
1	-4.593638	-1.223745	0.449854
1	-3.752371	-2.558575	0.784919
7	3.775753	-1.804318	-0.082121
1	4.601391	-1.225282	-0.223381
1	3.803379	-2.487036	-0.836916
1	3.987466	-2.341383	0.756646

 Cartesian coordinates of : 620-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	1.106934	-1.499100	0.850729
1	1.109549	-1.511252	1.870015
1	2.092576	-1.511284	0.591006
1	0.739892	-2.414937	0.568662
7	0.058632	-1.204441	-1.876904
1	0.928888	-1.157644	-2.405431
1	-0.043097	-2.187283	-1.619136
1	-0.670657	-1.029768	-2.566730
7	-1.106934	1.499100	-0.850729
1	-1.109549	1.511252	-1.870015
1	-0.739892	2.414937	-0.568662
1	-2.092576	1.511284	-0.591006
7	1.798630	1.204866	-0.538481
1	1.575396	2.187668	-0.374027
1	2.086169	1.158097	-1.515216
1	2.652521	1.030355	-0.010606
26	0.000000	0.000000	0.000000
7	-0.058632	1.204441	1.876904
1	0.670657	1.029768	2.566730
1	-0.928888	1.157644	2.405431
1	0.043097	2.187283	1.619136
7	-1.798630	-1.204866	0.538481
1	-2.652521	-1.030355	0.010606
1	-2.086169	-1.158097	1.515216
1	-1.575396	-2.187668	0.374027
7	-0.246603	-4.226135	-0.189461
1	-0.400818	-4.685120	0.707072
1	0.580312	-4.685220	-0.568504
1	-1.010117	-4.557900	-0.776711
7	0.246603	4.226135	0.189461
1	-0.580312	4.685220	0.568504
1	0.400818	4.685120	-0.707072
1	1.010117	4.557900	0.776711

 Cartesian coordinates of the nanomer : [Fe(NH3)9]2+

Cartesian coordinates of : 540-1_IS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

 7 1.774350 0.246299 -0.945060
 1 2.461651 0.779291 -0.402579
 1 1.791861 0.659907 -1.875934
 1 2.161204 -0.695568 -1.060443
 7 0.660647 1.657668 1.441249
 1 1.652489 1.869435 1.293693
 1 0.173821 2.552138 1.398921
 1 0.581521 1.367188 2.414766
 7 -1.872708 0.025514 0.866724
 1 -2.594653 0.588354 0.409644
 1 -1.900943 0.292967 1.849451
 1 -2.196168 -0.946806 0.844709
 7 0.381469 -1.728700 0.627818
 1 -0.463523 -2.306678 0.664337
 1 0.769932 -1.757593 1.570207
 1 1.069137 -2.203644 0.035492
 26 -0.041804 0.199173 -0.014705
 7 -0.929890 1.301962 -1.562998
 1 -0.964642 0.797962 -2.449169
 1 -0.444309 2.171975 -1.778277
 1 -1.901675 1.561426 -1.354880
 7 -3.940309 1.960434 -0.814916
 1 -4.344679 2.345952 0.035944
 1 -4.632506 1.300237 -1.162987
 1 -3.965263 2.732750 -1.478013
 7 2.748538 -2.860215 -1.239763
 1 2.249112 -3.554671 -1.791368
 1 3.237932 -3.391186 -0.522333
 1 3.485793 -2.526458 -1.857162
 7 -2.513052 -3.171549 0.860619
 1 -3.247658 -3.059830 1.556420
 1 -2.049295 -4.038722 1.123886
 1 -2.999063 -3.390062 -0.006368
 7 3.787843 2.116244 0.807137
 1 4.456559 1.451957 1.191135
 1 3.784068 2.889373 1.469686
 1 4.237972 2.498198 -0.022125

 Cartesian coordinates of : 630-1_IS

Atomic number (AN) and Cartesian coordinates

AN X Y Z

 7 1.484201 0.837279 1.192769
 1 1.805481 1.744204 0.828297

1	2.319580	0.258362	1.263753
1	1.216649	1.018641	2.159155
7	1.435169	-0.924237	-1.192628
1	1.159364	-1.092475	-2.159065
1	2.302556	-0.394459	-1.263463
1	1.703061	-1.847126	-0.825177
7	-1.574619	-0.804141	-1.200484
1	-1.566714	-0.460634	-2.159852
1	-2.505109	-0.573667	-0.837538
1	-1.554121	-1.819442	-1.285916
7	0.065219	1.927523	-1.369161
1	-0.795616	2.460020	-1.481991
1	0.398676	1.772947	-2.319125
1	0.739901	2.570893	-0.950593
26	-0.040614	0.001814	-0.002444
7	-1.526591	0.899273	1.191111
1	-1.445546	1.911658	1.275114
1	-1.541308	0.557609	2.151070
1	-2.468660	0.724289	0.826744
7	-0.055888	-1.927312	1.364012
1	0.585334	-2.607111	0.950383
1	-0.945645	-2.411493	1.469613
1	0.277820	-1.791626	2.316768
7	2.447108	3.684054	0.158657
1	1.935458	4.488743	0.514833
1	2.792448	3.974069	-0.753907
1	3.281526	3.632414	0.739728
7	-4.423007	0.123991	0.005338
1	-4.832267	-0.594404	0.599291
1	-4.853649	-0.015231	-0.906693
1	-4.822985	0.998260	0.340532
7	2.230073	-3.818728	-0.145872
1	2.588804	-4.103556	0.763146
1	3.046145	-3.829605	-0.754537
1	1.663140	-4.602344	-0.463222

 Cartesian coordinates of : 630-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	2.108911	-0.340780	1.021771
1	2.468613	0.350095	1.678491
1	2.726564	-0.289077	0.200698
1	2.316057	-1.238969	1.456678
7	0.774873	0.144831	-1.750118
1	1.790474	0.045065	-1.798977
1	0.394689	-0.538256	-2.402553
1	0.565168	1.048927	-2.169541
7	-1.900535	0.210338	-0.047851
1	-2.017342	1.081905	-0.568871
1	-2.547784	0.282757	0.735521
1	-2.260077	-0.550670	-0.628182
7	0.303004	2.014888	0.712345
1	0.184591	2.372243	1.659137

1	-0.407149	2.494022	0.145764
1	1.199767	2.386252	0.402938
26	0.095374	-0.073149	0.497449
7	-0.565087	-0.304529	2.802449
1	-1.016005	0.522798	3.190573
1	0.201796	-0.498003	3.445138
1	-1.233061	-1.056060	2.968006
7	-0.159095	-2.141220	0.167670
1	-1.022153	-2.319080	-0.358582
1	-0.230834	-2.709785	1.010372
1	0.588160	-2.573408	-0.373731
7	-2.880110	-2.585041	-1.476650
1	-2.668490	-3.579429	-1.532578
1	-3.032411	-2.302337	-2.442485
1	-3.799619	-2.545918	-1.041566
7	-1.973625	3.375806	-1.078152
1	-1.386726	4.172883	-1.316373
1	-2.692447	3.758248	-0.467008
1	-2.458989	3.152893	-1.944625
7	4.079609	-0.212931	-1.468006
1	4.867648	0.011049	-0.863501
1	4.176298	0.425855	-2.254605
1	4.297917	-1.131670	-1.848014

Cartesian coordinates of the decamer : [Fe(NH3)10]2+

Cartesian coordinates of : 640-2_IS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.451817	1.472676	0.293302
1	-1.145949	2.202358	-0.355961
1	-1.693679	1.959845	1.154459
1	-2.331499	1.086322	-0.057099
7	-0.001952	0.279516	2.919369
1	0.001855	1.253467	3.218767
1	-0.810905	-0.123774	3.389272
1	0.801935	-0.130809	3.391864
7	1.453924	-1.421673	0.545560
1	1.640523	-1.823344	1.462672
1	2.354538	-1.077940	0.200748
1	1.181329	-2.208824	-0.047194
7	1.450968	1.473483	0.294379
1	2.330937	1.087592	-0.055826
1	1.692371	1.960517	1.155737
1	1.145016	2.203183	-0.354823
26	-0.000132	0.031825	0.486079
7	0.001020	-0.271577	-1.912733
1	-0.807262	0.097787	-2.409348
1	0.001688	-1.273761	-2.098020
1	0.809270	0.098753	-2.408680
7	-1.453388	-1.422598	0.544429

1	-1.639971	-1.824677	1.461370
1	-1.180035	-2.209396	-0.048432
1	-2.354128	-1.079377	0.199426
7	-0.000583	3.828535	-1.478372
1	0.803449	3.958624	-2.088514
1	-0.000553	4.643857	-0.868984
1	-0.804713	3.958611	-2.088388
7	0.002088	-3.820601	-1.270928
1	0.001972	-4.571833	-0.583529
1	0.806847	-4.015676	-1.863296
1	-0.802016	-4.016107	-1.864042
7	4.228436	-0.085434	-0.500222
1	4.708812	0.807181	-0.407111
1	4.396856	-0.372058	-1.461969
1	4.778872	-0.727873	0.066012
7	-4.228394	-0.087963	-0.501763
1	-4.777909	-0.734872	0.060261
1	-4.395969	-0.368958	-1.465317
1	-4.710375	0.803206	-0.403256

**Cartesian coordinates of all the proposed isomers of
[Fe²⁺(NH₃)_{n=1-10}] at MP2-6-31++G(d,p) level of theory at
singlet spin-state**

Cartesian coordinates of the monomer : [Fe(NH₃)₂]²⁺

Cartesian coordinates of : 100_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.370326	0.000014	0.000001
1	-1.787327	-0.941252	-0.039482
1	-1.788097	0.504612	-0.795155
1	-1.788164	0.436239	0.834594
26	0.575226	0.000012	0.000001

Cartesian coordinates of the dimer : [Fe(NH₃)₂]₂²⁺

Cartesian coordinates of : 200_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.550752	-0.649749	0.000000
1	-1.604630	-1.273515	-0.812563
1	-2.452337	-0.155018	0.000013
1	-1.604615	-1.273533	0.812550
26	0.000000	0.557716	0.000000
7	1.550751	-0.649750	-0.000000
1	1.604636	-1.273506	0.812570
1	2.452336	-0.155018	-0.000027
1	1.604608	-1.273543	-0.812543

Cartesian coordinates of the trimer : [Fe(NH₃)₃]₂²⁺

Cartesian coordinates of : 300-1_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.700566	1.773544	-0.000001
1	-1.263719	2.000362	-0.827613
1	0.049987	2.478162	0.000046
1	-1.263786	2.000331	0.827574
7	-1.185816	-1.493381	0.000001
1	-2.171257	-1.195506	-0.000079
1	-1.100671	-2.094570	-0.827555

1	-1.100772	-2.094497	0.827621
7	1.886297	-0.280113	-0.000000
1	2.364329	0.094201	-0.827591
1	2.121148	-1.282442	-0.000005
1	2.364329	0.094194	0.827593
26	0.000039	-0.000022	0.000000

Cartesian coordinates of : 300-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
26	0.000001	-0.290190	0.000041
7	-0.000005	1.697667	-0.001501
1	-0.000014	2.107866	0.937493
1	0.807753	2.123736	-0.462269
1	-0.807757	2.123730	-0.462284
7	2.010977	-0.516966	-0.000232
1	2.503152	-0.022666	0.748603
1	2.309597	-1.491696	0.110531
1	2.478051	-0.213878	-0.859257

