Electronic Suplementary Information for the article "*Relation between structural patterns and magnetism in small iron oxide clusters; reentrance of magnetic moment at high oxidation rates.*"

R. H. Aguilera-del-Toro,[1] F. Aguilera-Granja,[2] M. B. Torres,[3,*] and A. Vega[1]

[1]*Departamento de Física Teórica, Atómica y Óptica, Universidad de Valladolid, E-47011 Valladolid, Spain*

[2]*Instituto de Física, Universidad Autónoma de San Luis Potosí, México*

[3]*Departamento de Matemáticas y Computación, Universidad de Burgos, Spain*

PACS numbers: 75.75+a; 36.40Cg; 75.30.Pd; 75.50.-y

In Tables I to V, are garenthed the total energy differences with respect to the global minimum energy and spin multiplicities for each $Fe_nO_m^{0/\pm}$ $(n = 2-6)$ oxide. Adiabatic ionization potentials and electron affinities are shown in the last two columns.

Table VI shows some calculated fragmentation energies predicted in this work, that are not found among the first two for any (n, m) values.

Optimized cartesian coordinates of Fe_nO_m, $Fe_nO_m^+$ and $Fe_nO_m^-$ $(n = 2-6)$ oxides studied in this work. The total binding energy of each isomer is included before its corresponding cartesian geometrical structure.

TABLE I. Total energy differences (in eV) with respect to the global minimum energy and spin multiplicities of $Fe_2O_m^{0/\pm}$ clusters, shown in Figure 1. Adiabatic ionization potentials (in eV) and electron affinities (in eV) are shown in the last two columns.

	Cationic		Neutral		Anionic		IP(eV)	AE (eV)
	ΔE (eV)	M	ΔE (eV)	M	ΔE (eV)	M		AE
2.1-I	**0.00**	8	**0.00**	1	**0.00**	8	7.29	1.20
2.1-II	0.00	2	0.06	1	0.33	2		
2.1-III	—	—	0.63	9	0.27	8		
2.2-I	**0.00**	10	**0.00**	1	**0.00**	2	8.00	1.41
2.2-II	0.48	2	0.88	1	0.24	8		
2.2-III	2.56	2	3.16	9	0.04	2		
2.3-I	**0.00**	2	**0.00**	1	**0.00**	8	8.80	2.50
2.3-II	0.40	2	0.90	7	0.75	8		
2.3-III	1.15	10	1.15	7	2.20	8		
2.4-I	**0.00**	2	**0.00**	1	**0.00**	2	10.10	3.36
2.4-II	2.34	4	1.08	7	1.50	6		
2.4-III	0.54	2	1.86	1	2.34	8		
2.5-I	**0.00**	4	**0.00**	3	**0.00**	6	10.45	3.99
2.5-II	0.28	2	0.28	1	0.07	6		
2.6-I	0.48	2	**0.00**	1	1.04	4	10.92	4.60
2.6-II	**0.00**	2	0.08	3	**0.00**	2		

TABLE II. Total energy differences (in eV) with respect to the global minimum energy and spin multiplicities of $Fe_3O_m^{0/\pm}$ clusters, shown in Figure 2. Adiabatic ionization potentials (in eV) and electron affinities (in eV) are shown in the last two columns.

	Cationic		Neutral		Anionic		IP (eV)	AE (eV)
	ΔE (eV)	M	ΔE (eV)	M	ΔE (eV)	M		
3.1-I	**0.00**	12	**0.00**	11	**0.00**	12	6.94	1.19
3.1-II	0.32	10	0.72	11	0.68	12		
3.1-III	0.60	12	1.36	11	1.24	12		
3.2-I	**0.00**	4	**0.00**	13	0.05	12	7.29	1.81
3.2-II	0.70	12	0.95	11	**0.00**	12		
3.2-III	0.45	12	1.05	13	1.70	12		
3.3-I	**0.00**	4	**0.00**	5	**0.00**	12	7.72	2.21
3.3-II	2.46	12	2.16	13	2.04	12		
3.3-III	2.04	6	2.82	7	2.52	6		
3.4-I	**0.00**	6	**0.00**	5	0.35	6	8.05	2.79
3.4-II	0.14	4	0.00	11	**0.00**	10		
3.4-III	0.14	4	0.14	3	0.14	12		
3.5-I	**0.00**	4	**0.00**	5	**0.00**	4	8.83	3.43
3.5-II	0.72	6	0.88	5	1.28	6		
3.5-III	2.16	6	1.44	5	0.96	6		
3.6-I	**0.00**	6	**0.00**	3	**0.00**	2	9.63	4.09
3.6-II	0.00	6	0.54	5	0.90	4		
3.6-III	0.72	6	2.43	5	3.60	4		
3.7-I	**0.00**	4	**0.00**	5	**0.00**	4	9.53	4.27
3.7-II	0.80	6	1.10	5	1.30	6		
3.7-III	1.50	2	1.40	1	1.50	2		
3.8-I	0.44	6	**0.00**	7	**0.00**	4	9.78	4.67
3.8-II	**0.00**	4	0.44	3	1.21	4		
3.8-III	1.21	2	1.98	1	3.08	4		
3.9-I	0.48	4	**0.00**	3	**0.00**	4	9.50	4.87
3.9-II	**0.00**	6	0.24	5	0.96	4		
3.9-III	1.56	8	2.28	5	3.12	4		

TABLE III. Total energy differences (in eV) with respect to the global minimum energy and spin multiplicities of $Fe_4O_m^{0/\pm}$ clusters, shown in Figure 3. Adiabatic ionization potentials (in eV) and electron affinities (in eV) are shown in the last two columns.

	Cationic		Neutral		Anionic		IP (eV)	AE (eV)
	ΔE (eV)	M	ΔE (eV)	M	ΔE (eV)	M		
4.1-I	0.05	14	**0.00**	15	—	—	6.83	0.94
4.1-II	**0.00**	14	0.75	13	**0.00**	16		
4.1-III	1.00	16	1.25	15	0.65	16		
4.2-I	**0.00**	16	**0.00**	15	0.12	16	7.01	1.59
4.2-II	0.18	16	0.24	15	0.12	16		
4.2-III	0.42	16	0.36	15	**0.00**	14		
4.3-I	**0.00**	16	**0.00**	15	—	—	7.23	2.01
4.3-II	0.00	16	0.14	15	**0.00**	16		
4.3-III	1.40	16	0.70	17	0.70	16		
4.4-I	**0.00**	2	**0.00**	1	**0.00**	2	7.36	2.40
4.4-II	0.72	2	0.40	17	0.40	16		
4.4-III	0.80	8	0.64	3	2.08	16		
4.5-I	**0.00**	2	**0.00**	1	**0.00**	2	7.39	2.73
4.5-II	0.63	2	0.09	1	0.27	2		
4.5-III	0.72	2	0.09	1	0.09	2		
4.6-I	**0.00**	2	**0.00**	3	**0.00**	2	8.02	3.30
4.6-II	1.60	2	1.40	1	1.50	2		
4.6-III	1.90	2	1.60	1	2.00	2		
4.7-I	**0.00**	2	**0.00**	1	**0.00**	2	8.43	3.44
4.7-II	1.43	2	0.99	1	0.88	2		
4.7-III	1.43	2	1.21	15	0.88	2		
4.8-I	**0.00**	12	**0.00**	5	**0.00**	12	9.19	3.82
4.8-II	0.60	14	0.72	13	0.72	2		
4.8-III	1.20	2	1.32	1	1.20	2		
4.9-I	**0.00**	9	**0.00**	9	**0.00**	10	9.12	4.46
4.9-II	1.82	11	1.43	13	1.43	14		
4.9-III	2.21	15	2.34	15	15.86	14		
4.10-I	**0.00**	7	**0.00**	9	**0.00**	10	9.67	4.90
4.10-II	0.70	1	1.40	11	1.68	10		
4.10-III	1.12	1	1.54	1	2.24	2		
4.11-I	**0.00**	9	**0.00**	13	**0.00**	10	9.53	4.78
4.12-I	**0.00**	5	**0.00**	7	**0.00**	6	9.38	5.00
4.13-I	**0.00**	1	**0.00**	3	**0.00**	2	9.39	5.23
4.14-I	**0.00**	3	**0.00**	1	**0.00**	2	9.48	4.54

TABLE IV. Total energy differences (in eV) with respect to the global minimum energy and spin multiplicities of $Fe_5O_m^{0/\pm}$ clusters, shown in Figure 4. Adiabatic ionization potentials (in eV) and electron affinities (in eV) are shown in the last two columns.

	Cationic		Neutral		Anionic		IP (eV)	AE (eV)
	ΔE (eV)	M	ΔE (eV)	M	ΔE (eV)	M		
5.1-I	0.12	16	**0.00**	17	**0.00**	18	6.57	1.78
5.1-II	**0.00**	18	0.18	17	0.36	18		
5.1-III	—	—	0.36	17	0.54	18		
5.2-I	0.21	18	**0.00**	17	**0.00**	18	6.89	1.96
5.2-II	0.07	18	0.07	17	0.28	18		
5.2-III	**0.00**	18	0.14	19	0.35	18		
5.3-I	**0.00**	20	**0.00**	17	**0.00**	18	7.03	1.88
5.3-II	0.16	20	0.32	19	2.96	18		
5.3-III	0.40	20	0.40	19	0.08	18		
5.4-I	**0.00**	20	**0.00**	19	**0.00**	18	6.25	2.44
5.4-II	3.15	16	1.62	17	1.26	18		
5.4-III	2.34	20	1.62	21	1.89	20		
5.5-I	**0.00**	4	**0.00**	5	0.10	4	6.87	2.88
5.5-II	0.80	6	0.00	5	**0.00**	4		
5.5-III	0.80	6	0.20	5	0.80	20		
5.6-I	0.44	4	**0.00**	3	**0.00**	16	8.77	2.33
5.6-II	**0.00**	4	0.99	5	0.33	6		
5.6-III	0.00	4	1.21	5	0.66	6		
5.7-I	**0.00**	6	**0.00**	5	**0.00**	4	8.05	3.25
5.7-II	0.12	2	0.24	3	0.24	4		
5.7-III	1.08	6	1.20	5	0.96	4		
5.8-I	**0.00**	4	**0.00**	3	**0.00**	4	8.16	3.64
5.8-II	0.91	4	1.56	5	1.56	6		
5.8-III	1.56	6	1.69	5	1.82	6		
5.9-I	**0.00**	4	**0.00**	3	**0.00**	4	8.75	3.73
5.9-II	0.56	4	0.00	3	0.00	4		
5.10-I	**0.00**	4	**0.00**	15	**0.00**	14	8.91	4.54
5.10-II	0.15	4	0.30	3	0.75	4		
5.10-III	0.90	4	1.20	3	1.80	2		
5.11-I	0.16	16	**0.00**	17	**0.00**	14	9.47	4.30
5.11-II	**0.00**	2	0.64	15	0.32	4		
5.11-III	0.16	2	0.80	3	0.80	14		
5.12-I	**0.00**	12	**0.00**	13	**0.00**	12	9.18	5.03
5.12-II	1.19	14	0.17	15	1.19	4		
5.12-III	0.51	14	0.85	13	0.51	14		
5.13-I	**0.00**	6	**0.00**	11	**0.00**	12	9.37	5.23
5.13-II	0.72	12	0.54	11	0.54	14		
5.13-III	1.44	12	1.26	3	1.44			
5.14-I	**0.00**	12	**0.00**	13	0.19	14	9.42	5.26
5.14-II	0.76	10	0.38	3	**0.00**	14		
5.14-III	0.76	2	0.76	1	0.57	14		
5.15-I	0.60	12	**0.00**	11	**0.00**	14	9.22	5.31
5.15-II	0.80	10	0.20	11	0.00	2		
5.15-III	**0.00**	2	0.40	13	0.20	2		
5.16-I	**0.00**	4	**0.00**	3	**0.00**	4	9.39	5.29
5.16-II	0.63	4	0.21	3	0.21	2		

TABLE V. Total energy differences (in eV) with respect to the global minimum energy and spin multiplicities of $Fe_6O_m^{0/\pm}$ clusters, shown in Figure 5. Adiabatic ionization potentials (in eV) and electron affinities (in eV) are shown in the last two columns.

	Cationic		Neutral		Anionic		IP (eV)	AE (eV)
	ΔE (eV)	M	ΔE (eV)	M	ΔE (eV)	M		
6.1-I	**0.00**	21	**0.00**	20	**0.00**	21	6.33	1.54
6.1-II	0.42	21	0.28	20	0.07	21		
6.1-III	—	—	0.35	20	0.35	19		
6.2-I	**0.00**	21	**0.00**	20	**0.00**	19	6.41	1.41
6.2-II	—	—	0.40	20	0.08	19		
6.2-III	0.16	19	0.40	20	0.16	21		
6.3-I	**0.00**	21	0.09	20	**0.00**	19	6.44	1.57
6.3-II	1.62	21	**0.00**	20	0.09	19		
6.3-III	0.90	21	0.99	20	0.72	21		
6.4-I	**0.00**	21	**0.00**	20	0.30	21	6.65	2.15
6.4-II	0.00	21	0.00	20	**0.00**	19		
6.4-III	1.50	21	1.10	0	0.60	21		
6.5-I	0.77	23	**0.00**	22	**0.00**	21	6.82	2.70
6.5-II	**0.00**	1	0.33	2	0.99	21		
6.5-III	0.44	23	0.44	22	1.10	21		
6.6-I	**0.00**	1	**0.00**	0	**0.00**	1	6.92	3.08
6.6-II	0.84	1	0.00	0	0.24	1		
6.6-III	0.24	1	0.12	0	0.60	1		
6.7-I	0.52	1	**0.00**	0	**0.00**	1	6.99	2.68
6.7-II	0.52	1	0.39	0	0.65	1		
6.7-III	**0.00**	1	0.39	0	0.13	1		
6.8-I	**0.00**	1	**0.00**	0	**0.00**	1	7.55	3.10
6.8-II	0.14	3	0.28	20	0.56	15		
6.8-III	5.60	1	0.70	0	0.98	1		
6.9-I	**0.00**	1	**0.00**	0	**0.00**	1	7.39	3.87
6.9-II	1.65	1	1.35	2	1.95	3		
6.9-III	2.40	7	1.80	16	2.10	1		
6.10-I	**0.00**	1	**0.00**	0	**0.00**	1	7.95	3.68
6.10-II	1.28	1	0.80	2	0.64	1		
6.10-III	1.12	1	0.96	0	0.96	1		
6.11-I	**0.00**	1	**0.00**	0	**0.00**	1	8.11	3.92
6.11-II	0.00	1	0.00	0	0.34	1		
6.11-III	1.70	19	0.85	18	1.02	3		
6.12-I	**0.00**	1	**0.00**	0	**0.00**	1	8.17	4.37
6.12-II	2.16	1	1.80	0	1.62	1		
6.12-III	2.88	25	1.98	24	1.26	23		
6.13-I	**0.00**	1	**0.00**	0	**0.00**	1	8.73	4.48
6.13-II	4.56	3	0.19	2	4.56	1		
6.13-III	4.56	1	0.19	0	4.94	1		
6.14-I	**0.00**	1	**0.00**	2	**0.00**	1	8.79	5.01
6.14-II	6.60	1	1.80	0	7.00	1		
6.14-III	8.80	21	3.80	0	8.20	21		
6.15-I	**0.00**	1	**0.00**	8	**0.00**	9	9.03	5.02
6.15-II	5.46	1	0.84	0	5.67	1		
6.15-III	5.25	3	0.84	2	5.46	1		
6.16-I	**0.00**	7	**0.00**	0	**0.00**	1	9.16	5.08
6.16-II	4.40	9	0.22	0	4.62	1		

TABLE VI. Some calculated fragmentation energies (in eV) predicted in this work, that are not found among the first two for any (n, m) values.