Cartesian coordinates of : 300-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.770482	-0.220588	0.374043
1	-2.448276	0.508429	0.128535
1	-1.751369	-0.218187	1.396418
1	-2.248661	-1.093647	0.128564
7	1.076282	-1.422977	0.374043

Cartesian coordinates of : 210-1_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.286113	-0.718551	0.000001
1	-3.417987	-1.321417	0.810343
1	-3.417681	-1.321950	-0.809993
1	-4.095188	-0.098343	-0.000356
7	-1.080052	0.943556	0.000073
1	-1.267475	1.547950	-0.806204
1	-1.914882	0.228676	0.000029
1	-1.267402	1.547773	0.806500
7	2.585465	-0.621100	0.000073
1	2.609325	-1.645919	0.000191
1	3.156768	-0.355403	0.808971
1	3.156819	-0.355596	-0.808854

26 0.727792 0.174880 -0.000064

Cartesian coordinates of : 210-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.054897	-1.466466	-0.016000
1	-1.016581	-1.078047	0.002028
1	0.011007	-2.111749	0.778303
1	-0.003872	-2.069678	-0.843720
7	-0.054937	1.466450	-0.016001
1	-1.016614	1.078005	0.002026
1	0.010951	2.111733	0.778304
1	-0.003925	2.069665	-0.843719
26	1.228643	0.000011	0.009404
7	-2.787889	-0.000008	0.011264
1	-3.222517	-0.798205	0.475867
1	-3.196537	-0.000354	-0.923707
1	-3.222568	0.798506	0.475275

Cartesian coordinates of the tetramer : [Fe(NH3)4]2+

Cartesian coordinates of : 400-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.588238	-1.284734	-0.000001
1	-1.610491	-1.912736	-0.806998
1	-2.514351	-0.854963	-0.000022
1	-1.610512	-1.912703	0.807022
7	1.284735	-1.588237	-0.000001
1	0.854964	-2.514350	0.000018
1	1.912704	-1.610509	-0.807023
1	1.912737	-1.610492	0.806996
7	-1.284735	1.588237	-0.000001
1	-1.912702	1.610511	-0.807025
1	-0.854964	2.514350	0.000021
1	-1.912738	1.610491	0.806995
26	0.000000	0.000000	0.000001
7	1.588238	1.284734	-0.000001
1	2.514351	0.854963	-0.000019
1	1.610510	1.912706	0.807020
1	1.610493	1.912734	-0.807000

Cartesian coordinates of : 400-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	2.020346	0.013669	0.612732
1	2.363951	0.860943	1.072395
1	2.596808	-0.068559	-0.226207
1	2.353121	-0.741707	1.218061
7	0.016870	-1.542644	-0.965953
1	0.238990	-2.442200	-0.530068
1	-0.866812	-1.713781	-1.448531
1	0.703766	-1.456112	-1.716960
26	-0.000002	-0.000002	0.315683
7	-0.016870	1.542639	-0.965959
1	-0.238857	2.442219	-0.530056
1	-0.703860	1.456164	-1.716886
1	0.866772	1.713689	-1.448641
7	-2.020342	-0.013660	0.612731
1	-2.353109	0.741771	1.217995
1	-2.363943	-0.860892	1.072475
1	-2.596813	0.068493	-0.226209

Cartesian coordinates of : 310-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-0.864667	-1.519990	-0.060307
1	-1.721094	-0.950790	0.012324
1	-0.928582	-2.215182	0.687920
1	-0.970547	-2.065664	-0.919409
7	-0.281514	1.310541	-0.144684
1	-1.293598	1.117656	-0.050011
1	-0.064386	2.021296	0.557268
1	-0.178073	1.795893	-1.039293
26	0.768852	-0.353038	0.002248
7	2.603722	0.504398	0.093858
1	2.815870	1.140199	-0.678609
1	3.375424	-0.169654	0.081342
1	2.772941	1.059581	0.936275
7	-3.276083	0.513907	0.106511
1	-3.795456	-0.103566	0.730083
1	-3.758712	0.441116	-0.788674
1	-3.514153	1.446099	0.444688

Cartesian coordinates of : 310-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.864667	-1.519990	-0.060307
1	-1.721094	-0.950790	0.012324
1	-0.928582	-2.215182	0.687920
1	-0.970547	-2.065664	-0.919409
7	-0.281514	1.310541	-0.144684
1	-1.293598	1.117656	-0.050011
1	-0.064386	2.021296	0.557268
1	-0.178073	1.795893	-1.039293
26	0.768852	-0.353038	0.002248
7	2.603722	0.504398	0.093858
1	2.815870	1.140199	-0.678609
1	3.375424	-0.169654	0.081342
1	2.772941	1.059581	0.936275
7	-3.276083	0.513907	0.106511
1	-3.795456	-0.103566	0.730083
1	-3.758712	0.441116	-0.788674
1	-3.514153	1.446099	0.444688

Cartesian coordinates of : 310-4_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.806673	1.779919	0.359282
1	1.495357	2.373558	-0.113353
1	1.110241	1.759901	1.334978
1	-0.048043	2.343808	0.365810
7	-0.856874	-0.760908	0.649648
1	-1.832987	-0.448546	0.339067
1	-0.901823	-1.783526	0.634989
1	-0.802419	-0.524884	1.642042
7	2.184258	-0.974504	0.168611
1	3.072561	-0.557510	-0.124609
1	2.241826	-1.942010	-0.164218
1	2.253958	-1.049409	1.185558
26	0.564759	-0.012881	-0.455456
7	-3.501087	-0.031341	-0.128497
1	-3.693891	0.522956	-0.960224
1	-3.990418	0.445953	0.626481
1	-4.018876	-0.897554	-0.267976

Cartesian coordinates of : 310-5_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.394915	1.465281	-0.382327
1	-0.145994	2.251612	0.221473
1	-1.292551	1.095964	-0.029850
1	-0.612492	1.899597	-1.284591
7	1.685246	0.000018	1.344336
1	2.282554	-0.807403	1.547365
1	2.282568	0.807435	1.547344
1	0.985473	0.000034	2.089307
7	-0.394888	-1.465301	-0.382305
1	-1.292523	-1.095997	-0.029819
1	-0.145946	-2.251624	0.221495
1	-0.612469	-1.899627	-1.284563
26	0.915541	0.000001	-0.483551
7	-3.029250	0.000001	0.519345
1	-3.666988	0.000018	-0.276523
1	-3.324531	0.800034	1.078700
1	-3.324532	-0.800057	1.078663

Cartesian coordinates of : 220-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.758308	1.399858	0.076893
1	1.428224	2.244517	-0.395087
1	1.951682	1.705120	1.034983
1	2.681655	1.223948	-0.324896
7	1.878589	-1.591644	0.004327
1	2.533669	-1.546440	0.788475
1	2.474092	-1.632896	-0.826533
1	1.479524	-2.532933	0.068915
26	0.476871	-0.116997	-0.026927
7	-1.185235	0.971204	-0.083083
1	-1.305453	1.526126	-0.933649
1	-1.285567	1.648388	0.676247
1	-2.074332	0.380111	-0.027469
7	-3.630770	-0.497233	0.060148
1	-4.362899	0.199535	-0.066740
1	-3.848558	-0.946138	0.947398
1	-3.816928	-1.202716	-0.649531

Cartesian coordinates of : 220-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.332707	-2.288922	0.282447
1	-2.562095	-2.321394	1.273534

1	-1.992808	-3.221371	0.056520
1	-3.230714	-2.218341	-0.192760
7	-0.846920	0.000189	-0.634235
1	-1.010675	0.000373	-1.644778
1	-1.374664	-0.850185	-0.275771
1	-1.376764	0.849137	-0.275310
26	1.030543	0.001627	-0.139465
7	-2.338197	2.285000	0.283254
1	-3.239476	2.207671	-0.184646
1	-2.003867	3.217379	0.048870
1	-2.560235	2.322826	1.275821
7	2.995787	-0.000109	0.371114
1	3.290951	0.813621	0.919169
1	3.635636	-0.011050	-0.429157
1	3.284845	-0.804076	0.936540

Cartesian coordinates of the pentamer : [Fe(NH3)5]2+

Cartesian coordinates of : 500-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.543218	1.358758	-0.347252
1	-2.349656	1.166104	0.248133
1	-1.942249	1.409653	-1.287971
1	-1.304500	2.327621	-0.132951
7	-1.365529	-1.538219	-0.348802
1	-2.326516	-1.308390	-0.093752
1	-1.447898	-1.906230	-1.299901
1	-1.153849	-2.363126	0.213726
7	1.538594	-1.355672	-0.372098
1	2.296559	-1.231130	0.300263
1	2.006202	-1.312517	-1.280842
1	1.287175	-2.340239	-0.278241
7	0.026756	-0.004130	1.840348
1	0.921158	0.271187	2.248786
1	-0.168041	-0.912337	2.264147
1	-0.648174	0.623424	2.279845
26	-0.003513	-0.001479	-0.184842
7	1.350795	1.541550	-0.364527
1	1.212663	2.304599	0.299499
1	1.323010	2.002885	-1.277119
1	2.333681	1.290938	-0.251421

Cartesian coordinates of : 410-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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7	-0.869475	1.422008	-0.006746
1	-1.816284	1.017181	0.005577
1	-0.856950	2.034651	-0.824248
1	-0.841678	2.061409	0.789634
7	-0.869676	-1.421342	0.009195
1	-1.816153	-1.016805	-0.022451
1	-0.830758	-2.074019	-0.775774
1	-0.868965	-2.020279	0.836971
7	2.027220	1.443074	0.006087
1	1.709986	2.372449	-0.272169
1	2.818996	1.256940	-0.612152
1	2.455747	1.591762	0.922716
26	0.575849	0.000306	0.000198
7	2.025585	-1.444210	-0.007956
1	1.714177	-2.365020	0.303571
1	2.835298	-1.244798	0.582118
1	2.427262	-1.618015	-0.932339
7	-3.684288	0.000061	-0.002875
1	-4.114184	0.807661	-0.451970
1	-4.080738	-0.013072	0.935776
1	-4.113400	-0.795133	-0.474339

Cartesian coordinates of : 410-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.688864	-2.003248	-0.587371
1	-0.951745	-2.540983	0.239554
1	0.183648	-2.433294	-0.902505
1	-1.371303	-2.282213	-1.296688
7	0.871863	-0.114993	1.072703
1	0.847302	-0.961861	1.641638
1	1.839033	-0.100948	0.656381
1	0.873022	0.645058	1.753840
7	-0.311338	2.021854	-0.579872
1	-1.016673	2.450304	-1.184241
1	0.577258	2.269985	-1.021148
1	-0.332330	2.582169	0.273099
7	-2.195566	0.153958	0.812782
1	-3.061880	-0.085751	0.323713
1	-2.377461	1.080382	1.201120
1	-2.186528	-0.464260	1.625390
26	-0.536368	0.013041	-0.307630
7	3.598228	-0.088322	-0.009926
1	3.817091	-0.080871	-1.003584
1	4.079997	-0.906751	0.357271
1	4.105863	0.705214	0.376333

Cartesian coordinates of : 320-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.000018	-2.568367	0.110103
1	0.000026	-2.903973	1.076889
1	0.809849	-3.022145	-0.316704
1	-0.809930	-3.022134	-0.316627
7	1.987192	-0.357608	-0.057110
1	2.447304	-0.731398	-0.889919
1	2.302848	0.655925	-0.018444
1	2.476331	-0.802796	0.721929
7	-1.987210	-0.357586	-0.057055
1	-2.476329	-0.802730	0.722021
1	-2.302846	0.655954	-0.018425
1	-2.447355	-0.731407	-0.889831
26	-0.000010	-0.584382	-0.037357
7	-2.995560	2.338200	0.042882
1	-2.799641	2.888695	0.875861
1	-4.008477	2.234518	0.029316
1	-2.784482	2.951444	-0.741137
7	2.995620	2.338146	0.042918
1	2.799496	2.888756	0.875773
1	2.784777	2.951296	-0.741237
1	4.008536	2.234422	0.029641

Cartesian coordinates of : 320-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.265036	1.557783	0.047838
1	2.204002	1.137171	-0.009840
1	1.270806	2.125039	0.898629
1	1.220461	2.242168	-0.710697
7	1.161373	-1.334718	0.127225
1	1.124250	-1.846367	1.011624
1	2.128421	-0.982871	0.047919
1	1.061648	-2.057047	-0.588571
7	-1.808793	-0.988132	-0.091638
1	-1.901397	-1.549337	-0.940831
1	-1.907268	-1.664113	0.668197
1	-2.700966	-0.411567	-0.053549
26	-0.159020	0.127104	-0.008602
7	-4.281348	0.482321	0.012968
1	-4.640440	0.601969	0.957819
1	-4.367364	1.397606	-0.423021
1	-4.971434	-0.098444	-0.459671
7	4.000046	-0.018818	-0.080081
1	4.416501	0.677355	-0.697472
1	4.449876	0.133282	0.821871
1	4.393219	-0.898600	-0.412940

Cartesian coordinates of : 320-4_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.547750	-0.817197	0.588904
1	1.567558	-1.838642	0.529956
1	1.613695	-0.621819	1.588913
1	2.477874	-0.507372	0.176950
7	-1.547753	-0.817189	0.588911
1	-2.477876	-0.507367	0.176954
1	-1.567561	-1.838635	0.529973
1	-1.613698	-0.621802	1.588918
7	0.000006	1.807133	0.484487
1	0.000008	1.815717	1.505881
1	-0.809257	2.375014	0.219357
1	0.809271	2.375009	0.219354
26	-0.000001	-0.017425	-0.292831
7	4.112399	-0.084579	-0.492408
1	4.609024	-0.957120	-0.663598
1	4.684103	0.412352	0.187843
1	4.209314	0.443684	-1.356769
7	-4.112400	-0.084579	-0.492410
1	-4.209314	0.443682	-1.356772
1	-4.684106	0.412353	0.187839
1	-4.609024	-0.957121	-0.663599

Cartesian coordinates of : 230-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.473354	0.150647	-0.581776
1	-2.266172	-0.043952	0.109759
1	-1.120119	1.101552	-0.395526
1	-1.923521	0.197126	-1.499776
7	1.473354	0.150649	-0.581774
1	2.266172	-0.043951	0.109760
1	1.120118	1.101553	-0.395523
1	1.923520	0.197129	-1.499775
26	0.000000	-1.082197	-0.490018
7	3.647373	-0.335296	1.193593
1	3.488022	-0.179951	2.186814
1	4.383258	0.321047	0.938735
1	4.084710	-1.252754	1.134146
7	-0.000001	2.918698	-0.093390
1	0.800716	3.280101	0.423350
1	-0.800718	3.280100	0.423353
1	-0.000003	3.444974	-0.966277
7	-3.647372	-0.335297	1.193594
1	-3.488020	-0.179952	2.186815
1	-4.084709	-1.252755	1.134147
1	-4.383257	0.321047	0.938737

Cartesian coordinates of : 500-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.567932	2.012105	-0.200561
1	-0.091980	2.622036	-0.682187
1	1.407226	2.105255	-0.772208
1	0.776486	2.493424	0.677781
7	-1.742089	1.165770	0.070335
1	-1.632017	1.973368	0.683667
1	-1.983937	1.540313	-0.850067
1	-2.610836	0.751495	0.405185
7	2.087676	0.094758	0.255263
1	2.654885	0.001086	-0.590918
1	2.409066	-0.637122	0.888839
1	2.428412	0.942052	0.708479
26	-0.004673	-0.008762	-0.000006
7	0.743117	-1.954319	-0.210498
1	0.252378	-2.433255	-0.965884
1	0.647835	-2.548090	0.616612
1	1.719347	-2.051290	-0.485947
7	-1.642089	-1.305041	0.085527
1	-1.496111	-2.312752	0.053996
1	-2.323997	-1.139142	-0.656665
1	-2.137102	-1.172475	0.969004

Cartesian coordinates of the hexamer : [Fe(NH3)6]2+

Cartesian coordinates of : 600_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.207408	-0.983960	1.374740
1	1.449734	-1.940597	1.113714
1	0.809633	-1.082254	2.309563
1	2.112915	-0.543486	1.542442
7	-1.206570	-1.683094	-0.165242
1	-0.808555	-2.541635	0.217215
1	-2.112299	-1.608502	0.299704
1	-1.448390	-1.935477	-1.124323
7	-1.207421	0.983952	-1.374739
1	-0.809706	1.082144	-2.309599
1	-1.449660	1.940626	-1.113771
1	-2.112970	0.543528	-1.542342
7	1.207530	-0.697897	-1.539720
1	1.449021	0.006512	-2.237932
1	0.810257	-1.458823	-2.091941

1	2.113449	-1.062492	-1.242292
26	-0.000000	0.000001	-0.000001
7	1.206568	1.683097	0.165234
1	2.112277	1.608523	-0.299754
1	1.448428	1.935461	1.124310
1	0.808530	2.541645	-0.217185
7	-1.207515	0.697900	1.539729
1	-2.113363	1.062674	1.242301
1	-0.810148	1.458697	2.092059
1	-1.449150	-0.006553	2.237846

Cartesian coordinates of : 510-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.934264	1.424079	-0.374260
1	-0.977233	1.857524	-1.298875
1	-0.865361	2.214672	0.266486
1	-1.873988	1.035300	-0.225850
7	-0.934258	-1.424086	-0.374256
1	-1.873976	-1.035309	-0.225812
1	-0.977254	-1.857515	-1.298877
1	-0.865335	-2.214690	0.266474
7	0.452970	-0.000002	1.832100
1	0.892354	0.805350	2.279606
1	0.892445	-0.805304	2.279608
1	-0.501141	-0.000054	2.195009
26	0.522008	0.000000	-0.190322
7	1.979481	1.451346	-0.331457
1	2.348517	1.569802	-1.277780
1	2.811658	1.287130	0.235819
1	1.677361	2.389790	-0.069203
7	1.979486	-1.451339	-0.331465
1	2.811718	-1.287052	0.235710
1	2.348428	-1.569884	-1.277813
1	1.677407	-2.389761	-0.069085
7	-3.765061	0.000002	-0.006816
1	-4.163884	-0.802607	0.477644
1	-4.218513	-0.000011	-0.919246
1	-4.163899	0.802615	0.477626

Cartesian coordinates of : 420-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.435948	1.421418	0.201051
1	2.381055	1.036288	0.070721
1	1.456636	1.866084	1.120619
1	1.365245	2.200648	-0.454147
7	1.435945	-1.421425	0.201047

1	1.456630	-1.866099	1.120612
1	2.381053	-1.036293	0.070724
1	1.365245	-2.200649	-0.454158
7	-1.435949	1.421421	-0.201057
1	-2.381055	1.036289	-0.070716
1	-1.365243	2.200658	0.454132
1	-1.456645	1.866076	-1.120630
26	-0.000001	-0.000002	-0.000003
7	-1.435951	-1.421422	-0.201054
1	-1.456641	-1.866090	-1.120621
1	-1.365249	-2.200650	0.454147
1	-2.381058	-1.036289	-0.070724
7	4.248638	0.000006	-0.137243
1	4.628387	-0.801874	-0.638181
1	4.628391	0.801917	-0.638129
1	4.736694	-0.000024	0.757093
7	-4.248627	0.000005	0.137261
1	-4.628403	-0.802014	0.637957
1	-4.736693	0.000265	-0.757069
1	-4.628339	0.801776	0.638401

Cartesian coordinates of : 420-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.127049	2.315215	0.018230
1	0.992245	2.693774	-0.919739
1	2.140642	2.229190	0.117245
1	0.881259	3.088439	0.640662
7	1.002047	-0.455480	-1.039191
1	1.316015	0.087342	-1.843935
1	1.862084	-0.952747	-0.698695
1	0.414669	-1.187805	-1.439096
7	-0.768171	-1.043919	1.219524
1	-1.076634	-0.915632	2.185782
1	-0.188651	-1.883418	1.250000
1	-1.617940	-1.297908	0.699501
7	-1.573864	1.117218	-0.521278
1	-2.094182	1.872297	-0.069235
1	-2.229769	0.325373	-0.564794
1	-1.452476	1.432841	-1.483649
26	0.114752	0.580089	0.392206
7	-3.475979	-1.425218	-0.426195
1	-4.251492	-1.179591	0.187540
1	-3.411625	-2.440084	-0.361715
1	-3.831578	-1.262996	-1.367179
7	3.434919	-1.861200	-0.146060
1	3.770635	-1.837801	0.813978
1	4.217490	-1.529757	-0.706349
1	3.353755	-2.850152	-0.372901

Cartesian coordinates of : 330-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	3.579744	-1.589972	-0.480979
1	3.826913	-2.543008	-0.218061
1	4.336822	-1.019969	-0.107968
1	3.707272	-1.571459	-1.491076
7	1.031834	0.703190	-0.800018
1	0.811248	0.998956	-1.751449
1	1.230909	1.593420	-0.273637
1	1.922761	0.204624	-0.862741
7	1.008191	-1.462624	1.087807
1	1.263432	-1.071154	1.996405
1	1.900104	-1.533069	0.557453
1	0.729905	-2.423940	1.296136
26	-0.342575	-0.382526	0.065727
7	-1.934137	0.473490	-0.785497
1	-2.007192	0.318954	-1.792762
1	-1.966514	1.488904	-0.681443
1	-2.855323	0.129513	-0.395691
7	-4.505282	-0.428611	0.209025
1	-5.181583	0.264895	-0.103958
1	-4.661168	-0.514351	1.210616
1	-4.826490	-1.308460	-0.188565
7	1.604920	3.198056	0.604071
1	2.582756	3.217301	0.885953
1	1.087789	3.494141	1.428644
1	1.508416	3.965695	-0.057613

Cartesian coordinates of : 321_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-4.416262	-0.601310	0.020022
1	-4.895443	0.090403	-0.551790
1	-4.851012	-0.531301	0.937465
1	-4.728116	-1.495911	-0.351506
7	2.942667	-1.346248	0.108024
1	2.467588	-2.231652	0.293681
1	3.433563	-1.495011	-0.776386
1	3.690064	-1.305856	0.806238
7	0.736555	1.991115	0.322096
1	-0.304094	1.896059	0.177506
1	1.031823	2.716472	-0.335519
1	0.845321	2.430083	1.239612
26	1.703726	0.264385	0.107351
7	0.374567	-0.509362	-1.088397
1	0.724008	-1.141917	-1.809101

1	-0.181698	0.186522	-1.586008
1	-0.325660	-1.068164	-0.515808
7	-2.125589	1.816883	-0.099636
1	-2.411164	2.311251	-0.942819
1	-2.497598	2.377372	0.665210
1	-2.671977	0.953608	-0.084921
7	-1.526703	-1.944221	0.472243
1	-2.417447	-1.458746	0.328308
1	-1.443296	-2.074014	1.477920
1	-1.658382	-2.881213	0.096332