	Fe_2	Fe_2O	Fe_2O_2	FeO_2^+	Fe_2O^+
Fe_3O^+	5.51	4.68	—	—	3.77
$Fe_3O_2{}^+$	8.93	5.86	4.59	8.93	3.99
$Fe_3O_3{}^+$	11.39	9.47	5.95	9.47	5.56
$Fe_3O_4{}^+$	12.93	9.93	7.57	7.57	5.30
$Fe_3O_5{}^+$	—	10.17	6.73	5.47	4.54
$Fe_3O_6{}^+$	—	—	8.86	5.14	—
Fe_4O^+	4.47	4.19	—	—	4.47
$Fe_4O_2{}^+$	5.20	4.76	4.04	—	4.76
$Fe_4O_3{}^+$	7.20	5.70	4.81	9.59	4.81
$Fe_4O_4{}^+$	9.67	7.88	5.94	9.57	6.33
$Fe_4O_5{}^+$	11.13	9.17	6.94	8.10	6.37
$Fe_4O_6{}^+$	12.42	10.35	7.95	8.45	7.18
Fe_5O^+	4.13	4.29	—	—	—-
$Fe_5O_2{}^+$	4.42	4.77	4.49	—	5.12
$Fe_5O_3{}^+$	4.57	5.11	5.02	9.85	5.11
$Fe_5O_4{}^+$	7.87	6.42	6.51	11.23	5.98
$Fe_5O_5{}^+$	9.58	6.82	4.93	9.47	6.07
$Fe_5O_6{}^+$	9.48	8.62	5.41	7.69	7.26
$Fe_5O_7{}^+$	10.64	9.12	7.81	7.79	7.31
$Fe_5O_8{}^+$	12.36	9.32	7.36	6.61	8.22
Fe_6O^+	4.34	4.93	—	—	—-
$Fe_6O_2{}^+$	4.94	5.22	5.38	—	5.69
$Fe_6O_3{}^+$	5.59	6.08	5.93	11.56	6.36
$Fe_6O_4{}^+$	5.90	6.58	6.64	11.66	6.64
$Fe_6O_5{}^+$	6.47	5.96	6.20	10.69	5.89
$Fe_6O_6{}^+$	6.93	6.16	5.22	9.31	6.05
$Fe_6O_7{}^+$	8.63	5.20	5.52	9.64	5.46
$Fe_6O_8{}^+$	10.13	7.04	4.71	7.96	5.90