Cartesian coordinates of : 240_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.466844	2.244224	-0.404411
1	-3.081235	3.181734	-0.489529
1	-4.246394	2.340032	0.243118
1	-3.893861	2.047955	-1.306803
7	-1.851661	0.060186	0.665557
1	-2.375671	-0.824197	0.433082
1	-1.936173	0.156017	1.679901
1	-2.424137	0.851250	0.269679
7	1.851654	0.060169	-0.665555
1	2.375706	-0.824184	-0.433054
1	1.936164	0.155970	-1.679902
1	2.424092	0.851269	-0.269699
26	-0.000004	0.059579	0.000001
7	-3.347197	-2.372621	0.065770
1	-4.300427	-2.167278	0.357725
1	-3.084975	-3.203477	0.591182
1	-3.427883	-2.680243	-0.900498
7	3.347371	-2.372508	-0.065760
1	3.427783	-2.680384	0.900450
1	4.300671	-2.166966	-0.357349
1	3.085421	-3.203252	-0.591484
7	3.466687	2.244344	0.404397
1	3.893393	2.048348	1.306996
1	3.081103	3.181905	0.489076
1	4.246459	2.339894	-0.242903

Cartesian coordinates of the heptamer : [Fe(NH3)7]2+

Cartesian coordinates of : 610-1_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.995128	-0.016221	1.450819
1	-0.983242	-0.825994	2.071241

1	-1.938177	-0.010628	1.044110
1	-0.981723	0.779752	2.088822
7	1.956364	0.018423	1.453172
1	1.612263	0.006789	2.413791
1	2.600974	-0.771569	1.411854
1	2.572753	0.831035	1.420926
7	-3.866095	-0.001363	0.000002
1	-4.266064	-0.938050	-0.000271
1	-4.291272	0.459358	-0.802881
1	-4.291304	0.458891	0.803136
26	0.473626	0.000158	0.000000
7	-0.995137	-0.016809	-1.450803
1	-0.983267	-0.826843	-2.070886
1	-0.981725	0.778895	-2.089141
1	-1.938183	-0.011035	-1.044090
7	1.956356	0.017790	-1.453188
1	1.612255	0.005278	-2.413797
1	2.601211	-0.771969	-1.411236
1	2.572492	0.830619	-1.421599
7	0.399719	2.073098	-0.000427
1	0.829864	2.530745	-0.804823
1	0.830027	2.531094	0.803683
1	-0.557829	2.426154	-0.000408
7	0.453601	-2.073993	0.000428
1	-0.493617	-2.453750	0.000432
1	0.896203	-2.519511	0.804888
1	0.896338	-2.519856	-0.803767

Cartesian coordinates of : 520-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.456504	1.414176	-0.513753
1	2.362424	1.065206	-0.179065
1	1.302899	2.301452	-0.035949
1	1.626435	1.684129	-1.484529
7	0.085409	0.000003	1.733958
1	0.566976	0.805019	2.135114
1	-0.831317	0.000021	2.182459
1	0.566949	-0.805022	2.135130
7	-1.467872	-1.427522	-0.362260
1	-1.592113	-1.842403	-1.287563
1	-2.390657	-1.048686	-0.118488
1	-1.329715	-2.229888	0.251384
7	1.456495	-1.414205	-0.513747
1	1.626435	-1.684154	-1.484523
1	1.302883	-2.301483	-0.035948
1	2.362412	-1.065241	-0.179050
26	-0.004176	-0.000010	-0.286646
7	-1.467863	1.427512	-0.362288
1	-2.390655	1.048683	-0.118528
1	-1.592088	1.842399	-1.287590
1	-1.329707	2.229874	0.251362

7	-4.262720	0.000028	0.285773
1	-4.613529	-0.803051	0.804873
1	-4.797939	0.000225	-0.580971
1	-4.613450	0.802931	0.805197
7	4.204664	0.000030	0.356103
1	4.524684	-0.802827	0.894987
1	4.524631	0.802780	0.895178
1	4.790701	0.000146	-0.477175

Cartesian coordinates of : 430-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.456467	1.414191	-0.513752
1	1.302907	2.301461	-0.035921
1	1.626299	1.684156	-1.484542
1	2.362424	1.065222	-0.179162
7	-1.467879	1.427527	-0.362046
1	-1.329770	2.229786	0.251749
1	-1.592025	1.842567	-1.287289
1	-2.390697	1.048666	-0.118427
7	-1.467870	-1.427539	-0.362035
1	-1.329776	-2.229766	0.251805
1	-1.591979	-1.842628	-1.287261
1	-2.390699	-1.048673	-0.118467
7	0.085575	0.000012	1.734078
1	0.567220	-0.804977	2.135198
1	-0.831105	-0.000043	2.182671
1	0.567116	0.805065	2.135195
26	-0.004189	-0.000001	-0.286523
7	1.456468	-1.414192	-0.513743
1	2.362424	-1.065213	-0.179163
1	1.626298	-1.684171	-1.484530
1	1.302914	-2.301455	-0.035899
7	-4.262872	0.000003	0.285305
1	-4.797883	-0.000056	-0.581567
1	-4.613778	0.803019	0.804436
1	-4.613754	-0.802961	0.804533
7	4.204750	0.000001	0.355706
1	4.524823	-0.802819	0.894614
1	4.524807	0.802787	0.894674
1	4.790681	0.000038	-0.477647

Cartesian coordinates of : 340-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.184147	1.998071	-0.706707
1	-0.611492	2.510872	-0.326295

1	0.277234	2.350455	-1.661454
1	1.018875	2.381359	-0.205323
7	-0.468923	-0.014775	1.347654
1	-0.164598	0.805670	1.872318
1	-1.493005	-0.042629	1.439140
1	-0.119582	-0.810985	1.881413
26	0.030334	-0.009550	-0.582632
7	0.370960	-1.995665	-0.675155
1	-0.369809	-2.574969	-0.279742
1	0.489586	-2.353382	-1.625092
1	1.242004	-2.290784	-0.175588
7	2.837579	-2.940625	0.662633
1	2.621276	-3.723681	1.275292
1	3.456681	-2.342600	1.203791
1	3.424308	-3.333477	-0.070230
7	2.538908	3.189535	0.637773
1	3.084181	3.635821	-0.096538
1	3.214163	2.658191	1.181370
1	2.245608	3.949746	1.247174
7	-1.836069	-0.100625	-1.287729
1	-2.058370	-0.932242	-1.835446
1	-2.120044	0.680703	-1.879350
1	-2.494643	-0.104259	-0.497993
7	-3.669400	-0.112787	1.329607
1	-4.139602	-1.012670	1.246186
1	-4.337894	0.564919	0.966486
1	-3.653959	0.070331	2.331801

Cartesian coordinates of : 331_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.587344	0.999291	-1.034862
1	5.452110	0.726087	-0.572529
1	4.711330	1.982743	-1.265537
1	4.600618	0.512535	-1.927824
7	0.108600	0.460444	-0.842502
1	-0.583243	1.060849	-0.311848
1	0.695614	1.100925	-1.377387
1	-0.446210	-0.046241	-1.532196
7	2.439136	0.685987	0.905590
1	2.061380	1.622904	1.052705
1	3.188699	0.795424	0.173293
1	2.948986	0.482192	1.768540
26	1.058974	-0.678775	0.423120
7	-0.144759	-2.254542	0.157031
1	0.147579	-2.881142	-0.595467
1	-1.126683	-1.967687	-0.087536
1	-0.233522	-2.867497	0.970493
7	-2.873795	-1.520433	-0.551869
1	-3.273870	-0.586696	-0.445536
1	-3.432838	-2.118567	0.053695

1	-3.109136	-1.817336	-1.496763
7	-1.797110	2.012066	0.631912
1	-2.723229	1.686446	0.340488
1	-1.744790	2.988481	0.349088
1	-1.819418	2.033370	1.648712
7	-4.790065	1.194118	-0.249245
1	-5.288429	0.686744	-0.976532
1	-4.932579	2.174759	-0.480142
1	-5.331144	1.041321	0.598789

Cartesian coordinates of the octamer : [Fe(NH3)8]2+

Cartesian coordinates of : 620-1_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.250136	-0.823193	1.420882
1	-1.175033	-0.437501	2.361834
1	-1.175246	-1.831374	1.554117
1	-2.223983	-0.665740	1.149393
7	-1.250139	-0.818463	-1.423610
1	-1.175250	-1.826196	-1.560195
1	-2.223985	-0.661912	-1.151595
1	-1.175038	-0.429644	-2.363274
7	1.250136	0.823193	-1.420882
1	1.175033	0.437500	-2.361834
1	2.223983	0.665740	-1.149393
1	1.175246	1.831374	-1.554117
7	1.249515	-1.642614	-0.002733
1	2.223503	-1.329244	-0.002212
1	1.174243	-2.262000	-0.809259
1	1.174245	-2.264680	0.801729
26	0.000000	0.000000	0.000000
7	1.250139	0.818463	1.423610
1	1.175038	0.429644	2.363274
1	1.175250	1.826196	1.560196
1	2.223985	0.661912	1.151595
7	-1.249515	1.642614	0.002733
1	-1.174245	2.264680	-0.801729
1	-1.174243	2.262000	0.809259
1	-2.223503	1.329244	0.002212
7	-4.168077	-0.000068	-0.000000
1	-4.587763	0.462935	0.804896
1	-4.588029	-0.928510	-0.001545
1	-4.587764	0.465611	-0.803351
7	4.168077	0.000068	0.000000
1	4.588029	0.928510	0.001545
1	4.587763	-0.462935	-0.804896
1	4.587764	-0.465611	0.803351

Cartesian coordinates of : 620-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.705496	-0.426271	-1.163366
1	-2.386190	0.265060	-0.828770
1	-2.221943	-1.304793	-1.205705
1	-1.548932	-0.183257	-2.141375
7	-0.856247	-1.902690	1.201604
1	-1.774212	-1.639553	1.560856
1	-1.020678	-2.798897	0.742532
1	-0.320142	-2.145169	2.035142
7	1.705498	-0.426114	1.163354
1	1.548944	-0.182994	2.141339
1	2.386189	0.265178	0.828671
1	2.221949	-1.304630	1.205786
7	-0.824906	1.019546	1.194437
1	-0.255825	1.862602	1.268978
1	-0.994971	0.751343	2.163691
1	-1.736348	1.338460	0.846302
26	-0.000001	-0.445615	-0.000000
7	0.824579	1.019926	-1.194193
1	0.255444	1.862977	-1.268389
1	0.994444	0.751985	-2.163555
1	1.736086	1.338778	-0.846177
7	0.856581	-1.902285	-1.201857
1	1.021381	-2.798474	-0.742883
1	1.774408	-1.638798	-1.561206
1	0.320447	-2.144880	-2.035342
7	-3.711228	1.817510	-0.008390
1	-3.717781	2.646461	0.583240
1	-4.513415	1.274399	0.305472
1	-3.975163	2.164618	-0.928666
7	3.711222	1.817526	0.008386
1	4.514496	1.272700	-0.299677
1	3.971873	2.169641	0.927693
1	3.719953	2.643204	-0.587776

Cartesian coordinates of : 530-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	-1.432736	0.729037	1.018054
1	-1.236915	1.695677	0.754317
1	-1.532623	0.741377	2.033637
1	-2.367495	0.510194	0.659110
7	0.000049	0.471173	-1.471229
1	0.808501	0.305241	-2.070036
1	-0.808313	0.305123	-2.070123
1	-0.000037	1.478900	-1.279504

7	1.463238	-1.849452	-0.232857
1	1.585879	-2.614304	0.432946
1	2.383808	-1.397916	-0.284861
1	1.329895	-2.317654	-1.128364
7	-1.463112	-1.849504	-0.232894
1	-1.585696	-2.614395	0.432875
1	-1.329758	-2.317658	-1.128425
1	-2.383712	-1.398021	-0.284860
26	0.000032	-0.517206	0.280228
7	1.432749	0.729059	1.018136
1	2.367510	0.510294	0.659146
1	1.532663	0.741298	2.033717
1	1.236890	1.695720	0.754513
7	4.272757	-0.312219	-0.147961
1	4.672865	-0.981882	-0.802689
1	4.778473	-0.472225	0.721444
1	4.603070	0.591277	-0.481192
7	-0.000298	3.536247	-0.414689
1	-0.804388	3.896318	-0.926201
1	0.803803	3.896416	-0.926116
1	-0.000374	4.064416	0.456422
7	-4.272727	-0.312498	-0.147909
1	-4.603088	0.590922	-0.481298
1	-4.778397	-0.472360	0.721548
1	-4.672840	-0.982301	-0.802492

Cartesian coordinates of : 530-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.107270	-0.079433	-1.205034
1	-2.393970	-0.906198	-1.728682
1	-2.430900	0.700496	-1.776924
1	-2.700355	-0.067894	-0.367203
7	0.003569	-2.051228	-0.762259
1	-0.804951	-2.559245	-0.405226
1	0.143382	-2.426667	-1.701843
1	0.808355	-2.387614	-0.219030
7	1.881047	0.049157	-0.363733
1	2.164041	0.888558	0.148114
1	2.442708	0.061063	-1.216397
1	2.216232	-0.763746	0.159252
7	-0.557384	-0.007260	1.296292
1	-0.199857	0.808048	1.793637
1	-0.182128	-0.806146	1.807020
1	-1.569357	-0.016870	1.469085
26	-0.129420	-0.015712	-0.668631
7	-0.121683	2.022075	-0.799969
1	-0.962730	2.484809	-0.456694
1	0.001582	2.389204	-1.745112
1	0.656789	2.416679	-0.257733
7	2.584328	-2.910386	0.895533
1	3.273041	-3.258302	0.230793

1	2.148838	-3.748531	1.276200
1	3.133441	-2.541041	1.669211
7	2.390656	3.061575	0.863028
1	3.055190	3.447902	0.194879
1	2.962851	2.736618	1.639902
1	1.900758	3.872736	1.235948
7	-3.773763	-0.048295	1.553334
1	-3.699778	0.276448	2.515785
1	-4.186032	-0.976504	1.627349
1	-4.508720	0.531258	1.151731

Cartesian coordinates of : 440-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.023763	1.738533	0.509111
1	-0.502081	2.480923	0.031161
1	-1.234714	2.114439	1.434179
1	-1.933604	1.640580	0.046258
7	-1.737748	-1.024867	0.509545
1	-1.640819	-1.927111	0.031566
1	-2.486633	-0.498721	0.046929
1	-2.104012	-1.251425	1.434788
7	1.737758	1.024876	0.509522
1	2.486643	0.498728	0.046907
1	1.640823	1.927116	0.031535
1	2.104028	1.251445	1.434760
26	0.000006	0.000004	0.527483
7	1.023773	-1.738526	0.509095
1	1.234725	-2.114437	1.434162
1	0.502091	-2.480915	0.031144
1	1.933613	-1.640568	0.046242
7	-1.010922	-3.875953	-0.814154
1	-1.331745	-4.555432	-0.126959
1	-1.751985	-3.836733	-1.511110
1	-0.242030	-4.338807	-1.294950
7	3.894097	-1.007055	-0.787371
1	4.273979	-1.901211	-0.482307
1	4.636825	-0.341071	-0.583162
1	3.869383	-1.065558	-1.803320
7	-3.894084	1.007022	-0.787374
1	-4.637152	0.341856	-0.581745
1	-3.869733	1.063836	-1.803427
1	-4.273277	1.901929	-0.483661
7	1.010882	3.875967	-0.814163
1	1.330244	4.555914	-0.126751
1	0.242342	4.338080	-1.296232
1	1.752972	3.837049	-1.510042

Cartesian coordinates of : 341_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.057846	-1.236480	1.283110
1	3.755832	-0.722455	0.740615
1	3.468594	-2.146374	1.481237
1	3.005363	-0.772711	2.186464
7	2.396702	1.428179	-1.278834
1	3.251985	0.958265	-0.975778
1	2.355067	1.315364	-2.289068
1	2.572963	2.420880	-1.138902
26	-0.840902	-0.747292	0.119120
7	0.823850	-1.659798	-0.492664
1	1.614548	-1.515451	0.188852
1	1.173922	-1.289790	-1.377180
1	0.755921	-2.669046	-0.635875
7	5.395361	0.292734	-0.403535
1	5.795412	0.994745	0.214618
1	5.635772	0.598274	-1.343502
1	5.956848	-0.542500	-0.254779
7	-2.639614	-0.074209	0.652688
1	-2.909446	-0.286390	1.614381
1	-3.428088	-0.436281	0.065414
1	-2.660416	0.949688	0.585821
7	0.073505	0.936171	0.483084
1	-0.576771	1.730199	0.441080
1	0.867806	1.120386	-0.169837
1	0.486241	0.967931	1.416511
7	-2.262531	3.132311	0.444530
1	-3.182950	3.222256	0.018325
1	-1.689919	3.807273	-0.058771
1	-2.368250	3.524730	1.378241
7	-4.890980	-1.116770	-0.945646
1	-4.990908	-0.758598	-1.892173
1	-5.737604	-0.828458	-0.460525
1	-4.967432	-2.127302	-1.031427

Cartesian coordinates of : 242_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.038841	3.701210	-0.412293
1	0.941028	3.937731	-0.278180
1	-0.555855	4.403390	0.112607
1	-0.234323	3.897119	-1.391324
7	-0.660438	-2.012851	-0.266930
1	-1.584893	-2.181934	0.261153
1	-0.824252	-2.298395	-1.234596
1	-0.018991	-2.692811	0.149686
7	-1.034560	1.144347	0.452014

1	-2.003261	1.159143	0.023343
1	-0.605696	2.062154	0.120547
1	-1.128428	1.210481	1.467555
26	-0.003754	-0.272853	-0.100647
7	1.755733	0.073498	-0.500279
1	2.287370	-0.836425	-0.670800
1	2.288994	0.552067	0.276279
1	1.862577	0.615661	-1.360621
7	3.356485	-2.256020	-1.031500
1	3.604482	-2.844491	-0.239555
1	4.237362	-1.865280	-1.359524
1	3.062843	-2.895324	-1.766412
7	3.360387	1.303232	1.585519
1	4.079703	1.908439	1.196590
1	3.864482	0.578102	2.090436
1	2.900241	1.856138	2.304131
7	-3.683720	1.388442	-0.696520
1	-3.940598	0.788370	-1.476200
1	-3.765256	2.337712	-1.053411
1	-4.436308	1.294280	-0.018707
7	-3.034460	-2.684596	1.099442
1	-3.838887	-2.781177	0.483925
1	-3.347044	-2.102443	1.872594
1	-2.891781	-3.609164	1.501152

Cartesian coordinates of the nanomer : [Fe(NH₃)₉]²⁺

Cartesian coordinates of : 630-1_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.299885	-1.662319	1.184147
1	1.057198	-2.256683	0.830176
1	-0.509155	-2.276865	1.270755
1	0.562182	-1.456077	2.147638
7	-1.300181	-1.079443	-1.187172
1	-1.371568	-0.750062	-2.149488
1	-1.072514	-2.069269	-1.277324
1	-2.261713	-1.052089	-0.831150
7	-0.285858	1.663291	-1.186147
1	0.035933	1.561277	-2.148283
1	0.218123	2.482214	-0.829233
1	-1.257076	1.960455	-1.276830
7	1.583178	-0.584833	-1.185216
1	2.320331	0.113044	-1.282005
1	1.334316	-0.821286	-2.145343
1	2.048104	-1.424513	-0.823247
26	-0.001777	-0.001039	-0.001021
7	1.286213	1.089681	1.184867
1	2.218406	0.687725	1.281002
1	0.971178	1.224467	2.145222

1	1.434008	2.038673	0.824528
7	-1.591775	0.568811	1.183313
1	-2.486769	0.219623	0.823637
1	-1.712328	1.576953	1.277283
1	-1.550238	0.230856	2.144426
7	2.811410	-3.327893	0.003195
1	3.744116	-3.094508	-0.332031
1	2.508909	-4.100015	-0.587399
1	2.971102	-3.746921	0.917332
7	1.496376	4.090151	0.002181
1	0.933585	4.715120	0.575902
1	1.522512	4.531730	-0.914907
1	2.444644	4.194845	0.358019
7	-4.293194	-0.753324	0.002048
1	-4.552791	-1.547345	0.583959
1	-4.687252	-0.961862	-0.913355
1	-4.859407	0.018677	0.348764

Cartesian coordinates of : 630-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.611698	-1.632917	0.421080
1	2.106065	-1.706059	1.310029
1	2.316062	-1.313479	-0.253321
1	1.419329	-2.599827	0.160571
7	0.702782	0.602078	-1.202419
1	1.655666	0.318348	-1.449273
1	0.158406	0.495115	-2.057476
1	0.737186	1.609416	-1.036686
7	-1.629223	0.904317	0.425483
1	-1.320037	1.852976	0.209188
1	-2.155431	0.993632	1.293984
1	-2.324827	0.657556	-0.284693
7	0.996698	0.990263	1.587236
1	0.776903	1.039528	2.581383
1	0.804353	1.927488	1.220949
1	2.011736	0.897888	1.557730
26	-0.029092	-0.385847	0.443491
7	-0.783868	-1.356075	2.109620
1	-0.707603	-0.839089	2.985331
1	-0.345149	-2.254243	2.313034
1	-1.777914	-1.572340	2.034041
7	-1.063434	-1.681780	-0.780408
1	-1.920276	-1.250598	-1.145341
1	-1.369634	-2.556407	-0.354645
1	-0.538949	-1.976279	-1.603785
7	-3.750046	-0.205555	-1.796739
1	-4.052690	-1.082321	-2.216955
1	-3.705200	0.449434	-2.574617
1	-4.549652	0.097301	-1.243994
7	0.278150	3.768996	0.029280
1	1.221595	4.152892	0.023425

1	-0.203023	4.291902	0.759077
1	-0.136520	4.104468	-0.838253
7	3.704620	-0.541198	-1.784397
1	4.243601	-1.397344	-1.668480
1	4.346371	0.203692	-1.520861
1	3.594387	-0.448526	-2.792276