NEUTRAL OXIDES

Fe_2O

I - 8.49

Fe 1.199610 -0.054538 0.000000

Fe -1.198756 -0.053094 0.000000

O 0.051233 1.316439 0.000000

II - 8.43

Fe 1.789778 0.000003 0.000014

Fe -1.792905 0.000003 0.000013

O 0.002818 -0.000005 -0.000024

III - 7.86

Fe 1.204182 -0.363609 0.000003

Fe -1.100826 0.156852 0.000001

O 2.242135 0.989055 0.000007

Fe_2O_2

I- 14.28

Fe 1.119429 0.000002 0.000001

Fe -1.223430 0.000001 0.000002

O -0.052005 1.447329 0.000001

O -0.052003 -1.447327 0.000004

II- 13.40

Fe 0.969203 0.000000 0.000000

Fe -2.637756 0.000000 0.000000

O -0.880524 0.000000 0.000000

O 2.656843 0.000000 0.000000

III-11.12

Fe 1.131963 -0.368666 -0.052123

Fe -1.131871 -0.368676 0.052141

O 0.767855 1.520234 -0.052787

O -0.767786 1.520229 0.052799

Fe_2O_3

I-19.00

Fe 0.266962 0.221868 1.103330

Fe 0.468181 0.407912 -1.301419

O 1.329948 -0.694020 -0.066080

O -0.597672 1.321368 -0.073164

O 0.148471 0.092854 2.770781

II-18.10

Fe 0.995427 0.052252 -0.019501

Fe -1.252458 0.052319 -0.049285

O 0.038823 0.052189 1.486963

O 0.049281 -1.260469 -0.785844

O 0.049091 1.365295 -0.785622

III-17.85

Fe 1.821770 -0.368482 -0.088352

Fe -0.777474 -0.469468 -0.155099

O 0.467487 0.832211 -0.256355

O 2.352652 -1.201145 -1.416311

O 2.323202 -0.879196 1.403902

Fe_2O_4

I-23.82

Fe 0.692954 0.798219 1.210649

Fe 0.764771 0.868158 -1.314551

O 1.709171 -0.045755 -0.048446

O -0.251155 1.712358 -0.055432

O 0.662211 0.769951 2.874202

O 0.795319 0.896742 -2.978141

II-22.74

Fe -0.441641 0.826452 0.833394

Fe 1.409439 -0.819883 -0.786173

O 2.560199 0.034097 -1.608164

O -0.705223 2.447550 0.678628

O -0.266567 -0.242037 -0.586645

O -0.147459 0.257298 2.357974

III-21.96

Fe 1.062398 0.155170 0.067795

Fe -1.402271 0.365505 -0.009162

O -0.055419 1.610228 0.250174

O -0.274610 -1.092612 -0.182954

O 2.865898 0.663583 -0.170216

O 2.697638 -0.692635 0.475605

Fe_2O_5

I-27.58

Fe 0.390555 0.463119 1.386954

Fe -0.044619 -0.479928 -0.862302

O 1.380934 -0.584288 0.285207

O -1.023686 0.586160 0.259411

O -0.765744 -1.935443 -1.091935

O 0.681850 1.098487 2.882716

O 0.358775 0.290694 -2.252736

II-27.30

Fe 0.051694 0.526398 1.200370

Fe 0.382515 -0.251890 -1.407537

O 0.387342 1.300163 -0.485757

O -1.325417 1.187879 1.814293

O -0.050912 -0.995381 0.280242

O 1.393991 0.785096 2.123505

O 0.764535 -0.256517 -3.036070

Fe_2O_6

I-31.36

Fe 0.277157 0.567347 1.078116

Fe -0.033125 -0.332224 -1.387883

O 0.045287 1.302086 -0.576917

O -0.971246 0.783337 2.120939

O 0.249580 -1.065332 0.259924

O -1.501013 -0.691403 -2.026980

O 1.722523 0.985540 1.735423

O 1.190774 -0.569547 -2.456239

II-31.28

Fe 0.976446 0.154796 -0.422873

Fe -1.589229 0.336787 0.019293

O -0.423738 1.014284 -1.197812

O -0.191432 -0.537024 0.786198

O 2.045000 1.186981 0.257252

O 1.620296 -0.988890 -1.396529

O -2.232874 1.485798 0.987649

O -2.669578 -0.682590 -0.663805

Fe_3O

I-12.08

Fe 1.465511 0.366181 0.157375

Fe -0.401860 0.889440 -0.988633

Fe 0.473203 2.238252 0.930159

O -0.994875 2.433583 -0.167498

II-11.36

Fe 1.200082 0.055166 -0.052929

Fe -1.131597 -0.049586 -0.154952

Fe -0.050423 2.022347 -0.258139

O -0.057831 0.783252 1.299047

III-10.72

Fe 1.060912 -0.026205 0.000000

Fe -1.060916 -0.026197 0.000000

Fe -0.000001 3.463326 0.000000

O 0.000005 1.609585 0.000000

Fe_3O_2

I-18.15

Fe 1.341302 0.141158 0.062320

Fe -1.203349 0.160014 -0.155697

Fe -0.136890 2.217008 -0.154005

O 0.058249 -1.193454 0.039712

O 1.697844 1.954764 0.043836

II-17.20

Fe 1.087286 -0.128655 0.147856

Fe -1.345151 -0.048799 0.048236

Fe -0.052246 1.923323 -0.151989

O -0.151673 1.001680 1.417497

O -0.145174 -1.352775 -0.568745

III-17.10

Fe 1.154355 0.050206 -0.047043

Fe -1.259383 0.050177 -0.046905

Fe -0.052253 2.135023 -0.102690

O -0.052549 0.782013 1.403439

O -0.052577 0.695633 -1.531120

Fe_3O_3

I-24.48

Fe 1.262518 0.053723 0.053810

Fe -1.201360 -0.011539 0.053837

Fe -0.035018 2.417295 0.171976

O 0.065140 -1.350929 -0.053084

O 1.692085 1.828035 0.146720

O -1.726228 1.736155 0.146470

II-22.32

Fe 1.134662 0.055461 0.042751

Fe -1.238949 0.055526 0.042712

Fe -0.052091 2.342833 -0.149479

O -0.052104 0.998040 1.324996

O -0.051956 -1.228173 -0.666698

O -0.052117 3.174309 -1.622855

III-21.66

Fe 1.478804 0.366953 0.366724

Fe 3.589134 -0.571871 -0.364127

Fe -2.027113 -0.051009 -0.054492

O -0.137146 -0.149917 -0.145217

O 3.288174 0.770130 0.775905

O -3.723738 -0.062861 -0.161175

Fe_3O_4

I-28.70

Fe 1.308471 0.603863 0.260862

Fe -1.341401 0.644436 0.630783

Fe -0.437399 1.618081 -1.505164

O 0.060083 -0.475185 1.098782

O 1.208819 0.776873 -1.579635

O -2.168227 1.105170 -0.992259

O 0.046152 2.142483 0.438935

II-28.70

Fe 1.301134 -0.152459 0.053010

Fe -1.218712 -0.191309 0.036004

Fe -0.012492 2.547870 0.166035

O 0.062639 -1.509528 -0.057142

O 1.525139 1.647070 0.263597

O -1.525266 1.603047 0.172727

O -0.040217 4.160521 -0.067863

III-28.56

Fe 1.275311 -0.793351 -1.096702

Fe -0.954107 -0.677664 -0.361411

Fe 0.154848 1.356824 0.766133

O 0.675799 2.461411 2.243288

O 0.377125 0.887994 -0.973624

O -0.732151 1.916214 2.354974

O -0.052096 -2.103525 -1.200495

Fe_3O_5

I-32.80

Fe 1.301323 0.258551 -0.678240

Fe -0.849338 -1.013881 0.546770

Fe -0.705947 2.031413 -0.149734

O -1.639021 0.581997 0.261662

O 0.588499 1.822264 -1.361759

O -0.676201 3.401864 0.774448

O -1.824797 -2.166008 1.205561

O 0.881379 -1.288569 0.153314

II-31.92

Fe 1.189118 0.271492 0.053604

Fe -1.301076 0.367204 0.502620

Fe -0.370410 1.617888 -1.519289

O 0.052682 -0.481706 1.414604

O 1.448025 1.306235 -1.495488

O -2.110061 1.385108 -0.779974

O -0.035896 1.884306 0.461929

O -0.388227 -0.364135 -1.099519

III-31.36

Fe 1.417439 0.678538 -0.157964

Fe -0.992069 -0.431578 -0.052399

Fe -0.675946 2.175582 -0.047581

O -0.060549 0.811478 1.120412

O -0.166349 0.834734 -1.309564

O -1.210351 3.721618 0.141478

O 3.024776 0.238470 -0.160139

O -1.689749 -1.932747 0.140983

Fe_3O_6

I-37.26

Fe 1.566328 0.157426 -0.560325

Fe -0.994290 -1.052556 0.467010

Fe -0.680169 2.143576 -0.064588

O -1.442474 0.687245 0.679455

O 0.804832 1.706858 -0.988190

O -0.879345 3.699914 0.480686

O 3.191933 -0.038063 -0.377567

O -1.598768 -2.355125 1.307753

O 0.466905 -1.234307 -0.580665

II-36.72

Fe 1.206832 0.088390 1.194259

Fe -0.702245 -0.159190 -1.307603

Fe 0.024907 2.345218 0.374934

O 1.587914 1.830280 1.190467

O 0.890649 -0.597247 -0.354509

O -0.681768 1.630094 -1.103053

O -1.943393 -0.873107 -0.490331

O 0.784617 -0.686802 2.567140

O -0.465229 -0.677107 -2.850108

III-34.83

Fe 1.263871 0.258106 0.048981

Fe -1.320258 0.349541 0.476486

Fe -0.361885 1.585769 -1.593770

O 0.049898 -0.456840 1.344911

O 1.516064 1.292211 -1.506064

O -2.115726 1.312386 -0.799008

O -0.046838 1.824294 0.367085

O -0.348659 -0.324596 -1.104853

O -0.505111 2.465783 -2.978570

Fe_3O_7

I-41.10

Fe 1.459487 -0.894885 0.252785

Fe -1.322747 -0.861976 -0.068906

Fe 0.047277 1.558288 0.160884

O 1.613081 0.805942 -0.366597

O -1.394722 0.786349 -0.721326

O 0.080888 -1.744983 -0.682173

O -0.158975 3.184042 0.052630

O 2.734699 -1.927035 0.168249

O -2.646081 -1.624934 0.488789

O -0.129942 -0.150613 1.202509

II-40.00

Fe 1.654928 0.148872 -0.904934

Fe -0.950049 -0.986676 0.466776

Fe -0.891426 1.923790 -0.149879

O -1.897236 0.467659 0.041446

O 0.571444 1.615813 -1.099247

O -1.197470 3.367898 0.578563

O 3.380480 -0.624901 -0.659857

O -1.426756 -2.137265 1.533990

O 0.463505 -1.174610 -0.564774

O 3.393346 0.604749 -1.511318

III-39.70

Fe 1.198771 0.363304 0.153454

Fe -1.502644 0.302248 0.576626

Fe -0.449393 1.594722 -1.558899

O -0.059128 -0.369657 1.433745

O 1.481244 1.308568 -1.346651

O -2.118207 1.311079 -0.907430

O -0.096228 1.815989 0.359508

O -0.262554 -0.266259 -0.989782

O -0.475113 2.456053 -2.951271

O 2.617680 -0.151832 0.780937

Fe_3O_8

I-43.67

Fe 1.320281 0.231939 -0.021609

Fe -1.319752 0.175916 0.519141

Fe -0.365380 1.513095 -1.623696

O 0.166889 -0.289586 1.416642

O 1.397170 0.896445 -1.727683

O -2.004466 1.298217 -0.754062

O 0.189218 1.742244 0.147794

O -0.362988 -0.461972 -0.939437

O -0.516746 2.757671 -2.662312

O 2.824726 0.051995 0.579865

O -2.564483 -0.694584 1.093170

II-43.23

Fe 1.772910 -1.262156 0.132503

Fe -1.618619 -1.306892 0.119342

Fe 0.050680 1.447690 0.269579

O 1.469873 0.471053 0.596290

O -1.386051 0.459644 0.468468

O 0.084678 -1.830383 0.169549

O 0.057528 2.984039 -0.279486

O 3.053192 -2.636960 0.062238

O 3.556485 -1.329821 -0.485193

O -2.851038 -2.733557 0.042265

O -3.380082 -1.468700 -0.575844

III-41.69

Fe 1.309242 -0.185729 0.046812

Fe -1.358966 -0.161469 -0.040731

Fe 0.044818 2.165395 0.015985

O 0.634264 -1.833027 0.054041

O -0.851321 -2.022013 0.039475

O 2.454665 1.177612 0.063757

O 1.927159 2.578797 0.050645

O -2.580558 1.295682 -0.052972

O -1.811812 2.575006 -0.052776

O 0.051279 0.562999 1.213706

O 0.121250 0.550581 -1.198641

Fe_3O_9

I-46.32

Fe 1.291136 0.149849 0.202746

Fe -1.375417 0.257112 0.685483

Fe -0.371370 1.470826 -1.405986

O 0.142997 -0.577447 1.408305

O 1.431098 0.895211 -1.461771

O -2.013415 1.508460 -0.497819

O 0.177219 1.646984 0.456545

O -0.512864 -0.369322 -0.890407

O -0.692482 1.737802 -3.276945

O 2.798318 0.057527 0.787615

O -2.654385 -0.369759 1.494300

O -0.458682 2.986658 -2.554260

II-46.08

Fe 1.631469 -1.411468 0.056404

Fe -1.709834 -1.405395 -0.011351

Fe -0.057646 1.503120 0.010349

O 1.358545 0.377311 0.047727

O -1.404134 0.345088 -0.156014

O -0.042903 -2.015403 0.157903

O 0.590970 3.268967 -0.259716

O -0.769482 3.210603 0.375998

O 2.789936 -2.863988 -0.281035

O 3.480293 -1.703512 0.378306

O -2.874404 -2.852392 -0.370301

O -3.535901 -1.723223 0.362117

III-44.04

Fe 1.693947 -1.412883 0.051890

Fe -1.624017 -1.328944 0.049747

Fe 0.058870 1.514184 0.020993

O 0.044511 3.311869 -0.047638

O 0.054126 4.676211 0.050444

O -4.398602 -2.866204 -0.051508

O -3.190187 -2.232659 0.050396

O 4.385581 -3.074111 0.052215

O 3.179717 -2.428187 0.050911

O 0.019985 -2.057439 0.056491

O 1.509862 0.402937 0.052166

O -1.389150 0.454674 0.048409

Fe_4O

I-15.80

Fe 1.202379 -0.202172 0.047564

Fe -1.311630 0.051869 0.143294

Fe -0.049303 1.234524 1.724920

Fe -0.154433 -1.299347 1.617554

O 1.605436 1.403801 0.891517

II-15.05

Fe 1.211953 0.062018 0.045687

Fe -1.211909 0.061969 0.045719

Fe 0.000032 1.142073 1.852107

Fe 0.000067 -1.199982 1.617415

O -0.000015 1.599895 -0.050827

III-14.55

Fe 1.803663 -0.182930 -0.000001

Fe -1.600009 0.033913 -0.000001

Fe -0.183099 1.803675 0.000000

Fe 0.033962 -1.600057 0.000005

O 1.638463 1.638278 -0.000002

Fe_4O_2

I-21.66

Fe 1.097202 -0.051430 -0.045001

Fe -1.201222 -0.051551 -0.045217

Fe -0.052141 1.233010 1.814030

Fe -0.052229 -1.273876 1.713226

O -0.051946 1.615282 -0.050269

O -0.052177 -0.054051 3.132619

II-21.42

Fe 1.268076 0.194046 -0.191158

Fe -1.270961 0.152956 -0.053994

Fe -0.051148 1.255074 1.717914

Fe -0.157997 -1.093120 1.614408

O -0.054793 -0.265181 -1.406111

O 1.744926 1.307563 1.211851

III-21.30

Fe 1.234399 0.023586 -0.617819

Fe -1.295796 -0.049954 -0.538876

Fe -0.059763 2.122237 0.091447

Fe 0.050109 -1.774001 0.261150

O 1.728723 1.729738 -0.057475

O -1.831006 1.632423 0.050638

Fe_4O_3

I-27.72

Fe 1.200369 -0.573145 0.199896

Fe -1.304570 -0.573182 0.199921

Fe -0.052100 1.204090 1.435490

Fe -0.051995 -0.951726 2.335451

O 1.603680 0.147569 1.928828

O -1.707859 0.147660 1.928931

O -0.052051 -1.094254 -1.063924

II-27.58

Fe 1.612816 0.157423 0.258567

Fe -0.679815 -0.466024 0.158215

Fe 0.031989 1.232979 1.936677

Fe 0.170165 -1.300599 2.219868

O -0.472828 0.063953 3.284863

O 1.319548 1.905306 0.785146

O 0.908779 -1.639419 0.460975

III-27.02

Fe 1.438232 -0.028807 -0.072249

Fe -1.260093 -0.047868 0.063120

Fe -0.074710 1.195643 1.802259

Fe -0.059071 -1.239403 1.822072

O -0.047106 -0.050688 -1.296214

O 1.506263 1.580737 0.982663

O 1.522649 -1.620654 1.001979

Fe_4O_4

I-33.92

Fe 1.964327 0.046936 0.045901

Fe -2.042805 -0.045575 -0.086273

Fe -0.057058 2.031289 0.049371

Fe -0.038419 -2.030717 0.048897

O 1.731672 1.832126 0.063522

O -1.830417 1.740830 -0.046605

O -1.825204 -1.832141 -0.046252

O 1.736722 -1.738122 0.061958

II-33.52

Fe 1.390388 0.035616 -0.060143

Fe -1.342131 0.021163 -0.094796

Fe -0.156482 1.200986 1.776577

Fe -0.143956 -1.225981 1.726928

O 0.049689 0.054734 -1.278553

O 1.501853 1.463420 1.023636

O 1.519715 -1.428261 0.975290

O -1.683065 -0.027659 1.810080

III-33.28

Fe 1.829917 0.271590 0.044025

Fe -1.919681 -0.197094 -0.046323

Fe 0.250299 2.194293 0.051328

Fe -0.251726 -1.822212 0.046192

O 2.074507 2.106788 -0.044845

O -1.417962 1.507423 0.032563

O -2.060137 -2.002860 -0.047693

O 1.506234 -1.506755 0.054599

Fe_4O_5

I- 38.79

Fe 1.544972 -0.583796 0.456162

Fe -1.050252 -0.257897 -0.575576

Fe -0.078053 1.203108 1.618627

Fe -0.493732 -1.528172 2.136414

O 1.738749 1.111030 1.207048

O -0.790648 0.073842 2.883441

O 0.580113 -0.791737 -1.096549

O -1.320789 1.301918 0.266889

O 1.109912 -2.028546 1.509687

II-38.70

Fe 2.136800 -0.052966 0.878977

Fe 0.053241 1.927215 -0.154152

Fe 0.286974 -0.044968 2.439227

Fe -0.988390 -0.256660 -0.044861

O 1.810619 1.473239 -0.052093

O -1.190994 1.076428 -1.310178

O -0.776127 1.182267 1.526062

O 0.469765 -1.182593 0.652551

O 2.103992 -0.155179 2.773220

III-38.70

Fe 1.991463 -0.090648 0.821096

Fe -1.916465 -0.203610 0.779528

Fe 0.061666 1.776865 0.569005

Fe 0.025192 -2.052113 1.079969

O -1.825458 -2.038376 0.997502

O 1.914086 1.739979 0.568277

O 1.805748 -1.809113 1.415639

O -1.725858 1.608898 0.903795

O 0.053206 -0.245860 0.045661

Fe_4O_6

I-44.00

Fe 1.387769 0.144970 -0.128751

Fe -1.431417 0.045458 -0.066621

Fe 0.069082 1.500928 1.781457

Fe -0.046995 -1.240003 1.828740

O -0.046109 0.065610 -1.229577

O 1.584596 1.726884 0.892237

O 1.427733 -1.416545 0.879878

O -1.594569 -1.504266 1.007661

O -1.438953 1.643574 0.879781

O 0.040164 0.149985 2.971168

II-42.60

Fe 0.998646 1.269171 0.049075

Fe 1.518990 -1.367337 0.360617

Fe -1.519530 1.566861 -0.360030

Fe -1.001080 -1.070371 -0.047305

O 0.343186 -0.267113 1.291254

O -0.344530 0.467471 -1.290868

O 2.462995 0.064515 -0.149398

O -2.463865 0.135535 0.150412

O -0.241974 2.737284 0.151942

O 0.240583 -2.537482 -0.150041

III-42.40

Fe -1.306415 0.610657 0.248406

Fe 1.367506 0.622349 0.334222

Fe -0.111209 -1.606806 -0.258190

Fe 0.120892 1.405104 2.442753

O -1.919948 -1.084036 -0.039979

O 1.618487 -1.188993 0.267319

O 0.027249 2.030064 0.501704

O 0.067025 0.248916 -1.089065

O 1.934986 1.076739 2.009133

O -1.611477 0.883907 2.030902

Fe_4O_7

I-47.85

Fe 1.540833 0.052810 -0.361646

Fe -1.407285 0.038147 -0.021060

Fe 0.144410 1.814502 1.905067

Fe 0.059427 -1.234070 1.828413

O -0.050310 0.052435 -1.219907

O 1.509442 1.536477 0.807685

O 1.457110 -1.414382 0.781957

O -1.527837 -1.493547 1.084391

O -1.301508 1.626168 0.891814

O 0.153758 0.147998 2.864369

O 0.170878 2.967142 3.072297

II-46.86

Fe 1.302609 0.312073 -0.141260

Fe -1.300098 0.214573 -0.020474

Fe 0.048399 1.518515 1.788012

Fe 0.043754 -1.304976 1.806128

O -0.037898 -0.367839 -1.239881

O 1.851589 1.395327 1.293737

O 1.489048 -1.295585 0.752683

O -1.496608 -1.418883 0.880887

O -1.760171 1.297425 1.406812

O 0.054928 0.075155 2.941687

O -0.047308 1.728215 -0.156899

III-46.64

Fe -1.406421 0.781152 0.047878

Fe 1.542242 0.785687 -0.046328

Fe 0.079988 -1.215901 0.269820

Fe 0.131996 0.873022 2.020658

O -1.781212 -1.003322 0.054642

O 1.924043 -0.997719 -0.057075

O 0.075512 2.043935 0.400102

O 0.035225 0.161026 -1.172767

O 1.970769 1.103068 1.701880

O -1.726983 1.095750 1.817705

O 0.143801 -0.990895 2.122001

Fe_4O_8

I-51.48

Fe 1.541995 0.058351 -0.348503

Fe -1.616413 0.062188 -0.153939

Fe -0.043088 1.570695 1.924966

Fe -0.002985 -1.586609 1.996344

O -0.091582 0.130403 -1.112397

O 1.401076 1.430376 0.771032

O 1.302066 -1.300528 0.798492

O -1.426587 -1.411470 0.951953

O -1.534913 1.521869 0.907522

O -0.049698 0.014175 2.836421

O 2.694490 -0.050683 -1.506807

O 0.160728 -2.792437 3.091051

II-50.76

Fe 1.210391 0.252866 -0.223683

Fe -1.241816 0.267640 -0.045667

Fe -0.022666 1.522983 1.684925

Fe 0.046790 -1.439778 1.929868

O -0.060099 -0.458268 -1.347725

O 1.784013 1.322121 1.204463

O 1.399890 -1.318784 0.795386

O -1.407572 -1.317991 0.906980

O -1.829399 1.377325 1.390837

O 0.057167 0.061534 2.866207

O -0.061313 1.762414 -0.277688

O 0.057008 -2.780350 2.847315

Fe_4O_9

III-55.51

Fe 1.463553 0.059861 -0.367099

Fe -1.604785 0.043350 -0.085114

Fe -0.027578 1.702078 1.970538

Fe 0.010229 -1.520608 2.024122

O -0.144496 0.048086 -1.165350

O 1.284904 1.447034 0.765220

O 1.307679 -1.300251 0.797108

O -1.461444 -1.403785 1.001609

O -1.504640 1.518968 0.965688

O 0.046721 0.102721 2.793863

O 2.723112 0.052836 -1.410551

O 0.047920 -2.854871 2.969877

O -0.042410 3.070023 2.868041

I-54.08

Fe 1.240679 0.267693 -0.162125

Fe -1.305465 0.260451 -0.083993

Fe 0.021171 1.683805 1.707166

Fe 0.037002 -1.486479 1.925985

O -0.064507 -0.366471 -1.319435

O 1.836633 1.345200 1.213153

O 1.414136 -1.311473 0.796641

O -1.409290 -1.319046 0.884347

O -1.824366 1.327921 1.327561

O 0.055088 0.065194 2.745321

O -0.043142 1.778727 -0.188379

O 0.058770 -2.882577 2.777314

O 0.049718 3.081055 2.570204

II-53.17

Fe 1.245700 0.380807 -0.266091

Fe -1.303270 0.365786 -0.195030

Fe 0.019599 1.508681 1.662467

Fe 0.040832 -1.483239 1.822645

O -0.056238 -0.250381 -1.423765

O 1.808413 1.378522 1.200066

O 1.428889 -1.217834 0.609798

O -1.418167 -1.237246 0.686090

O -1.793355 1.348106 1.303569

O 0.057489 0.060327 2.799620

O -0.042287 1.910174 -0.286360

O 0.056819 -2.777176 3.195094

O 0.049997 -3.477655 1.914131

Fe_4O_{10}

I-59.36

Fe 1.574049 -0.064654 -0.352165

Fe -1.624572 0.022487 -0.267628

Fe 0.097610 1.621034 1.935104

Fe -0.029650 -1.576390 1.998735

O -0.047299 -0.045297 -1.108580

O 1.424593 1.317704 0.774749

O 1.313938 -1.391472 0.804229

O -1.421660 -1.320065 0.899927

O -1.306871 1.389169 0.840899

O 0.050904 0.038350 2.771907

O 2.879172 -0.161358 -1.313673

O 0.151244 -2.955243 2.849125

O 0.050981 3.035596 2.742039

O -2.967298 0.165225 -1.176548

II-57.96

Fe 1.403170 0.070625 -0.481994

Fe -1.610983 0.059761 0.011009

Fe -0.014467 1.708566 1.931797

Fe -0.004381 -1.469371 2.011442

O -0.367384 0.047382 -1.176248

O 1.198339 1.502199 0.684730

O 1.211245 -1.302446 0.765301

O -1.522930 -1.361580 1.012436

O -1.543873 1.515691 0.964267

O 0.054612 0.140767 2.792928

O 0.052084 -2.696976 3.072599

O 0.047556 2.979269 2.937698

O 3.206575 0.051333 -0.951848

O 2.334465 -0.051305 -2.158419

III-57.82

Fe 1.261069 0.059029 -0.475612

Fe -1.753723 0.039371 -0.367015

Fe 0.073536 1.717568 2.153142

Fe -0.162789 -1.404131 1.953827

O -0.259461 -0.043594 -1.396865

O 1.014546 1.440500 0.676371

O 1.104355 -1.311059 0.673507

O -1.615460 -1.191388 0.964986

O -1.671834 1.716324 1.682825

O 0.170818 0.124513 2.894923

O 2.527007 0.155420 -1.512257

O -0.180733 -2.599201 3.074169

O 0.463973 3.007723 3.050948

O -2.033427 1.817381 0.225281

Fe_4O_{11}

I-62.10

Fe 1.542510 -0.043683 -0.351627

Fe -1.646174 0.061422 -0.264748

Fe 0.055758 1.605819 1.978961

Fe -0.042730 -1.600955 1.934812

O -0.069720 0.045283 -1.117048

O 1.411415 1.318968 0.762590

O 1.311680 -1.411595 0.787186

O -1.442080 -1.317128 0.868022

O -1.400581 1.405898 0.836847

O 0.040222 -0.032647 2.763247

O 2.848186 -0.254719 -1.297090

O -0.051166 -3.001272 2.759289

O 0.064930 3.600772 2.204572

O -2.982043 -0.059755 -1.180339

O -0.058101 2.953342 3.486435

Fe_4O_{12}

II-60.45

Fe 1.563396 0.047888 -0.364611

Fe -1.612301 0.054498 -0.261987

Fe 0.043775 1.621202 1.973123

Fe 0.057789 -1.595779 1.958057

O -0.040992 0.050590 -1.137227

O 1.386912 1.398771 0.780105

O 1.379234 -1.328515 0.759901

O -1.378428 -1.320512 0.794103

O -1.384055 1.393597 0.864404

O 0.053643 -0.018106 2.764643

O -3.000038 0.168022 -1.108483

O 2.968720 -0.139660 -1.177050

O -0.723583 2.872360 3.400011

O 0.336405 3.477845 2.658221

O -0.039238 -2.860441 3.409996

O 0.043633 -3.600710 2.174121

Fe_4O_{13}

III-63.04

Fe 1.558797 -0.009862 -0.336483

Fe -1.644841 -0.054267 -0.238995

Fe -0.015044 1.591875 1.986873

Fe 0.013485 -1.619445 2.029036

O -0.098041 -0.058668 -1.096509

O 1.330908 1.382994 0.791001

O 1.311260 -1.347663 0.819027

O -1.467466 -1.379013 0.876416

O -1.394809 1.309937 0.858463

O 0.056694 0.002694 2.814717

O -2.956991 0.050058 -1.198975

O -0.037385 2.816804 3.509180

O 0.026488 3.513500 2.230166

O -0.278002 -2.838553 3.559999

O 0.058769 -3.537111 2.331244

O 2.641724 -0.055975 -1.852464

O 3.467616 0.059294 -0.625641

Fe_4O_{14}

I-62.40

Fe 1.618428 0.035226 -0.210750

Fe -1.568708 0.039043 -0.266375

Fe -0.059377 1.478075 2.145525

Fe 0.023178 -1.707921 1.935804

O 0.040933 0.078770 -1.065593

O 1.312566 1.312383 1.006197

O 1.412174 -1.405528 0.844533

O -1.310509 -1.392286 0.781496

O -1.406075 1.326593 0.970207

O -0.039133 -0.167588 2.860656

O -0.930511 2.560390 3.612721

O 0.284621 3.165630 3.163898

O 0.828258 -2.971090 3.296523

O -0.385551 -3.487839 2.745540

O 2.867584 -0.690688 -1.631253

O 3.390813 0.484467 -1.006639

O -2.755030 0.964343 -1.624719

O -3.294755 -0.292405 -1.208427

Fe_5O

I-18.84

Fe 1.933064 0.044082 0.159045

Fe -1.991428 0.051109 0.266723

Fe -0.051367 1.165348 -0.678869

Fe -0.052996 -1.163740 -0.582396

Fe -0.019702 0.050359 1.616882

O 1.817272 0.066191 1.990124

II-18.66

Fe 1.203971 -0.467263 -0.160414

Fe -1.457467 -0.263452 -0.052533

Fe -0.054078 1.552539 -0.050650

Fe -0.161151 -2.239815 0.575686

Fe -0.056624 -0.369313 1.975183

O 1.223618 0.898297 1.302206

III-18.48

Fe -1.300261 0.783960 0.000017

Fe 1.300260 0.783964 0.000019

Fe 0.000012 -1.397464 0.000015

Fe -0.000001 -0.027781 1.879310

Fe 0.000002 -0.027772 -1.879277

O -0.000003 2.134833 -0.000029

Fe_5O_2

I-25.06