Cartesian coordinates of : 540-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.445671	-1.378784	-0.886666
1	-1.237004	-2.221898	-0.350825
1	-1.592797	-1.695289	-1.845325
1	-2.360741	-1.046111	-0.564728
7	1.444957	-1.379560	-0.886948
1	1.235816	-2.222745	-0.351411
1	1.592009	-1.695840	-1.845694
1	2.360176	-1.047478	-0.564819
7	1.422845	1.474720	-0.530193
1	1.128818	2.240339	0.082943
1	1.636102	1.918905	-1.424167
1	2.321962	1.121221	-0.193463
7	0.000150	-0.323369	1.366183
1	-0.808384	0.041297	1.868412
1	0.809224	0.040450	1.868157
1	-0.000356	-1.335705	1.528050
26	0.000041	0.028201	-0.612505
7	4.226723	-0.103273	0.127618
1	4.619430	0.771912	0.468551
1	4.783292	-0.328215	-0.694882
1	4.498618	-0.792004	0.825941
7	-0.001575	-3.581004	1.373889
1	-0.806154	-3.755411	1.973536
1	0.802953	-3.756062	1.973415
1	-0.001935	-4.360871	0.718710
7	-1.421947	1.475504	-0.529901
1	-2.321255	1.122493	-0.193166
1	-1.635003	1.919894	-1.423822
1	-1.127437	2.240906	0.083272
7	-4.226874	-0.100752	0.127288
1	-4.499272	-0.789148	0.825745
1	-4.783397	-0.325620	-0.695262
1	-4.619184	0.774736	0.467901
7	0.001285	3.876076	1.168901
1	0.001362	4.667740	0.528657
1	0.804987	4.030989	1.773962
1	-0.802135	4.031369	1.774239

Cartesian coordinates of : 450-3_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	0.114761	-1.463691	-0.142821
1	0.815893	-1.927863	0.439785
1	0.455707	-1.499460	-1.106712
1	-0.743552	-2.028312	-0.114814
7	0.680886	1.275426	-1.163029
1	1.604568	1.645277	-0.913121
1	0.830112	0.577256	-1.902909
1	0.180368	2.048829	-1.600563
7	1.422647	0.522846	1.545666
1	2.157300	1.080447	1.097863
1	1.815257	-0.411473	1.712333
1	1.290686	0.935605	2.469701
26	-0.225551	0.411203	0.375993
7	-2.069819	0.400796	-0.426887
1	-2.492043	-0.523679	-0.309662
1	-2.097686	0.576460	-1.430331
1	-2.733582	1.085631	-0.008422
7	-2.734762	-2.879443	-0.030429
1	-3.435815	-2.850259	-0.767726
1	-3.263087	-2.876003	0.839404
1	-2.344499	-3.817650	-0.090465
7	3.511320	2.382783	-0.071023
1	4.347747	1.802877	-0.082245
1	3.649242	3.033769	0.699597
1	3.589041	2.961334	-0.905192
7	1.121901	-1.045652	-3.289509
1	2.058679	-1.443950	-3.284776
1	1.125483	-0.390008	-4.068646
1	0.514489	-1.801109	-3.600087
7	2.434468	-2.479813	1.974336
1	1.877009	-3.229405	2.378570
1	3.027785	-2.166107	2.740011
1	3.072813	-2.939780	1.328746
7	-3.993013	2.373244	0.754423
1	-4.366691	2.115830	1.664275
1	-4.798091	2.405684	0.133755
1	-3.691539	3.339322	0.850717

Cartesian coordinates of : 450-4_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

7	0.002247	1.482514	0.382928
1	0.832318	2.077273	0.312752
1	0.003556	1.098095	1.333459
1	-0.828501	2.076977	0.315167
7	-0.005341	-1.484865	0.388189

1	0.825022	-2.080024	0.324568
1	-0.009651	-1.098820	1.338531
1	-0.834852	-2.079706	0.315981
7	2.011549	-0.008814	-1.107008
1	2.420001	-0.836885	-0.659403
1	2.422899	0.823519	-0.670191
1	2.367241	-0.015805	-2.063874
26	0.000959	-0.003339	-0.919839
7	-2.008441	0.001753	-1.115782
1	-2.359386	0.010376	-2.074401
1	-2.418080	0.829475	-0.669314
1	-2.423526	-0.830748	-0.681712
7	-2.977058	2.831876	0.062720
1	-3.824626	2.523001	0.534307
1	-3.295370	3.242217	-0.812895
1	-2.655695	3.624981	0.613891
7	2.986898	-2.827253	0.068028
1	3.846698	-2.513155	0.513350
1	3.283573	-3.262327	-0.803239
1	2.671841	-3.603043	0.646762
7	-0.003109	0.005529	3.267640
1	0.754560	0.554872	3.668261
1	0.084695	-0.906789	3.711001
1	-0.854842	0.400132	3.661471
7	2.997533	2.815203	0.052576
1	3.495974	3.066860	-0.798740
1	3.724073	2.571041	0.722281
1	2.620835	3.697411	0.393104
7	-3.007855	-2.808948	0.055996
1	-3.269106	-2.922001	1.033038
1	-2.687609	-3.727889	-0.242757
1	-3.891941	-2.681183	-0.432598

Cartesian coordinates of : 360_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.703827	0.162790	-0.194039
1	2.541328	0.241150	0.422303
1	1.697286	0.991696	-0.798541
1	1.852190	-0.651040	-0.799936
7	-0.710933	-1.556952	-0.194039
1	-1.061822	-2.321429	0.422302
1	-1.489911	-1.278524	-0.799937
1	0.010191	-1.965740	-0.798541
7	-0.992893	1.394163	-0.194039
1	-1.479506	2.080279	0.422302
1	-1.707476	0.974044	-0.798542
1	-0.362278	1.929564	-0.799936
26	0.000000	0.000000	0.727105
7	1.317721	2.866338	-1.940794
1	1.094591	3.797995	-1.596479

1	0.926648	2.827861	-2.879733
1	2.325620	2.885381	-2.083120
7	1.823461	-2.574348	-1.940794
1	1.985675	-2.216431	-2.879734
1	1.336003	-3.456736	-2.083120
1	2.741865	-2.846941	-1.596479
7	-3.141180	-0.291989	-1.940796
1	-3.661621	0.571356	-2.083123
1	-3.836455	-0.951054	-1.596482
1	-2.912321	-0.611429	-2.879735
7	-1.708633	-3.752825	1.575780
1	-2.276842	-3.494509	2.378434
1	-0.973674	-4.348670	1.948362
1	-2.296604	-4.369484	1.020505
7	-2.395728	3.356130	1.575780
1	-1.887918	3.719052	2.378437
1	-3.279227	3.017560	1.948357
1	-2.635781	4.173660	1.020507
7	4.104358	0.396694	1.575781
1	4.252895	1.331110	1.948362
1	4.932386	0.195825	1.020506
1	4.164755	-0.224547	2.378435

Cartesian coordinates of the decamer : [Fe(NH₃)₁₀]²⁺

Cartesian coordinates of : 640-5_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.856791	-0.012286	0.974313
1	2.584764	0.592722	0.584078
1	2.213865	-0.967052	0.920361
1	1.833433	0.205423	1.969541
7	0.764114	-1.208768	-1.381074
1	1.462716	-0.865225	-2.039088
1	1.219499	-1.982095	-0.886751
1	0.047898	-1.640948	-1.963581
7	-1.739219	0.285219	-0.989626
1	-1.682725	0.486065	-1.987040
1	-2.341759	1.016542	-0.603702
1	-2.271393	-0.585866	-0.916156
7	0.805969	1.726201	-1.115336
1	0.322215	2.611917	-0.971271
1	0.771475	1.585762	-2.124360
1	1.791791	1.914027	-0.903104
26	0.059931	0.157211	-0.008514
7	-0.627099	1.496041	1.396811
1	0.005301	2.276638	1.571327
1	-0.799937	1.103668	2.321486
1	-1.518084	1.924368	1.120274
7	-0.650478	-1.456432	1.048903
1	-1.456688	-1.885485	0.583627

1	-0.953175	-1.292576	2.007813
1	0.059228	-2.187297	1.113190
7	3.924302	2.150392	-0.358607
1	3.907554	3.058526	-0.818485
1	4.602051	1.605734	-0.887634
1	4.371575	2.329402	0.538097
7	-3.432675	2.726845	0.443550
1	-4.248480	2.247140	0.817932
1	-3.736714	3.110519	-0.448806
1	-3.314044	3.541245	1.042800
7	-3.232849	-2.615721	-0.531926
1	-2.918054	-3.572080	-0.680508
1	-3.816768	-2.411450	-1.340307
1	-3.883716	-2.671214	0.248766
7	2.187858	-3.422612	0.530822
1	1.723617	-4.267974	0.204117
1	2.357838	-3.591336	1.520492
1	3.111502	-3.458753	0.103440

Cartesian coordinates of : 640-6_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.820995	1.483369	-1.603632
1	-0.407118	1.586793	-2.529621
1	-0.724624	2.405433	-1.164742
1	-1.818427	1.372722	-1.783431
7	-1.648695	0.006997	0.790596
1	-2.221574	0.849373	0.761909
1	-2.291563	-0.766638	0.600588
1	-1.360945	-0.085749	1.766321
7	0.818351	-1.431353	0.790485
1	1.809779	-1.601211	0.600453
1	0.375320	-2.348690	0.761746
1	0.754796	-1.135848	1.766231
7	0.830477	1.424340	0.790490
1	1.846430	1.499314	0.761700
1	0.606387	1.221521	1.766241
1	0.481871	2.367884	0.600508
26	-0.000011	-0.000004	-0.433801
7	1.695038	-0.030741	-1.603749
1	2.097909	0.888379	-1.783622
1	1.577607	-0.440928	-2.529709
1	2.445420	-0.575203	-1.164884
7	-0.874236	-1.452628	-1.603641
1	-1.720957	-1.830185	-1.164746
1	-0.279726	-2.261121	-1.783476
1	-1.170750	-1.145877	-2.529616
7	3.940344	-1.833770	-0.125138
1	4.508562	-1.405849	0.602699
1	4.513679	-1.781595	-0.964823
1	3.919102	-2.825111	0.105016
7	-3.558387	-2.495407	-0.124972

1	-4.406156	-1.981395	0.105806
1	-3.471669	-3.201855	0.602452
1	-3.800258	-3.017541	-0.964841
7	0.000157	-0.000119	3.755146
1	-0.613486	0.698076	4.170905
1	0.911663	0.182215	4.170840
1	-0.297660	-0.880672	4.170866
7	-0.382028	4.329321	-0.124940
1	0.487025	4.806550	0.105666
1	-1.037061	4.607414	0.602611
1	-0.713464	4.799835	-0.964745

Cartesian coordinates of : 640-7_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.029301	1.697852	0.057796
1	0.501288	2.199104	0.776284
1	1.247580	2.410848	-0.637313
1	1.935568	1.441318	0.457824
7	0.341147	0.660739	-2.578932
1	-0.172966	1.485327	-2.888080
1	1.320329	0.898464	-2.736665
1	0.137747	-0.044179	-3.287105
7	-1.151093	-1.537271	-1.231811
1	-1.486207	-1.536984	-2.194407
1	-1.997644	-1.580300	-0.657568
1	-0.693419	-2.440569	-1.115695
7	-1.748378	1.188210	-0.491838
1	-2.524936	0.601849	-0.181517
1	-2.091967	1.670403	-1.321041
1	-1.639147	1.913248	0.223356
26	-0.024584	0.079004	-0.629453
7	-0.378724	-0.544315	1.294360
1	-0.087252	0.094494	2.032483
1	0.088852	-1.434129	1.492584
1	-1.372308	-0.712023	1.456587
7	1.690662	-1.049260	-0.625685
1	2.003039	-1.425434	-1.519827
1	1.586831	-1.859728	-0.009886
1	2.488628	-0.526216	-0.252097
7	-1.133657	3.375606	1.875379
1	-1.983900	3.195489	2.404738
1	-1.309309	4.251707	1.387498
1	-0.439140	3.608960	2.581972
7	1.132076	-3.411206	1.612897
1	1.829707	-3.983932	1.142102
1	0.341158	-4.036170	1.752956
1	1.513159	-3.258140	2.544379
7	-3.776142	-1.248389	0.712332
1	-4.126665	-0.706913	1.500128
1	-3.804388	-2.213643	1.035461