Fe 1.949196 0.000046 0.146584

Fe -1.949517 0.000002 0.146512

Fe -0.000214 1.185382 -0.578703

Fe -0.000186 -1.185371 -0.578641

Fe -0.000198 0.000268 1.775413

O 1.861347 0.000391 1.943178

O -1.861348 0.000293 1.943340

II-24.99

Fe -1.292420 0.683275 -0.017238

Fe 1.262223 0.779941 -0.064065

Fe -0.048773 -1.407307 -0.185205

Fe 0.146064 -0.053057 1.939132

Fe -0.054341 0.155989 -1.986838

O 1.711607 0.886425 1.750759

O -1.398472 -0.892849 1.200292

III-24.92

Fe 1.927963 -0.046496 -0.456496

Fe -1.931311 0.047461 -0.454463

Fe -0.031568 1.396678 -0.808129

Fe 0.027385 -1.396510 -0.803876

Fe -0.001307 0.003261 1.378750

O 1.208314 1.330248 0.783760

O -1.210829 -1.326060 0.788139

Fe_5O_3

I-31.52

Fe 1.873801 -0.054170 0.570972

Fe -1.581895 -0.043982 -0.260216

Fe 0.048297 1.606494 -0.257818

Fe 0.055951 -1.883095 0.573768

Fe -0.148029 0.147742 1.956773

O 1.101064 1.524823 1.392665

O -1.521892 -1.102690 1.389864

O 1.791423 -1.792277 -0.042842

II-31.20

Fe -1.231613 1.094962 -0.047474

Fe 1.088735 0.509011 -0.159187

Fe 0.779679 -2.026650 -0.532180

Fe -0.330111 -0.682821 1.621836

Fe -0.258385 -0.122402 -2.031608

O -1.934045 0.174826 1.396079

O 1.428645 -1.102422 0.999519

O -0.053204 -1.951896 -2.164162

III-31.12

Fe 2.117112 -0.571357 0.258910

Fe -1.860034 -0.062804 -0.044888

Fe 0.375852 0.987811 -0.640253

Fe 0.153700 -1.405956 -0.886619

Fe 0.049356 0.204842 1.712465

O 1.890547 0.161297 1.927893

O -1.814750 0.051810 1.759314

O -0.976797 0.065813 -1.730521

Fe_5O_4

I-37.89

Fe 1.409896 1.192707 0.043436

Fe -1.228059 1.389753 0.058168

Fe 1.224867 -1.392356 -0.027805

Fe -1.412329 -1.194692 0.002296

Fe 0.008075 -0.044525 1.616451

O 2.032870 -0.182081 1.219803

O -2.022667 0.124490 1.254806

O 0.157910 2.253631 -0.799923

O -0.171942 -2.226857 -0.896400

II-36.27

Fe -0.775408 0.467915 -0.058231

Fe 1.540282 1.509529 0.254760

Fe -0.775345 -1.892409 -0.155489

Fe 0.572188 -0.154046 2.039716

Fe 0.257972 -0.256438 -2.037923

O -0.572905 -1.506400 1.613166

O 1.817220 1.185485 2.033002

O 1.083725 1.282958 -1.499641

O -0.259913 -2.015508 -1.916587

III-36.27

Fe -1.195655 0.885253 -0.056571

Fe 1.190813 0.853649 -0.058874

Fe -0.043909 -1.515632 -0.031226

Fe -0.014701 -0.056838 2.033272

Fe -0.017950 0.053139 -2.028758

O -0.046116 -1.815687 1.837415

O 1.521220 0.773922 1.832150

O -1.534511 0.800866 1.833021

O -0.052051 -1.776402 -1.856667

Fe_5O_5

I-42.80

Fe -1.913630 0.678797 -0.103656

Fe 1.801057 0.971120 0.248700

Fe 0.456238 -1.067987 -0.399222

Fe 0.045805 0.059531 1.993665

Fe -0.347424 0.670902 -2.109973

O 1.637443 1.108021 2.020617

O -1.568449 0.870425 1.639780

O -0.070818 -1.651624 1.207211

O 1.400305 0.294280 -1.494011

O -2.137821 0.882182 -1.946208

II-42.80

Fe 0.372667 2.100698 -0.052064

Fe -2.667977 0.575043 -0.052121

Fe 2.902601 0.900041 -0.052088

Fe -1.925157 -1.752198 -0.052070

Fe 1.507725 -1.409083 -0.052092

O 2.142218 2.555708 -0.052117

O -1.392047 1.829324 -0.052088

O -0.160325 -2.046327 -0.052078

O 3.260029 -0.889162 -0.052058

O -3.600456 -1.004655 -0.052097

III-42.60

Fe -1.563677 0.572355 -0.786867

Fe 1.195461 0.996988 -0.242395

Fe -0.472681 -1.554336 -0.044633

Fe -0.422289 0.674693 1.718440

Fe 0.157070 -0.360863 -2.239630

O -0.878837 -1.059194 1.689211

O -1.545430 -1.206357 -1.696816

O 1.316718 -0.889287 -0.684956

O 0.979077 1.812598 1.418885

O -0.032339 1.516492 -1.637590

Fe_5O_6

I-49.17

Fe -1.298151 0.677901 -0.051610

Fe 1.395044 0.849617 -0.042157

Fe -0.041603 -1.416284 -0.054420

Fe 0.071777 0.053597 2.249164

Fe -0.031592 0.010956 -2.289038

O 1.634768 0.995901 1.741431

O -1.542844 0.789309 1.711159

O -0.052952 -1.714658 1.704559

O 1.497540 0.895164 -1.843389

O -1.507225 0.994835 -1.835423

O 0.149547 -1.752912 -1.834733

II-48.18

Fe -1.841216 1.108372 0.021588

Fe 0.605128 0.254349 1.099896

Fe 0.699088 -2.321040 -0.067825

Fe -1.342343 -1.193481 1.608000

Fe -0.467042 -0.617118 -1.609484

O 0.466815 -1.722919 1.727760

O -0.353314 1.762705 0.887015

O -0.269928 -2.467846 -1.634867

O -1.617258 0.757799 -1.815696

O -2.657982 -0.051769 1.213193

O 1.121459 -0.362126 -0.680013

III-47.96

Fe -2.210634 0.803235 0.132055

Fe 1.719848 0.040701 -0.186569

Fe -0.470403 -2.020778 0.157537

Fe 0.248268 0.253850 1.964597

Fe -0.603407 -0.056392 -1.505594

O 0.059712 -1.573674 1.823080

O 1.944410 0.897475 1.386179

O -1.409120 0.979377 1.733656

O 0.869400 -1.280651 -1.192657

O -1.520666 1.502053 -1.505960

O -2.019025 -1.105174 -0.585357

Fe_5O_7

I-53.40

Fe -1.505963 1.503883 -0.232357

Fe 1.676781 0.857906 0.205695

Fe 0.261567 -2.057940 -0.240027

Fe 0.052633 0.048063 2.059288

Fe -0.178459 -0.059322 -1.812551

O 0.051181 -1.684143 1.508946

O -1.324356 1.098561 1.512376

O -0.573835 -1.821486 -1.931697

O -1.823705 0.687357 -1.920565

O 1.519516 -0.661361 -0.904865

O 1.720364 0.882344 2.046631

O 0.369794 1.650030 -0.902670

II-53.16

Fe -0.896143 1.830982 -0.012156

Fe 1.867283 1.310809 0.252873

Fe -0.366685 -2.042622 -0.103616

Fe 0.273987 0.017605 2.029882

Fe 0.154148 -0.162082 -1.830779

O 2.018959 0.672573 1.966658

O -1.128083 1.123721 1.618206

O -0.128416 -1.715462 1.619989

O 1.729883 0.443396 -1.400369

O -1.062401 1.113695 -1.722888

O -0.370610 -1.847673 -1.960964

O 0.678462 2.671265 0.069906

III-52.20

Fe -1.927903 0.367567 -0.050817

Fe 2.027192 1.297690 0.052512

Fe -0.476465 -1.794275 -0.160582

Fe 0.370552 0.256454 1.889861

Fe 0.144594 -0.068879 -2.046360

O 0.356346 -1.509505 1.378878

O 2.027698 1.104846 1.866193

O -1.284176 0.958756 1.497951

O -0.035359 -1.939377 -1.903491

O -1.505735 0.797733 -1.750873

O 1.718934 0.700984 -1.606129

O -2.244574 -1.413543 -0.031095

Fe_5O_8

I-57.59

Fe -1.405552 0.872860 0.015407

Fe 1.387781 1.510135 0.126213

Fe -0.725913 -1.933770 -0.151067

Fe 0.361919 -0.087214 2.027739

Fe 0.215165 -0.231197 -2.098000

O 0.157926 -1.803110 1.386541

O 1.857122 0.981119 1.828849

O -1.268333 0.684743 1.805008

O -0.260730 -1.975732 -1.914556

O -1.261121 0.691984 -1.921800

O 1.617808 0.688113 -1.504418

O -2.147761 -0.927894 -0.056026

O -0.255636 2.256603 -0.047651

II-56.03

Fe -1.084813 0.954900 0.140824

Fe 1.760966 1.109662 -0.681897

Fe 0.259827 -1.302295 0.119468

Fe -1.209856 -0.668645 2.406176

Fe -0.187244 -0.015950 -2.418853

O -1.400034 1.082809 1.956074

O 0.249553 -1.642398 1.936205

O 1.312548 0.873697 -2.469564

O -1.509471 0.879636 -1.693401

O -0.037937 -1.614929 -1.715215

O 0.374122 2.024610 0.062822

O 1.907058 -0.555172 0.038207

O -1.617464 -0.895190 0.379290

III-55.90

Fe -1.297150 1.601322 0.264148

Fe 1.333624 1.302447 -0.279696

Fe -0.079693 -1.574980 -0.212915

Fe 0.884996 0.053568 1.815720

Fe -0.680297 0.247685 -2.099404

O 0.255721 1.986277 1.205719

O -0.991767 -0.166408 0.889236

O 0.891057 -1.714411 1.319378

O -0.256207 1.969679 -1.306528

O -1.212473 -1.465182 -1.742294

O 1.110126 -0.238233 -1.296532

O 2.510768 0.783123 0.924749

O -2.919597 1.826988 0.472460

Fe_5O_9

I-61.32

Fe -1.375932 0.840978 0.059422

Fe 1.435892 0.876163 0.046999

Fe -0.002650 -1.535702 -0.015520

Fe 0.120924 0.050750 2.365434

Fe -0.049296 0.085184 -2.332424

O 1.605207 0.903046 1.964685

O -1.372433 0.882185 1.926362

O 0.068721 -1.633286 1.847428

O 1.402628 0.908891 -1.934162

O -1.501250 0.891260 -1.851787

O -0.062434 -1.595706 -1.930353

O 0.033082 2.014765 0.029936

O 1.716453 -0.906203 -0.060007

O -1.761400 -0.969377 0.049675

II-61.32

Fe -1.517916 0.755851 0.144246

Fe 0.953305 2.226865 0.090838

Fe -0.078554 -1.785213 -0.025642

Fe 0.467233 0.118333 2.125456

Fe 0.385360 0.302397 -2.026687

O 1.423338 1.711858 1.839327

O -1.315928 0.564428 1.929817

O 0.470041 -1.720436 1.690793

O 1.288441 1.832750 -1.723997

O -1.324629 0.677353 -1.810077

O 0.363423 -1.532446 -1.809305

O -0.884045 2.448126 0.133757

O -1.740319 -1.190017 -0.039173

O 0.593212 0.164581 0.030444

Fe -1.713169 0.878913 0.051426

Fe 0.875498 2.189958 0.231487

Fe -0.167810 -1.820103 -0.095049

Fe 0.469313 0.267010 2.040492

Fe 0.363348 0.053901 -1.956977

O 1.530771 1.705438 1.913214

O -1.218770 0.579090 1.911471

O 0.691107 -1.401612 1.423446

O 1.410699 1.312515 -1.278701

O -1.284459 0.671264 -1.748923

O 0.356761 -1.772781 -1.824857

O -0.896090 2.499498 0.075390

O -1.750164 -1.167423 0.041743

O -3.358392 1.073668 0.159733

Fe_5O_{10}

I-64.95

Fe -1.240929 0.785639 -0.054854

Fe 1.401355 0.825465 -0.045008

Fe 0.023620 -1.530360 -0.029331

Fe 0.051123 0.051072 2.550442

Fe -0.044366 0.060174 -2.431936

O 1.479821 0.805002 1.821310

O -1.330695 0.868047 1.824021

O 0.062653 -1.571027 1.834541

O 1.410455 0.860553 -1.952129

O -1.480808 0.900779 -1.954465

O -0.016715 -1.594604 -1.935849

O 0.067781 2.105068 -0.050172

O 1.807760 -0.994910 -0.065445

O -1.746836 -0.997708 -0.031865

O 0.061439 0.050492 4.169871

II-64.65

Fe -1.561162 0.770386 0.064583

Fe 0.986871 2.105827 0.046442

Fe -0.076763 -1.835669 -0.023035

Fe 0.357498 0.159210 2.139902

Fe 0.368718 0.259270 -2.083766

O 1.449230 1.508722 1.925123

O -1.319590 0.578942 1.954641

O 0.568650 -1.532940 1.837060

O 1.322100 1.747322 -1.757029

O -1.331348 0.669380 -1.812967

O 0.358716 -1.523282 -1.833369

O -0.839250 2.423891 0.155030

O -0.043608 -3.482691 0.035048

O -1.719940 -1.156853 0.048208

O 0.579999 0.078058 0.006593

III-63.75

Fe -1.469434 0.798284 0.135270

Fe 1.368916 0.990270 0.155836

Fe -0.263708 -1.649606 -0.040319

Fe 0.107235 0.046283 2.352120

Fe -0.058596 0.071676 -2.224457

O 1.617487 1.002325 2.023344

O -1.490441 0.800065 1.944241

O 0.058338 -1.645648 1.731410

O 1.392718 0.883560 -1.791737

O -1.510605 0.891551 -1.805991

O -0.164429 -1.627643 -1.950001

O -0.075682 2.023189 0.137791

O 2.465115 -0.677264 0.073095

O -1.937176 -0.990203 0.021399

O 1.753671 -1.869689 -0.175158

Fe_5O_{11}

I-69.12

Fe -1.265367 0.895807 0.048261

Fe 1.473436 0.786254 -0.048143

Fe 0.012613 -1.530580 0.006322

Fe 0.161692 0.053359 2.694014

Fe -0.017676 0.050346 -2.687283

O 1.520766 0.782107 1.838432

O -1.192457 0.891534 1.934469

O 0.064072 -1.515274 1.894838

O 1.400443 0.779831 -1.933208

O -1.316034 0.888549 -1.839330

O -0.050756 -1.517600 -1.881746

O 0.154889 2.092816 -0.006479

O 1.803563 -1.040596 -0.052706

O -1.732513 -0.899165 0.059975

O 0.234773 0.053828 4.326238

O -0.063636 0.051614 -4.320572

II-68.48

Fe -1.335885 2.022141 0.044739

Fe 1.518501 0.809630 0.063995

Fe 0.900028 -2.233295 -0.053905

Fe -0.184161 -0.133067 2.005210

Fe -0.366623 -0.145323 -2.189706

O 1.372990 0.677425 1.947355

O -1.498694 0.964649 1.499759

O -0.048391 -1.813935 1.421768

O 1.135621 0.659004 -1.737909

O -1.550298 0.772240 -1.234732

O -0.266557 -1.682552 -1.304165

O 0.398286 2.326551 0.050684

O 2.127815 -0.970610 -0.042187

O -0.604592 -0.255277 -3.797537

O -2.325190 3.287315 -0.246554

O 1.407315 -3.752633 -0.363676

III-68.32

Fe -1.297538 1.721280 -0.020677

Fe 1.575519 0.979802 -0.059580

Fe 0.820886 -2.146340 -0.059213

Fe -0.265867 -0.145984 2.031456

Fe -0.381964 -0.170356 -2.348062

O 1.267834 0.674371 1.754839

O -1.557034 0.986026 1.601687

O -0.037876 -1.819858 1.483484

O 1.093531 0.605844 -1.919358

O -1.608721 0.885569 -1.608792

O -0.379414 -1.608782 -1.288836

O 0.357383 2.346889 -0.132986

O 2.050388 -0.964236 -0.137251

O -0.579227 -0.571270 -3.919599

O 3.103428 1.616017 0.038912

O 1.299593 -3.676964 -0.358152

Fe_5O_{12}

I-72.59

Fe -1.324563 1.924070 0.031717

Fe 1.610868 0.860005 -0.058329

Fe 0.783431 -2.152847 -0.022266

Fe -0.185543 -0.074044 2.332735

Fe -0.308460 -0.135685 -2.325860

O 1.302263 0.688108 1.802751

O -1.445903 0.794756 1.410976

O -0.163196 -1.601255 1.391820

O 1.195844 0.659412 -1.898426

O -1.495215 0.788687 -1.347062

O -0.269193 -1.650370 -1.375095

O 0.385502 2.304682 -0.040746

O 2.080158 -0.972185 -0.057053

O -0.457237 -0.149739 3.935253

O -0.576749 -0.363295 -3.914267

O -2.337980 3.190958 0.145397

O 1.229422 -3.716290 -0.062367

II-72.42

Fe -1.220554 0.958213 0.056411

Fe 1.438617 0.853913 -0.034500

Fe 0.006110 -1.777453 0.024366

Fe 0.161900 0.048305 2.696330

Fe -0.011292 0.042923 -2.665290

O 1.513292 0.799991 1.833723

O -1.182051 0.909626 1.927681

O 0.066698 -1.532757 2.013855

O 1.395602 0.804070 -1.904161

O -1.297761 0.912631 -1.813617

O -0.051281 -1.534376 -1.968383

O 0.159410 2.181896 0.019814

O 1.604040 -1.016718 -0.039559

O -1.527673 -0.893823 0.061479

O 0.238499 0.074849 4.323803

O -0.057471 0.064144 -4.294076

O -0.054815 -3.413705 0.043593

III-71.74

Fe -1.230838 0.884667 0.031456

Fe 1.623189 0.975348 0.012107

Fe -0.041538 -1.719767 0.046876

Fe 0.151857 0.052167 2.707797

Fe -0.048054 0.126224 -2.403761

O 1.524029 0.817038 1.952359

O -1.189957 0.878053 1.906591

O 0.055419 -1.529758 1.982269

O 1.405394 0.896998 -1.975918

O -1.444609 0.996755 -1.838993

O -0.076412 -1.512522 -1.950699

O 0.213056 2.055492 0.052073

O 1.545803 -0.842649 -0.037039

O -1.633913 -0.930694 0.068089

O 0.159384 0.060710 4.327855

O 3.084484 1.730909 -0.048777

O -0.061893 -3.366045 0.034180

Fe_5O_{13}

I-75.96

Fe -1.353351 1.900759 0.003832

Fe 1.747485 0.967334 -0.058826

Fe 0.782500 -2.128876 -0.022578

Fe -0.161163 -0.067560 2.304807

Fe -0.279294 -0.092524 -2.326542

O 1.299086 0.710006 1.796995

O -1.438389 0.800788 1.409174

O -0.147725 -1.620314 1.416903

O 1.203693 0.681391 -1.888261

O -1.515771 0.820184 -1.409268

O -0.240488 -1.619918 -1.395429

O 0.347048 2.245972 -0.041040

O 2.022136 -0.915392 -0.058229

O -0.375450 -0.170660 3.912129

O -0.580446 -0.259479 -3.914997

O 3.184024 1.724013 -0.056999

O -2.420468 3.128829 0.045700

O 1.209109 -3.698356 -0.045210

II-75.42

Fe -1.503720 0.949597 0.036093

Fe 1.631961 0.848548 -0.047139

Fe -0.011488 -1.497403 -0.004425

Fe 0.108389 0.066255 2.662858

Fe -0.028352 0.067888 -2.672806

O 1.500291 0.791672 1.917403

O -1.271928 0.884097 1.990491

O 0.042882 -1.509500 1.852430

O 1.404718 0.789214 -2.002519

O -1.375201 0.879417 -1.931808

O -0.057574 -1.508577 -1.861052

O 0.092318 1.806911 -0.020008

O 1.759068 -0.916189 -0.051271

O -1.741447 -0.804040 0.046928

O 0.153752 0.050093 4.283206

O -0.061729 0.051204 -4.293716

O 3.066111 1.644887 -0.064201

O -2.877150 1.844320 0.060023

III-74.70

Fe -1.399098 1.036897 0.038863

Fe 1.644329 0.903550 -0.025233

Fe 0.041796 -1.729304 0.010142

Fe 0.127215 0.052177 2.661152

Fe 0.001477 0.005046 -2.526960

O 1.517816 0.781125 1.918548

O -1.210340 0.924649 1.973033

O 0.047467 -1.531651 1.964252

O 1.430266 0.763446 -2.031789

O -1.337675 0.880351 -1.930823

O -0.053400 -1.602830 -1.959299

O 0.142640 1.940645 -0.032119

O 1.628028 -0.949089 -0.046332

O -1.500481 -0.779818 0.049061

O 0.160974 0.058244 4.289041

O 2.960253 1.912400 -0.066133

O -2.772017 1.941619 0.056758

O -0.022349 -3.371234 0.045860

Fe_5O_{14}

I-78.66

Fe -1.259187 1.935729 -0.058681

Fe 1.825856 0.917733 -0.153799

Fe 0.741287 -2.143495 -0.057082

Fe -0.184792 -0.076323 2.253396

Fe -0.368294 -0.145182 -2.365402

O 1.263697 0.663570 1.707645

O -1.417487 0.779777 1.283807

O -0.143935 -1.656267 1.415805

O 1.136041 0.567648 -1.946899

O -1.528920 0.890998 -1.483092

O -0.373189 -1.606530 -1.337922

O 0.446972 2.265131 -0.125892

O 2.048439 -1.002306 -0.143013

O -0.458168 -0.133561 3.852279

O -0.675190 -0.375066 -3.942475

O -2.169114 3.273651 0.045583

O 1.204265 -3.694690 -0.143693

O 3.490842 1.825666 -0.928450

O 3.598333 1.713528 0.489338

II-78.28

Fe -1.403895 1.025928 0.033017

Fe 1.674928 0.899164 0.042031

Fe 0.034119 -1.719956 -0.012539

Fe 0.156550 0.047312 2.680951

Fe 0.021051 0.058328 -2.658457

O 1.572863 0.789357 1.946298

O -1.187506 0.898769 2.008421

O 0.066970 -1.518347 1.959194

O 1.412988 0.781880 -1.966180

O -1.318135 0.887900 -1.882270

O -0.059457 -1.534967 -1.925273

O 0.164086 1.895658 0.033591

O 1.632355 -0.915687 -0.039184

O -1.512467 -0.780488 0.056732

O 0.250095 0.055857 4.299870

O -0.052252 0.051655 -4.273746

O 3.105916 1.702574 -0.037203

O -2.776851 1.916120 0.069221

O -0.037923 -3.353957 0.034481

III-77.90

Fe -1.379892 1.092724 -0.030788

Fe 1.648150 0.785383 -0.034991

Fe 0.059410 -1.817841 0.005266

Fe 0.198876 0.060146 2.655089

Fe 0.044769 0.046678 -2.670422

O 1.604924 0.770367 1.845151

O -1.114328 0.965003 2.032010

O 0.054761 -1.512612 1.938580

O 1.450686 0.772186 -1.917964

O -1.290865 0.912194 -1.955111

O -0.068535 -1.522060 -1.919377

O 0.140997 1.944933 0.035909

O 1.665109 -1.044361 -0.047914

O -1.420384 -0.677998 0.040181

O 0.273004 0.048212 4.282754

O 0.042935 0.057920 -4.296755

O -2.784467 1.927966 0.053825

O 0.587350 -3.691402 -0.046830

O -0.807219 -3.815308 0.050384

Fe_5O_{15}

I-81.40

Fe -1.514523 1.012023 -0.029699

Fe 1.625447 0.872896 -0.038818

Fe -0.052373 -1.573780 0.070946

Fe 0.039305 0.202258 2.666397

Fe -0.002918 0.041921 -2.667047

O 1.453042 0.884066 1.922599

O -1.317983 0.997796 1.938674

O -0.045857 -1.409338 1.928912

O 1.421207 0.770302 -1.990500

O -1.352225 0.888660 -1.969159

O -0.057871 -1.501144 -1.824178

O 0.093356 1.837906 -0.047393

O 1.691010 -0.890991 0.036512

O -1.722590 -0.741502 0.047653

O 0.055904 0.257457 4.285464

O -0.038775 -0.046472 -4.284688

O 3.073683 1.638014 -0.059444

O -2.877228 1.920643 -0.046079

O 0.154529 -3.498695 -0.095224

O 0.475868 -4.125466 -1.242774

II-81.20

Fe -1.441532 1.002862 0.031522

Fe 1.646097 0.868353 -0.045317

Fe -0.032195 -1.726914 0.002005

Fe 0.128660 0.057459 2.666668

Fe -0.004811 0.049371 -2.672140

O 1.515388 0.783671 1.910556

O -1.225695 0.898148 1.971009

O 0.043646 -1.515346 1.887118

O 1.421099 0.776631 -1.994469

O -1.329861 0.887448 -1.923123

O -0.056789 -1.522858 -1.879926

O 0.143969 1.865755 -0.027085

O 1.630763 -0.903078 -0.045801

O -1.612718 -0.764929 0.045413

O 0.160780 0.062617 4.287901

O -0.049414 0.052101 -4.293411

O 3.100174 1.613704 -0.063652

O -2.807856 1.900894 0.056374

O 0.572816 -3.696176 0.043922

O -0.825086 -3.589939 0.051562

III-81.00

Fe -1.311035 1.953703 -0.056989

Fe 1.791656 0.888272 -0.155748

Fe 0.777385 -2.158565 -0.062723

Fe -0.160767 -0.113427 2.234592

Fe -0.367494 -0.158348 -2.345630

O 1.293580 0.636854 1.717914

O -1.384069 0.792035 1.326225

O -0.122621 -1.698751 1.399912

O 1.142795 0.566826 -1.969986

O -1.520835 0.877938 -1.492922

O -0.359988 -1.619215 -1.311799

O 0.398437 2.257931 -0.125338

O 2.083402 -0.988852 -0.153555

O -0.368155 -0.260642 3.839503

O -0.663399 -0.465425 -3.912454

O 1.308741 -3.690953 -0.144863

O 3.470481 1.817610 -0.935578

O 3.572288 1.715789 0.481293

O -2.236742 3.477372 0.771048

O -2.337364 3.490390 -0.675183

Fe_5O_{16}

I-84.00

Fe -1.528916 1.070643 -0.072361

Fe 1.593850 0.851229 -0.001668

Fe 0.033440 -1.645922 0.055386

Fe 0.016915 0.163885 2.663613

Fe -0.021674 0.043117 -2.658495

O 1.413031 0.898808 1.894777

O -1.321887 0.989568 2.000785

O -0.041677 -1.419962 1.941504

O 1.358242 0.797922 -1.930590

O -1.396059 0.883249 -1.997705

O -0.061180 -1.509292 -1.835348

O -0.003421 1.917183 -0.028576

O 1.717817 -0.955645 0.025234

O -1.609550 -0.690304 0.040457

O 0.069515 0.165328 4.290976

O -0.039893 -0.047006 -4.278803

O 3.268775 1.833008 -0.109810

O -2.922471 1.929667 -0.047742

O 0.149407 -3.573654 -0.049428

O 0.470421 -4.222161 -1.190357

O 3.837215 2.127484 -1.304818

II-83.79

Fe -1.529811 1.051918 -0.035829

Fe 1.575698 0.883599 -0.043718

Fe 0.029027 -1.823101 -0.018862

Fe 0.043521 0.041003 2.648722

Fe -0.089450 0.045207 -2.666755

O 1.414134 0.798820 1.863018

O -1.310348 0.878304 2.041716

O -0.053153 -1.524170 1.939461

O 1.301432 0.794027 -1.939164

O -1.439137 0.887555 -1.943400

O -0.151672 -1.532715 -1.919957

O -0.018735 1.916470 0.042282

O 1.573782 -0.976323 -0.042692

O -1.494994 -0.713197 0.051742

O 0.175901 0.056491 4.271543

O -0.144771 0.057399 -4.291166

O -2.958502 1.846055 0.051653

O 0.617166 -3.702007 0.043076

O -0.786127 -3.788218 0.050812

O 3.473263 1.304461 -0.057088

O 3.706866 2.653485 -0.048798

Fe -1.476946 0.984591 0.035534

Fe 1.614275 0.876262 -0.048273

Fe -0.007932 -1.741160 0.002596

Fe 0.113569 0.053185 2.668786

Fe -0.025025 0.043918 -2.673864

O 1.480791 0.784777 1.853334

O -1.247894 0.888983 1.985537

O 0.050661 -1.520040 1.905969

O 1.388445 0.778269 -1.940776

O -1.352790 0.878004 -1.930062

O -0.053145 -1.527837 -1.899496

O 0.058825 1.877545 -0.024294

O 1.626520 -0.946631 -0.048784

O -1.596346 -0.786317 0.047436

O 0.151063 0.061399 4.295398

O -0.064725 0.051597 -4.300209

O -2.868655 1.839706 0.058865

O 0.602189 -3.684971 0.048049

O -0.808713 -3.589399 0.047357

O 3.612712 1.131104 -0.056948

O 2.962042 2.386605 -0.055859

Fe_6O

I-22.75

Fe 1.294360 1.351622 -0.052194

Fe 1.294358 -1.351637 -0.052195

Fe -1.063693 1.286448 0.053798

Fe -1.063694 -1.286452 0.053796

Fe -0.157233 -0.000006 1.814485

Fe 0.272395 -0.000005 -1.699284

O 1.730979 -0.000009 1.297902

II-22.47

Fe 1.300957 1.300956 0.090094

Fe 1.098814 -1.163567 -0.052754

Fe -1.163567 1.098814 -0.052754

Fe -1.290695 -1.290695 -0.157766

Fe 0.073727 0.073727 1.821631

Fe -0.078327 -0.078326 -1.828726

O 1.384009 1.384009 1.938026

III-22.40

Fe 0.789047 -0.602749 -0.779658

Fe -1.555551 -0.122455 -1.020216

Fe 0.046950 1.711862 -0.744974

Fe 1.712707 0.471786 1.092044

Fe -0.807081 0.155900 1.176153

Fe 0.172704 2.338353 1.536033

O 0.485019 0.683499 2.595745

Fe_6O_2

I-29.12

Fe 1.183311 1.648846 -0.263121

Fe -1.183456 1.648988 -0.263157

Fe 1.197071 -1.104285 0.384423

Fe -1.197350 -1.103985 0.384647

Fe 0.000046 0.471967 1.805955

Fe -0.000048 -0.046085 -1.503795

O 1.831656 0.564163 1.205029

O -1.831604 0.564657 1.205025

II-28.72

Fe -1.812630 -0.275073 -0.063069

Fe 1.720100 0.399008 0.362529

Fe 0.255644 -1.515750 0.060662

Fe -0.051281 0.468120 1.982236

Fe 0.042434 0.249182 -1.615070

Fe -0.056142 1.932227 0.165707

O -1.070925 -1.085749 1.509224

O -1.817104 0.486107 -1.728545

III-28.72

Fe 1.165850 1.400842 -0.154879

Fe -1.165903 1.400838 0.154866