1	-4.515934	-1.191961	0.014499
7	4.070188	0.703125	0.758251
1	4.778106	0.201840	0.225595
1	4.206032	0.404624	1.721487
1	4.378697	1.672890	0.737779

Cartesian coordinates of : 550_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.708558	0.006875	-0.552177
1	2.424794	0.034128	0.176087
1	1.875645	0.819449	-1.150338
1	1.901906	-0.825029	-1.114799
7	-0.234188	2.026232	0.045451
1	-1.187729	2.367570	-0.108059
1	0.335076	2.344790	-0.745697
1	0.114716	2.552301	0.845166
7	-0.197899	-2.038149	0.093166
1	-1.142587	-2.393296	-0.082448
1	0.399526	-2.370298	-0.671094
1	0.128988	-2.540779	0.916862
26	-0.161167	-0.003250	0.246939
7	-2.136167	-0.017404	0.763126
1	-2.308691	-0.023809	1.767307
1	-2.634151	0.805769	0.411491
1	-2.622118	-0.844635	0.404003
7	-3.388983	2.797202	-0.303009
1	-4.183177	2.717903	0.328535
1	-3.142020	3.784144	-0.274680
1	-3.773638	2.649897	-1.233447
7	-3.330832	-2.853693	-0.324477
1	-3.181375	-3.798796	0.022347
1	-3.471843	-2.956663	-1.326900
1	-4.243566	-2.591964	0.041968
7	1.912598	-2.842681	-2.224127
1	2.928910	-2.794817	-2.242196
1	1.619878	-2.643795	-3.178081
1	1.708549	-3.830433	-2.087805
7	0.525056	0.027985	2.140511
1	0.254595	-0.778519	2.702400
1	0.217068	0.831163	2.687695
1	1.552946	0.051765	2.172219
7	1.808782	2.810378	-2.326550
1	2.610697	2.421434	-2.817588
1	2.143476	3.693395	-1.947081
1	1.156258	3.066863	-3.064063
7	3.689845	0.090003	2.149714
1	4.214282	-0.764970	1.977541
1	3.726659	0.214837	3.159505
1	4.269892	0.839663	1.779333

Cartesian coordinates of : 460-2_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.338670	-1.397679	0.845320
1	0.395126	-1.526818	1.550608
1	-0.265926	-2.180089	0.190396
1	-1.246562	-1.492480	1.311297
7	0.411508	-0.442624	-1.873735
1	1.417076	-0.299983	-2.032542
1	0.251813	-1.457224	-1.874811
1	-0.055796	-0.083016	-2.705596
7	1.672794	0.692935	0.495293
1	2.357603	0.545669	-0.248684
1	1.933462	0.060486	1.254918
1	1.834264	1.654347	0.849295
26	-0.196161	0.309609	-0.140150
7	-2.162184	0.309009	-0.587638
1	-2.687102	-0.099966	0.190934
1	-2.405358	-0.261107	-1.396419
1	-2.581841	1.240889	-0.774541
7	-3.382689	-1.305737	2.007964
1	-4.077155	-1.893913	1.552526
1	-3.903503	-0.509373	2.368780
1	-3.107054	-1.826082	2.837967
7	3.504620	0.117760	-2.250448
1	4.167227	-0.584878	-1.930212
1	3.977491	1.010008	-2.124621
1	3.460953	-0.006903	-3.259761
7	-0.094971	-3.594139	-1.632859
1	0.677600	-4.157923	-1.284753
1	-0.056848	-3.702258	-2.644485
1	-0.936678	-4.094903	-1.356182
7	2.074665	-1.554426	2.940405
1	2.279237	-0.839477	3.634999
1	2.979920	-1.928058	2.664336
1	1.635697	-2.305884	3.468068
7	-3.428124	2.983592	-1.173838
1	-3.508679	3.625367	-0.389770
1	-4.383870	2.789173	-1.461573
1	-3.026287	3.529718	-1.931061
7	2.184714	3.500651	1.535757
1	2.067409	4.256232	0.866119
1	3.160564	3.541383	1.818238
1	1.655761	3.781849	2.356867

Cartesian coordinates of : 361_LS

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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7	1.766942	-0.919951	-0.465516
1	2.621908	-1.357601	-0.062802
1	2.077601	-0.273441	-1.199326
1	1.234253	-1.666893	-0.925195
7	-1.080120	-0.782742	0.358816
1	-1.618907	-1.141301	1.173589
1	-1.674449	-0.095480	-0.120244
1	-0.947437	-1.566406	-0.287117
7	0.441215	1.708318	-0.130906
1	0.629572	2.560304	0.436941
1	-0.520687	1.786190	-0.491077
1	1.071467	1.739122	-0.937919
26	0.633120	0.018986	0.803023
7	2.600842	1.370063	-2.576254
1	2.537249	2.378062	-2.702880
1	2.300266	0.978560	-3.466275
1	3.600357	1.184258	-2.525819
7	-0.181843	-3.184861	-1.681280
1	-0.816178	-2.987318	-2.452137
1	-0.623869	-3.934144	-1.153027
1	0.625489	-3.624779	-2.118222
7	-2.534708	1.677436	-1.064585
1	-3.349320	1.050762	-1.104393
1	-2.399926	1.989223	-2.024319
1	-2.863799	2.500925	-0.564344
7	-2.591069	-1.774236	2.759962
1	-3.367671	-1.152454	2.969806
1	-2.101140	-1.899749	3.641914
1	-3.014006	-2.676951	2.559801
7	0.991200	4.165871	1.507123
1	1.972993	4.429138	1.530217
1	0.687127	4.177454	2.477131
1	0.513537	4.948597	1.067581
7	4.226314	-2.182593	0.703932
1	4.750335	-1.650564	1.393858
1	4.884438	-2.363661	-0.049829
1	4.056943	-3.087849	1.134783
7	-5.108886	-0.087893	-1.274232
1	-5.811570	0.344216	-0.680824
1	-5.207854	-1.088199	-1.129955
1	-5.417045	0.080449	-2.227943

Cartesian coordinates of : 352

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.275099	-0.008735	-2.750212
1	4.020810	-0.692678	-2.651562
1	3.736121	0.855435	-3.023209
1	2.747203	-0.300328	-3.568123
7	2.726873	-1.667808	2.401128
1	3.238789	-2.464563	2.029048

1	3.442294	-1.001999	2.684267
1	2.325202	-1.996588	3.276515
26	0.001847	0.365995	-0.016221
7	1.984202	0.511359	-0.056697
1	2.407958	0.291377	-0.977055
1	2.393864	-0.140928	0.615247
1	2.339629	1.451633	0.199390
7	3.030531	3.263887	0.691021
1	4.035944	3.220622	0.545602
1	2.911498	3.553342	1.658102
1	2.712774	4.050807	0.131594
7	-1.978686	0.524766	-0.063649
1	-2.399825	0.326378	-0.990078
1	-2.326699	1.462694	0.210296
1	-2.397298	-0.138488	0.592552
7	-0.003159	-1.403352	0.791771
1	-0.849665	-1.565649	1.348368
1	0.816748	-1.546264	1.392959
1	0.024085	-2.163750	0.084581
7	-2.827071	-1.708463	2.267002
1	-3.017014	-1.118282	3.073799
1	-2.579452	-2.614531	2.658696
1	-3.731819	-1.859865	1.826595
7	-3.002400	3.271548	0.733554
1	-2.479013	3.863632	1.372650
1	-3.906930	3.133823	1.176967
1	-3.186917	3.850843	-0.081231
7	-3.261582	0.037237	-2.767765
1	-2.763454	0.277700	-3.620414
1	-4.092245	0.623737	-2.768671
1	-3.601629	-0.909999	-2.909839
7	0.052367	-3.669760	-1.192618
1	-0.879923	-4.032753	-1.373379
1	0.559567	-4.437254	-0.759213
1	0.478167	-3.548714	-2.107457

**Cartesian coordinates of all the proposed isomers of
[Fe²⁺(NH₃)_{n=1-10}] obtained only at M06-2X-6-31++G(d,p) level
of theory at singlet spin state**

Cartesian coordinates of the tetramer : [Fe(NH₃)₄]²⁺

Cartesian coordinates of : 310-m

Atomic number (AN) and Cartesian coordinates			
AN	X	Y	Z

7	0.091470	-1.735072	0.000077
1	0.255096	-2.339508	-0.811135
1	-0.912767	-1.514502	0.000068
1	0.255098	-2.339436	0.811341
7	0.075445	0.865237	-1.500944
1	0.231450	1.870845	-1.621562
1	0.234697	0.464458	-2.430533
1	-0.926531	0.748131	-1.301317
7	0.075451	0.865369	1.500870
1	-0.926527	0.748247	1.301256
1	0.231457	1.870987	1.621399
1	0.234705	0.464671	2.430493
26	1.082273	0.004681	-0.000002
7	-2.721850	-0.005749	0.000002
1	-3.150671	-0.471449	0.802725
1	-3.150673	-0.471519	-0.802679
1	-3.158029	0.918860	-0.000038

Cartesian coordinates of the pentamer : [Fe(NH₃)₅]²⁺

Cartesian coordinates of : 410-m

Atomic number (AN) and Cartesian coordinates			
AN	X	Y	Z

7	0.855358	1.723951	0.000023
1	0.906825	2.349007	-0.808115
1	1.731708	1.188740	0.000016
1	0.906818	2.348975	0.808185
7	0.132971	-0.669122	-1.508740
1	-0.258790	-1.596052	-1.684190
1	0.136146	-0.209826	-2.423166
1	1.119635	-0.816487	-1.263597
7	0.132972	-0.669165	1.508718
1	1.119637	-0.816518	1.263573
1	-0.258783	-1.596102	1.684144

1	0.136144	-0.209894	2.423157
26	-0.717803	0.393528	0.000004
7	-2.558406	-0.566743	-0.000004
1	-3.143326	-0.335592	-0.808259
1	-3.143311	-0.335633	0.808275
1	-2.513963	-1.588025	-0.000030
7	3.075918	-0.697576	-0.000007
1	3.619380	-0.376986	0.803614
1	3.619376	-0.376968	-0.803623
1	3.213676	-1.709773	-0.000019

Cartesian coordinates of the hexamer : [Fe(NH₃)₆]²⁺

Cartesian coordinates of : 510-m

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.798116	-1.424646	0.910718
1	-0.869652	-1.508748	1.927015
1	-0.669568	-2.383176	0.584935
1	-1.732460	-1.145258	0.589715
7	-0.785465	1.433560	0.920320
1	-1.725550	1.144966	0.626261
1	-0.833281	1.539549	1.935969
1	-0.670967	2.385191	0.569968
7	-0.310930	0.027388	-1.622062
1	-0.088945	-0.758261	-2.234951
1	-0.123684	0.859104	-2.183855
1	-1.328194	0.003196	-1.493122
26	0.574525	0.000388	0.238946
7	1.994316	-1.494299	-0.176317
1	2.497334	-1.813028	0.655979
1	2.731236	-1.224344	-0.829892
1	1.601338	-2.348872	-0.574052
7	2.033245	1.461071	-0.164347
1	2.506139	1.344398	-1.062379
1	2.790815	1.477326	0.523326
1	1.690357	2.422634	-0.179002
7	-3.439674	-0.003219	-0.391649
1	-3.767388	0.806832	-0.919758
1	-4.025363	-0.006801	0.445043
1	-3.773436	-0.803779	-0.930432