Fe 1.165848 -1.400845 -0.154881

Fe -1.165906 -1.400838 0.154866

Fe -0.123282 0.000000 1.758899

Fe 0.123225 0.000002 -1.758912

O 1.704120 -0.000007 1.087197

O -1.704177 -0.000003 -1.087212

Fe_6O_3

I-35.64

Fe 1.199557 1.235570 0.785511

Fe -1.265834 1.202622 0.786683

Fe 1.199059 -1.190179 -0.408036

Fe -1.200505 -1.205578 -0.412890

Fe -0.007468 -0.577895 1.927345

Fe -0.016289 0.568113 -1.515891

O 1.825610 -0.519832 1.307663

O -1.841099 -0.569367 1.309901

O -0.046147 2.147403 -0.380048

II-35.73

Fe 1.307075 1.476382 -0.052115

Fe -1.415328 1.434166 -0.052112

Fe 1.917636 -1.072611 -0.052070

Fe -1.935694 -1.133226 -0.052064

Fe -0.023876 -0.371878 1.179917

Fe -0.023887 -0.371904 -1.284098

O 2.875702 0.469199 -0.052109

O -2.949864 0.372604 -0.052064

O -0.072215 2.676566 -0.052094

III-34.74

Fe 1.304973 1.206097 -0.114386

Fe -1.100711 1.380011 -0.159905

Fe 1.304324 -1.207362 -0.038555

Fe -1.101420 -1.372043 -0.061835

Fe -0.088208 0.066069 1.881744

Fe -0.367806 -0.055617 -1.912575

O 1.731768 0.048573 1.508746

O -1.810286 0.049037 1.101035

O 1.518021 -0.051909 -1.636995

Fe_6O_4

I-42.20

Fe 1.298457 1.335346 -0.045424

Fe -1.402921 1.303624 0.157544

Fe 1.404789 -1.123607 -0.362401

Fe -1.088035 -1.152488 -0.051971

Fe 0.058432 0.135286 1.746865

Fe -0.051007 0.041450 -1.971278

O 1.918598 -0.031536 1.171079

O -1.846314 -0.055271 1.428723

O 0.044401 -1.824773 -1.550496

O -0.134869 1.834163 -1.221873

II-42.20

Fe 1.351801 1.303127 0.046281

Fe -1.438963 1.301127 0.057390

Fe 1.352866 -1.407309 0.046010

Fe -1.438055 -1.404988 0.058291

Fe -0.029605 -0.051904 1.582836

Fe -0.049367 -0.052122 -1.397108

O -2.051323 -0.051656 1.273976

O 2.002965 -0.052077 1.233257

O -0.050110 1.965676 -1.093499

O -0.049690 -2.069750 -1.093234

III-41.10

Fe 1.338338 1.101480 0.150654

Fe -1.416035 1.209568 -0.286422

Fe 1.309582 -1.417501 0.182952

Fe -1.444461 -1.309410 -0.254300

Fe -0.065495 -0.167552 1.768358

Fe -0.039935 -0.040597 -1.870499

O 1.793053 -0.050330 1.710732

O -1.827540 -0.043069 1.219138

O 1.722332 -0.164737 -1.322363

O -1.898547 -0.158581 -1.814931

Fe_6O_5

I-47.74

Fe 1.278406 1.516653 0.073582

Fe -1.307360 1.409667 0.045132

Fe 1.193795 -1.338906 -0.059343

Fe -1.195346 -1.410941 -0.062856

Fe -0.039167 0.195978 1.814930

Fe -0.033186 -0.075136 -1.918844

O 1.887051 -0.064062 1.112223

O -1.928385 -0.157539 1.113633

O 0.002857 -1.933354 -1.511279

O 0.035324 1.727609 -1.494446

O -0.041126 2.166926 1.399905

II-47.41

Fe 1.300325 1.190785 -0.298783

Fe -1.265872 1.402620 -0.669593

Fe 2.092273 -0.983444 0.363204

Fe -1.923982 -0.916136 -0.271712

Fe 0.139418 -0.142062 1.713433

Fe -0.097626 -0.295525 -1.945697

O 1.842829 -0.869912 2.145926

O -1.412492 -1.102130 1.416669

O 1.705697 -0.379032 -1.416398

O -2.000709 0.071570 -1.928936

O -0.152829 1.720201 0.809456

III-47.30

Fe 1.829079 1.051937 -0.047421

Fe 1.303140 -1.297288 0.574187

Fe -2.246010 0.684854 -0.432570

Fe -1.200800 -1.628778 -0.369375

Fe -0.372276 0.386127 1.483012

Fe -0.044839 0.198871 -1.614833

O 1.621104 0.357834 1.678373

O -1.939747 1.399754 1.205565

O -0.452875 -1.727371 1.327373

O 1.508238 1.192360 -1.828598

O -1.839037 -0.574599 -1.836602

Fe_6O_6

I-52.92

Fe 1.608347 1.297132 0.216062

Fe -1.486040 1.196058 -0.050245

Fe 1.485950 -1.196054 0.050339

Fe -1.608308 -1.297179 -0.215545

Fe 0.149365 0.168947 1.891517

Fe -0.149436 -0.168986 -1.891243

O 2.034414 -0.180163 1.611165

O -1.632338 -0.287271 1.422236

O 1.632291 0.287675 -1.421799

O -2.034436 0.179785 -1.610962

O -0.047235 2.011681 0.883767

O 0.046962 -2.011682 -0.883581

II-52.92

Fe 0.047173 -0.053935 -0.524355

Fe -0.040985 0.086908 2.568098

Fe 1.397930 2.123340 -0.365004

Fe 1.196154 2.235073 2.760669

Fe -1.404604 2.072934 -0.361603

Fe -1.247553 2.244845 2.754141

O -0.037156 -0.889694 1.060860

O -0.037252 1.401656 3.994535

O 1.815556 2.865968 1.212873

O -1.831003 2.866232 1.189408

O 1.407189 0.680858 -1.494513

O -1.406318 0.582369 -1.423400

III-52.80

Fe 1.258556 1.289046 0.148379

Fe -1.502312 1.409020 0.271967

Fe 1.228253 -1.391766 0.077519

Fe -1.516400 -1.134533 0.054468

Fe 0.634376 -0.051291 2.133555

Fe -0.157168 -0.044232 -1.812948

O 2.344419 -0.080782 0.990858

O -2.865008 0.153233 0.249679

O -0.038970 -1.824835 -1.320650

O -0.072670 1.726574 -1.204400

O -0.159664 1.625621 1.613349

O -0.258195 -1.611349 1.457848

Fe_6O_7

I-57.98

Fe 0.860277 -0.590998 1.614856

Fe -1.643484 -0.575242 1.207411

Fe -0.357767 1.604401 1.372431

Fe 1.499884 -0.697427 -1.320561

Fe -1.507329 -0.816161 -1.414349

Fe 0.191531 1.657671 -1.590368

O -0.587736 0.164990 2.630065

O 1.741667 0.886558 -2.249076

O -1.426700 0.790022 -2.125436

O -0.048687 -1.709686 -1.817968

O -0.056899 2.676434 -0.058892

O 2.053925 -1.180757 0.381129

O -2.665255 -1.303663 -0.147461

II-57.59

Fe 0.682208 -0.435873 0.574193

Fe -1.819627 -0.254858 2.023868

Fe -0.564879 1.824792 1.869919

Fe 1.550899 -0.847697 -1.803943

Fe -1.199828 -0.880671 -1.224525

Fe 0.189163 1.715247 -1.406839

O -2.038935 1.373797 2.858870

O 1.514212 0.859599 -2.338998

O -1.423582 0.888793 -1.587248

O 0.052327 -1.733547 -2.350167

O 0.655986 1.519954 0.481225

O 2.120047 -1.403563 -0.155871

O -1.189734 -1.302926 0.659881

III-57.59

Fe 1.301061 -0.257141 0.293640

Fe -1.376914 -0.577108 1.737637

Fe -0.570889 1.919632 1.682740

Fe 0.960202 -0.981611 -2.133180

Fe -1.535395 -1.207988 -1.389391

Fe 0.170604 1.624717 -1.173689

O -1.533578 0.928208 2.860894

O 0.381052 -1.119699 1.532328

O 1.849155 0.557615 -1.326958

O -0.798944 0.383765 -2.247690

O -0.254853 -2.333863 -2.243194

O -0.371537 2.773019 0.115659

O -2.264845 -1.096637 0.249064

Fe_6O_8

I-62.86

Fe 1.400649 -0.776908 1.553046

Fe -1.698077 -0.968428 1.577016

Fe 0.051756 1.504771 1.236936

Fe 1.400617 -0.776975 -1.553428

Fe -1.698718 -0.968432 -1.580527

Fe 0.051636 1.504686 -1.236906

O 1.643092 1.088388 1.923624

O -1.524455 0.874451 1.722643

O -0.100751 -1.604755 2.151794

O 1.643010 1.088482 -1.923526

O -1.524363 0.874630 -1.723465

O -0.100559 -1.604721 -2.152877

O 2.039831 -1.411127 -0.000206

O -2.360876 -1.528525 -0.001672

II-62.58

Fe 1.273357 1.335857 0.000006

Fe 1.273360 -1.335858 0.000006

Fe -1.273361 1.335855 0.000006

Fe -1.273363 -1.335857 0.000006

Fe -0.000004 0.000001 1.761210

Fe -0.000007 0.000002 -1.761201

O 1.883871 0.000000 1.295706

O -0.000003 1.904793 1.351262

O -1.883881 -0.000001 1.295705

O -0.000002 -1.904792 1.351261

O 1.883866 0.000000 -1.295698

O -0.000004 1.904793 -1.351245

O -1.883881 -0.000001 -1.295698

O -0.000003 -1.904791 -1.351243

III-62.16

Fe 1.202235 1.653708 -0.038148

Fe 1.279849 -1.634515 -0.165253

Fe -1.225840 1.601130 -0.019957

Fe -1.306907 -1.641815 -0.147689

Fe -0.024426 -0.050885 1.916456

Fe -0.043719 -0.114832 -1.721760

O 1.307372 1.306859 1.716660

O -1.399304 1.280731 1.714126

O 1.285218 -1.287543 1.604847

O -1.314644 -1.309371 1.624283

O 1.741331 0.050727 -1.016273

O -0.056194 1.866995 -1.531091

O -1.828825 0.064836 -0.990587

O -0.038049 -2.043956 -1.594471

Fe_6O_9

I-68.10

Fe 1.518752 -0.886416 1.627751

Fe -1.617992 -0.882353 1.582350

Fe -0.011794 1.823705 1.622907

Fe 1.518768 -0.886602 -1.628117

Fe -1.618021 -0.882325 -1.583635

Fe -0.011617 1.823837 -1.622888

O 1.503596 0.892401 2.152920

O -1.504117 0.871820 2.009722

O -0.058294 -1.685645 2.021109

O 1.503748 0.892345 -2.153010

O -1.504147 0.872259 -2.009623

O -0.058123 -1.685596 -2.022096

O -0.057949 2.598732 0.000015

O 2.145814 -1.322793 -0.000225

O -2.364509 -1.307632 -0.000625

II-66.75

Fe 0.998659 1.986543 0.041022

Fe 1.404367 -1.143772 -0.152329

Fe -2.233549 0.462241 -0.238767

Fe -1.130053 -2.025138 0.671158

Fe 0.591971 0.588645 2.018533

Fe 0.154233 -0.117942 -2.031962

O 1.175716 2.349171 1.921934

O 0.747908 1.546528 -1.717254

O 0.373724 -1.303858 1.601800

O -0.186897 -1.938218 -0.983570

O 2.122385 0.322544 0.595540

O 1.856196 -0.882848 -1.868955

O -2.650282 -1.044348 0.675676

O -1.600928 0.261144 -1.927038

O -0.870935 1.290641 0.688130

III-66.30

Fe 1.067995 1.610158 0.124986

Fe 1.423231 -1.004030 0.034363

Fe -1.388128 1.258659 0.153281

Fe -1.003638 -1.339402 0.062350

Fe 0.148582 -0.484644 2.480266

Fe -0.041913 0.014665 -2.017185

O 1.537229 0.270239 1.477750

O -0.279375 2.383125 1.086603

O -1.422130 -0.147259 1.518186

O 0.342369 -2.009533 1.305075

O 1.931355 0.380673 -1.106131

O -0.244092 1.853566 -1.304112

O -1.942447 -0.160831 -1.060936

O 0.284512 -1.818860 -1.302733

O 0.159395 -0.380114 4.080407

Fe_6O_{10}

I-72.16

Fe 2.227386 0.162301 -0.414852

Fe -1.928854 0.057920 0.040236

Fe 0.263143 2.229935 -0.427982

Fe -0.049468 -1.911487 0.049794

Fe -0.347405 -0.283420 2.449530

Fe 1.992232 1.930502 2.143273

O 1.585694 1.510894 -1.404383

O 1.609245 -1.476019 -0.568209

O -1.403558 1.690291 -0.574760

O -1.709572 -1.616083 -0.674190

O 0.884058 0.890404 3.056038

O 0.049180 -1.941942 1.839778

O -1.989235 0.161978 1.828519

O 2.966629 2.857827 3.074137

O 1.008147 2.958035 0.977241

O 2.974513 0.888168 0.988976

II-71.36

Fe 0.770891 1.826703 -0.014911

Fe 2.032163 -1.311487 -0.092651

Fe -1.738969 1.623962 0.363932

Fe -2.105465 -1.206511 -0.048500

Fe 0.050856 -0.047700 1.872201

Fe 0.157299 -0.476284 -1.711515

O 1.245310 1.410436 1.674021

O -1.396904 1.099323 2.065027

O 1.508392 -1.132872 1.609672

O -1.092126 -1.426908 1.420770

O 1.715394 0.471496 -0.890859

O -0.587460 1.210398 -1.320563

O 1.306068 -1.913592 -1.709225

O -1.398490 -1.407684 -1.746558

O -0.539502 3.032323 0.366961

O -2.965558 0.381763 -0.065397

III-71.20

Fe 2.129694 1.193300 0.245325

Fe 1.196568 -1.466980 -0.057603

Fe -2.043431 1.003202 -0.312512

Fe -1.537539 -1.819495 0.679425

Fe 0.076898 0.157049 1.923686

Fe 0.264304 0.783897 -2.132161

O 1.510528 1.398267 1.897015

O -1.142273 1.399073 1.212281

O 1.213155 -1.251194 1.747022

O -1.305918 -1.059027 2.257236

O 1.506270 1.817939 -1.294957

O -1.410524 1.410622 -1.944180

O 0.686864 -0.948650 -1.793093

O -0.173758 -2.771632 0.058800

O 2.741206 -0.414658 -0.161805

O -2.632172 -0.710046 -0.169461

Fe_6O_{11}

I-75.82

Fe 1.517438 -0.881246 1.543267

Fe -1.615418 -0.870720 1.578356

Fe -0.034950 2.030081 1.828070

Fe 1.677205 -1.054303 -1.731243

Fe -1.615722 -0.843915 -1.497755

Fe 0.050373 1.819054 -1.443238

O 1.292456 0.867547 2.015506

O -1.419634 0.894378 1.896517

O -0.044035 -1.621159 2.016381

O 1.402800 0.688115 -1.915944

O -1.406637 0.889516 -1.918401

O -0.020809 -1.623505 -1.809187

O 0.042592 2.634689 0.144350

O 2.213038 -1.311286 -0.043073

O -2.436259 -1.305474 0.036957

O -0.151181 3.278017 2.877417

O 2.673018 -1.817946 -2.777645

II-75.82

Fe 1.546317 -0.994981 1.421940

Fe -1.621322 -0.879035 1.545084

Fe -0.055117 1.957997 1.629431

Fe 1.548395 -0.992478 -1.524440

Fe -1.620574 -0.877810 -1.650187

Fe -0.054678 1.959635 -1.731708

O 1.297368 0.792074 1.507867

O -1.393034 0.873314 2.007107