Cartesian coordinates of the heptamer : [Fe(NH3)7]2+

Cartesian coordinates of : 610-m

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.829914	-0.923442	-1.398746
1	1.796509	-0.741754	-1.107948
1	0.763978	-0.567898	-2.353094
1	0.763400	-1.936736	-1.497045
7	-1.705320	0.725791	-1.571194
1	-1.340135	1.542010	-2.063469
1	-1.864319	0.034288	-2.305699
1	-2.641885	1.008501	-1.278471
7	-1.706982	0.998395	1.412541
1	-1.865965	1.979850	1.179249
1	-1.342279	1.018139	2.365697
1	-2.643492	0.603468	1.511026
7	0.830028	1.673639	-0.098732
1	0.763417	2.323522	0.685322
1	0.764890	2.264259	-0.928031
1	1.796492	1.330672	-0.085224
26	-0.465787	0.000025	0.000447
7	0.828579	-0.750233	1.501169
1	1.795339	-0.592065	1.197551
1	0.760639	-1.753865	1.673338
1	0.763528	-0.325944	2.426696
7	-1.705520	-1.723238	0.157494
1	-2.638729	-1.615488	-0.242759
1	-1.872496	-2.007178	1.124174
1	-1.334788	-2.560186	-0.294129
7	3.684408	-0.001103	-0.001876
1	4.105671	0.520560	0.767746
1	4.103030	0.405194	-0.839525
1	4.104632	-0.928997	0.064096

Cartesian coordinates of : 520-m

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.515409	-1.446748	-0.318884
1	-1.293699	-2.269139	0.242876
1	-1.799275	-1.825950	-1.224886
1	-2.374137	-1.050022	0.087731
7	1.454495	-1.436549	-0.834553
1	1.241408	-2.388176	-0.534770
1	1.724199	-1.530419	-1.815632
1	2.309502	-1.168358	-0.335258
7	1.454497	1.436549	-0.834546

1	1.241416	2.388173	-0.534751
1	1.724203	1.530430	-1.815623
1	2.309501	1.168346	-0.335253
7	0.482360	-0.000000	1.554280
1	0.156080	0.808842	2.083929
1	1.504171	-0.000008	1.638984
1	0.156066	-0.808834	2.083933
26	-0.014870	0.000000	-0.446750
7	-1.515410	1.446748	-0.318890
1	-2.374146	1.050013	0.087699
1	-1.799253	1.825968	-1.224892
1	-1.293712	2.269128	0.242892
7	3.789942	0.000000	0.997082
1	4.526563	0.000053	0.290065
1	4.008690	-0.805629	1.584589
1	4.008666	0.805567	1.584684
7	-4.145053	-0.000001	0.744920
1	-4.414429	0.804768	1.310668
1	-4.414454	-0.804785	1.310635
1	-4.798693	0.000025	-0.037975

Cartesian coordinates of the octamer : [Fe(NH3)8]2+

Cartesian coordinates of : 620-m1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.588764	-2.112933	0.058074
1	0.398294	-2.392586	0.023354
1	-1.039662	-2.601372	-0.715717
1	-0.963618	-2.550191	0.900041
7	-2.185103	-0.062925	-1.484365
1	-1.846618	-0.307577	-2.415437
1	-2.916020	-0.747883	-1.287565
1	-2.686725	0.816091	-1.615981
7	-0.588754	2.112941	-0.058057
1	-0.963648	2.550228	-0.899989
1	0.398306	2.392593	-0.023373
1	-1.039613	2.601354	0.715773
7	0.916064	-0.029038	-1.402524
1	1.517997	0.783524	-1.242844
1	0.709604	-0.030945	-2.400641
1	1.508677	-0.846852	-1.234080
26	-0.664383	0.000003	-0.000000
7	0.916033	0.029040	1.402560
1	1.517953	-0.783539	1.242901
1	0.709563	0.030968	2.400676
1	1.508676	0.846832	1.234117
7	-2.185150	0.062934	1.484318
1	-2.916038	0.747912	1.287476
1	-1.846710	0.307576	2.415409
1	-2.686801	-0.816069	1.615903

7	2.596309	-2.595774	0.003845
1	3.490919	-2.106289	-0.009538
1	2.643627	-3.234389	-0.790709
1	2.651156	-3.204292	0.821155
7	2.596342	2.595746	-0.003854
1	2.643595	3.234407	0.790666
1	2.651250	3.204218	-0.821195
1	3.490956	2.106269	0.009626

Cartesian coordinates of : 620-m2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.294624	0.837797	1.451346
1	1.221885	0.446121	2.390403
1	1.222285	1.847010	1.581013
1	2.262406	0.668566	1.158727
7	1.294622	0.838099	-1.451174
1	1.222283	1.847338	-1.580631
1	2.262405	0.668807	-1.158590
1	1.221883	0.446617	-2.390312
7	-1.294624	-0.837797	-1.451346
1	-1.221885	-0.446121	-2.390403
1	-2.262406	-0.668566	-1.158727
1	-1.222285	-1.847010	-1.581013
7	-1.293655	1.676466	0.000175
1	-2.261629	1.339080	0.000139
1	-1.220772	2.293662	-0.808694
1	-1.220772	2.293494	0.809171
26	0.000000	0.000000	0.000000
7	-1.294622	-0.838099	1.451174
1	-1.221883	-0.446617	2.390312
1	-1.222283	-1.847338	1.580631
1	-2.262405	-0.668807	1.158590
7	1.293655	-1.676466	-0.000175
1	1.220772	-2.293494	-0.809171
1	1.220772	-2.293662	0.808694
1	2.261629	-1.339080	-0.000139
7	4.156762	-0.000132	0.000000
1	4.574792	-0.466005	0.806038
1	4.576103	0.930260	0.000096
1	4.574792	-0.465840	-0.806134
7	-4.156762	0.000132	-0.000000
1	-4.576103	-0.930260	-0.000096
1	-4.574792	0.466005	-0.806038
1	-4.574792	0.465840	0.806134

Cartesian coordinates of : 530-m

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.045011	1.239393	-1.452519
1	0.769241	2.083041	-0.936728
1	0.869873	1.440291	-2.438256
1	2.060062	1.177828	-1.369666
7	-1.698272	0.850227	-0.595485
1	-1.452837	1.763780	-0.204602
1	-2.136894	1.042270	-1.497204
1	-2.440631	0.453883	-0.007332
7	-1.195561	-1.964381	-0.009016
1	-0.772238	-2.560511	0.702571
1	-1.468424	-2.604394	-0.757486
1	-2.080480	-1.623787	0.392333
7	0.560720	0.241175	1.242516
1	1.542956	0.000624	1.422682
1	0.023277	-0.139569	2.020960
1	0.482902	1.259050	1.315706
26	-0.011032	-0.364684	-0.634054
7	-3.951543	-0.792649	1.043853
1	-4.059851	-1.546194	1.722445
1	-4.651622	-0.983522	0.327509
1	-4.290765	0.036182	1.530969
7	-0.058312	3.541160	0.552606
1	0.848975	3.926862	0.815372
1	-0.643901	3.687742	1.374983
1	-0.421320	4.199017	-0.138071
7	1.655250	-1.604742	-0.852831
1	2.355853	-1.344640	-0.145114
1	2.127947	-1.540064	-1.755374
1	1.485304	-2.601832	-0.720925
7	3.656853	-0.711231	1.470482
1	4.469524	-0.881795	0.878188
1	3.663871	-1.473654	2.147564
1	3.907003	0.118517	2.007654

Cartesian coordinates of the nanomer : [Fe(NH3)9]2+

Cartesian coordinates of : 630-m

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.274093	-1.833438	0.872021
1	2.239247	-1.525006	0.717780
1	1.219972	-2.773787	0.481047
1	1.182637	-1.959386	1.879731

7	-1.281574	-1.821879	-0.883332
1	-1.192291	-1.938957	-1.892305
1	-1.230297	-2.765939	-0.501010
1	-2.245368	-1.511277	-0.724621
7	-1.208826	1.103503	-0.868231
1	-1.203931	1.132507	-1.887487
1	-0.929639	2.043666	-0.563477
1	-2.189653	0.979851	-0.608327
7	1.342262	-0.378418	-1.636000
1	1.299230	0.454961	-2.222202
1	1.270352	-1.163391	-2.282898
1	2.299039	-0.409154	-1.267383
26	-0.000868	-0.386382	-0.000628
7	1.214995	1.092857	0.876820
1	2.195715	0.962232	0.619572
1	1.206933	1.120042	1.896066
1	0.943379	2.034440	0.571923
7	-1.344351	-0.384826	1.634377
1	-2.300742	-0.412568	1.264242
1	-1.301577	0.445579	2.224755
1	-1.274231	-1.173056	2.277489
7	4.161696	-0.447684	0.003322
1	4.607271	0.321854	-0.496558
1	4.588129	-1.286863	-0.390239
1	4.536785	-0.389095	0.950039
7	0.004457	3.972702	-0.001554
1	-0.075037	4.362629	0.936642
1	-0.741726	4.421061	-0.532240
1	0.862987	4.367303	-0.383598
7	-4.163707	-0.440722	0.002022
1	-4.594191	-1.280103	0.390675
1	-4.538783	-0.374420	-0.944170
1	-4.604948	0.328133	0.506764

Cartesian coordinates of : 631-m

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.911490	-1.202520	0.548784
1	1.872312	-0.862168	0.660196
1	0.946023	-1.937571	-0.156352
1	0.675032	-1.681018	1.417162
7	-1.349935	-0.733750	-1.390025
1	-0.959519	-0.815499	-2.327308
1	-1.450218	-1.686896	-1.025223
1	-2.304371	-0.386097	-1.509854
7	-1.622159	2.035461	-0.408814
1	-1.395916	2.530065	-1.271249
1	-1.696038	2.759886	0.304912
1	-2.574175	1.674025	-0.537419
7	1.184530	1.090698	-1.216177
1	1.153001	2.079316	-1.463779
1	1.268961	0.598252	-2.104652

1	2.079523	0.954198	-0.733332
26	-0.353019	0.417316	0.070330
7	0.636313	1.497043	1.592669
1	1.637455	1.280855	1.521063
1	0.366764	1.270848	2.549374
1	0.567683	2.512575	1.532560
7	-1.872877	-0.342575	1.319829
1	-1.879446	-1.363131	1.223324
1	-2.786182	-0.030755	0.980846
1	-1.857966	-0.140383	2.318140
7	3.635665	0.557533	0.853102
1	4.025945	1.500465	0.846467
1	4.213620	0.034361	0.172306
1	3.907313	0.183657	1.762867
7	5.566375	-0.881148	-1.048182
1	6.184266	-1.405537	-0.432280
1	6.148056	-0.160858	-1.470901
1	5.322491	-1.518244	-1.802301
7	-4.452083	0.565852	-0.735982
1	-4.864474	-0.364756	-0.681128
1	-4.706663	0.907633	-1.662712
1	-5.005591	1.132583	-0.093371
7	-1.786544	-3.482310	0.342741
1	-1.319172	-4.098450	-0.321581
1	-2.780102	-3.670806	0.213593
1	-1.565527	-3.876763	1.256453