O -0.042741 -1.650796 1.919123

O 1.298745 0.794434 -1.610400

O -1.392108 0.874809 -2.110995

O -0.040642 -1.647205 -2.022693

O -0.383115 2.447561 -0.051138

O 2.377139 -1.621555 -0.051274

O -2.346815 -1.273721 -0.052912

O 0.260061 3.175111 2.665444

O 0.260452 3.176762 -2.767823

III-74.97

Fe 1.417662 1.490985 0.050426

Fe 2.068259 -1.098694 0.051640

Fe -1.413112 1.490804 0.051080

Fe -2.064460 -1.098763 0.052543

Fe 0.002113 -0.052230 1.846544

Fe 0.002266 -0.053644 -1.744071

O 1.297439 1.200571 1.902470

O -1.293159 1.201133 1.902891

O 1.315567 -1.488909 1.536628

O -1.312889 -1.488522 1.538307

O 1.297456 1.199264 -1.801876

O -1.293352 1.199223 -1.801017

O 1.316013 -1.490365 -1.433262

O -1.312539 -1.489887 -1.432504

O 0.002466 2.647584 0.050734

O 2.993173 0.342874 0.051342

O -2.988907 0.342987 0.051782

Fe_6O_{12}

I-79.56

Fe 1.579546 -0.882224 1.604881

Fe -1.670175 -0.855959 1.700120

Fe -0.043162 1.900741 1.481898

Fe 1.652574 -0.980919 -1.613420

Fe -1.598279 -0.946995 -1.405555

Fe -0.146681 1.849983 -1.615683

O 1.376967 0.868869 1.840273

O -1.435002 0.888692 1.951006

O -0.055666 -1.385552 1.094176

O 1.300208 0.746309 -1.833524

O -1.513509 0.745365 -1.993712

O 0.012058 -1.631602 -1.818995

O -0.158160 2.773040 -0.066038

O 2.361498 -1.085279 0.052544

O -2.503180 -1.096011 0.154493

O 2.740544 -1.719642 -2.590094

O 2.118754 -1.734064 2.864680

O -2.148304 -1.719293 2.982313

II-77.76

Fe 1.430149 2.063682 0.272496

Fe -1.539192 2.021201 -0.028435

Fe 1.925846 -0.719542 0.259067

Fe -2.097998 -0.711494 0.129659

Fe 0.168158 -2.893737 0.563355

Fe -0.469650 0.682962 2.074967

O -0.045682 2.957402 -0.346160

O 2.892558 0.787850 0.242294

O -2.955239 0.878693 -0.255313

O 1.692133 -2.455336 -0.260418

O -1.329264 -2.330243 -0.158423

O 0.985532 1.726951 2.017628

O -1.623657 2.083364 1.783612

O 0.635512 -0.803619 1.519922

O -1.871279 -0.550548 1.926518

O 0.156869 -3.903569 1.839853

O 0.755115 0.474463 -0.998795

O -0.725461 0.431765 -1.101228

III-77.58

Fe 1.440056 1.433862 0.077631

Fe 1.397320 -1.494400 0.018436

Fe -1.396469 1.495991 -0.016898

Fe -1.437987 -1.431443 -0.075617

Fe 0.021034 -0.040464 2.034893

Fe -0.018823 0.042286 -2.033693

O 1.326060 1.275357 1.924883

O -1.272871 1.287357 1.828717

O 1.288364 -1.391327 1.868078

O -1.313642 -1.309475 1.778007

O 1.315774 1.311094 -1.775857

O -1.285749 1.393682 -1.866508

O 1.274411 -1.286018 -1.827577

O -1.324368 -1.272599 -1.923409

O 0.047659 2.662040 0.052657

O -0.046656 -2.660666 -0.051478

O 2.568117 -0.047443 0.050467

O -2.567045 0.048966 -0.049529

Fe_6O_{13}

I-83.41

Fe 1.260134 -0.866836 1.525410

Fe -1.953778 -0.774526 1.821452

Fe -0.260786 2.019234 1.713806

Fe 1.720559 -1.097639 -1.646584

Fe -1.399536 -1.238184 -0.978057

Fe -0.192668 1.581375 -1.435769

O 1.119553 0.870915 1.627727

O -1.701589 0.965754 1.929288

O -0.400540 -1.293948 0.946489

O 1.292644 0.603981 -1.836905

O -1.485046 0.397161 -1.715324

O 0.128498 -1.880640 -1.714347

O -0.343760 2.588624 0.051091

O 2.207064 -1.209342 0.049692

O -2.755010 -1.223609 0.316981

O -0.073860 3.048926 2.953676

O 2.735629 -1.717398 -2.756541

O 1.620923 -1.720481 2.850076

O -2.240454 -1.619588 3.166072

II-83.22

Fe 1.392363 -1.022573 1.517147

Fe -1.921239 -0.778980 1.779284

Fe -0.042809 1.821938 1.620700

Fe 1.832198 -0.977049 -1.673664

Fe -1.254834 -1.147480 -0.989929

Fe -0.059633 1.820197 -1.602532

O 1.280828 0.655035 2.051018

O -1.551542 0.925443 2.034321

O -0.281236 -1.211715 0.859665

O 1.380162 0.738241 -1.744684

O -1.310472 0.572755 -1.524037

O 0.237912 -1.735969 -1.802980

O -0.035253 2.582251 -0.000462

O 2.333017 -1.172332 0.047871

O -2.657699 -1.213796 0.254268

O 2.973530 -1.609044 -2.668251

O -0.238788 2.826868 -2.870573

O 1.731018 -2.131461 2.644631

O -2.127300 -1.720505 3.082163

III-83.22

Fe 1.516340 -0.988683 1.743435

Fe -1.715753 -0.877054 1.709065

Fe -0.050760 1.909997 1.689325

Fe 1.559048 -1.018646 -1.511267

Fe -1.683229 -0.906673 -1.533814

Fe -0.033063 1.875655 -1.571098

O 1.198476 0.705096 1.316246

O -1.436200 0.878790 2.036231

O -0.102165 -1.607794 2.055379

O 1.226295 0.689821 -1.172359

O -1.416102 0.839952 -1.911194

O -0.058159 -1.629367 -1.844813

O -0.366469 2.548413 0.050639

O 1.932096 -1.623526 0.128252

O -2.363655 -1.268737 0.083381

O 0.358809 2.957661 2.858925

O 2.654425 -1.287149 -2.678235

O 0.369914 2.900699 -2.762628

O 2.567863 -1.193777 2.963094

Fe_6O_{14}

I-86.80

Fe 1.626197 -0.988129 1.687560

Fe -1.517942 -0.888962 1.332668

Fe -0.035797 1.949494 1.760473

Fe 1.476953 -0.983773 -1.504682

Fe -1.793597 -0.848867 -1.630770

Fe -0.053473 1.929391 -1.508006

O 1.299073 0.758271 1.807631

O -1.412114 0.840540 1.811577

O -0.010857 -1.633382 1.935371

O 1.301059 0.764426 -1.505199

O -1.511529 0.884924 -1.516920

O -0.192612 -1.518515 -1.182897

O -0.061930 2.640799 0.137051

O 2.235288 -1.390787 0.034816

O -2.565085 -1.290371 -0.084389

O -0.044795 3.018521 2.980089

O 2.112370 -1.615793 -2.853317

O 0.049782 2.839127 -2.859535

O 2.779179 -1.620239 2.668534

O -2.449256 -1.425829 -2.984953

II-85.00

Fe 1.460069 1.538875 0.084737

Fe 1.447557 -1.534048 -0.105519

Fe -1.424236 1.403984 0.013151

Fe -1.411244 -1.505606 -0.058383

Fe 0.053653 0.168437 2.137826

Fe 0.062075 -0.168185 -2.181334

O 1.719027 0.087652 1.192348

O 0.063699 1.893886 1.328960

O -1.715271 0.077317 1.228679

O 0.027424 -1.621060 1.074743

O 1.713304 -0.140804 -1.280660

O 0.033239 1.598637 -1.092985

O -1.719114 -0.081617 -1.186430

O 0.004785 -1.918128 -1.330240

O 2.665843 2.560218 -0.181650

O 2.658077 -2.559355 0.156798

O -2.442846 2.659604 0.048840

O -2.625223 -2.542774 0.156416

O -0.369607 -0.270690 3.638099

O -0.358191 0.356286 -3.654245

III-83.00

Fe 1.389102 1.492869 -0.076818

Fe 1.387783 -1.492584 0.072424

Fe -1.407646 1.443294 -0.040098

Fe -1.309113 -1.514353 -0.019609

Fe -0.072713 0.229956 2.354889

Fe -0.024719 -0.008584 -2.362909

O 1.285607 1.203275 1.837681

O -1.408956 1.290196 1.832898

O 1.122724 -1.417527 1.840037

O -0.977220 -1.319991 1.799327

O 1.295058 1.413935 -1.828038

O -1.150637 1.311428 -1.844246

O 1.266815 -1.113205 -1.815508

O -1.268379 -1.289380 -1.899835

O -0.148304 0.275456 3.988511

O -0.047493 -0.036063 -3.994093

O 2.458212 -0.022481 0.038898

O -2.452852 -0.100057 -0.055254

O -0.040917 2.650164 0.129665

O 0.049507 -2.740294 -0.154698

Fe_6O_{15}

I-90.30

Fe 1.600915 -0.979272 1.666782

Fe -1.683662 -0.952794 1.661563

Fe -0.047243 1.907796 1.647754

Fe 1.600721 -0.979953 -1.559266

Fe -1.684419 -0.953322 -1.555043

Fe -0.047348 1.906820 -1.543140

O 1.299370 0.765547 1.715938

O -1.416956 0.796432 1.620786

O -0.047391 -1.614915 1.599159

O 1.299493 0.764825 -1.610579

O -1.417358 0.795914 -1.515740

O -0.047952 -1.615334 -1.493529

O -0.030834 2.695990 0.052052

O 2.265832 -1.317600 0.053696

O -2.343965 -1.321641 0.053437

O -0.059154 2.997959 2.865722

O 2.445102 -1.510368 -2.841427

O -0.059021 2.996333 -2.761757

O 2.444926 -1.509155 2.949358

O -2.521323 -1.412747 -2.861218

O -2.519336 -1.412633 2.968267

II-89.46

Fe 1.675435 -1.047703 1.682975

Fe -1.472745 -0.998519 1.195890

Fe -0.052741 1.833437 1.756140

Fe 1.608006 -0.962998 -1.538252

Fe -1.656406 -0.893371 -1.788325

Fe 0.017203 1.917622 -1.486890

O 1.309273 0.663789 1.525744

O -1.418095 0.641401 1.834190

O 0.044115 -1.731191 1.815385

O 1.374478 0.783218 -1.395497

O -1.404390 0.840908 -1.525050

O -0.059745 -1.586431 -1.402555

O -0.053010 2.643198 0.099612

O 2.264041 -1.434184 0.054117

O -2.451860 -1.389040 -0.273515

O 2.331839 -1.423051 -2.911612

O 0.064974 2.884460 -2.787335

O 2.563432 -1.509384 2.962039

O -2.325586 -1.320149 -3.192160

O -0.784083 3.300298 2.791125

O 0.380364 2.772448 3.467261

III-89.46

Fe 1.513151 -0.956738 1.614026

Fe -1.747973 -0.893272 1.724775

Fe -0.053546 1.975668 1.722489

Fe 1.728121 -0.993663 -1.616413

Fe -1.500965 -0.962317 -1.319813

Fe 0.040512 1.898283 -1.535446

O 1.296112 0.771869 1.498114

O -1.499659 0.815215 1.715733

O -0.110024 -1.597931 1.403933

O 1.395114 0.750000 -1.511320

O -1.334705 0.781804 -1.607187

O 0.062285 -1.616622 -1.806392

O -0.057176 2.666231 0.038677

O 2.224318 -1.400370 0.042837

O -2.466401 -1.318692 0.161034

O 2.654481 -1.500583 -2.856869

O 0.077830 2.874650 -2.836613

O 2.239589 -1.424341 2.975895

O -2.421422 -1.512754 3.061080

O -0.682323 3.447220 2.772671

O 0.270304 2.581169 3.496435

Fe_6O_{16}

I-93.06

Fe 1.595421 -1.012436 1.652460

Fe -1.662378 -1.024184 1.573261

Fe -0.052080 1.894129 1.720340

Fe 1.664001 -0.958109 -1.549747

Fe -1.588028 -0.970720 -1.596436

Fe 0.011078 1.889197 -1.533823

O 1.327762 0.701998 1.621113

O -1.431500 0.688033 1.507707

O -0.024162 -1.692458 1.404016

O 1.405753 0.783748 -1.539514

O -1.377322 0.782992 -1.422087

O 0.029448 -1.616997 -1.302157

O 0.058995 2.633270 0.044128

O 2.343032 -1.296521 0.052408

O -2.341062 -1.393846 -0.037756

O 2.334924 -1.611946 -2.864402

O -0.054346 2.855810 -2.826724

O 2.350262 -1.616647 2.941806

O -2.298347 -1.414092 -2.973504

O -2.472253 -1.514971 2.889029

O -0.781609 3.322595 2.756954

O 0.052930 2.390377 3.544246

II-92.84

Fe 1.614726 -1.007123 1.696522

Fe -1.666022 -0.941715 1.644449

Fe -0.053332 1.930090 1.714337

Fe 1.603152 -0.966818 -1.548477

Fe -1.666165 -0.936867 -1.540464

Fe -0.039554 1.915107 -1.548091

O 1.293209 0.706872 1.826127

O -1.443119 0.813396 1.605595

O -0.043601 -1.629747 1.505120

O 1.307421 0.786461 -1.515332

O -1.426166 0.804203 -1.416141

O -0.047563 -1.611350 -1.380287

O -0.037033 2.662103 0.023110

O 2.269426 -1.308288 0.089414

O -2.366179 -1.305098 0.059227

O 2.317366 -1.392163 -2.955458

O -0.060867 2.868013 -2.861272

O 2.361046 -1.631866 2.989269

O -2.453004 -1.416846 -2.864039

O -2.448693 -1.418491 2.974154

O 0.800948 3.494922 2.749527

O -0.439869 3.047249 3.293625

CATIONIC OXIDES

Fe_2O^+

I-9.45

Fe 1.157724 -0.034129 -0.000024

Fe -1.158159 -0.034754 0.000025

O -0.000818 1.410229 0.000000

II-9.45

Fe 1.822237 -0.052086 -0.085272

Fe -1.753290 -0.052137 -0.156060

O 0.054647 -0.051754 -0.054787

$Fe_2O_2^+$

I-14.36

Fe 1.271957 0.000002 0.000000

Fe -1.375654 0.000000 0.000001

O -0.051881 1.339129 0.000001

O -0.051879 -1.339127 0.000002

II-13.88

Fe 0.897664 -0.000024 -0.000006

Fe -2.661386 0.000024 0.000005

O -0.872797 -0.000027 -0.000005

O 2.544574 0.000009 0.000003

III-11.80

Fe 1.191339 -0.222733 -0.051933

Fe -1.246445 -0.262244 0.052182

O 1.313624 1.412067 -0.052249

O -1.290304 1.408594 0.051875

$Fe_2O_3^+$

I-18.20

Fe 0.480148 0.371193 1.157696

Fe 0.261768 0.264479 -1.444645

O 1.402566 -0.478131 -0.147461

O -0.481518 1.299716 -0.059840

O -0.067765 -0.275497 2.573868

II-17.80

Fe 0.994395 0.052082 -0.048485

Fe -1.348819 0.052064 -0.057276

O 0.066383 0.052089 1.414916

O 0.035104 -1.212590 -0.778692

O 0.035082 1.316721 -0.778717

III-17.05

Fe 1.931587 -0.614227 -0.054021

Fe -1.500929 0.194378 -0.262489

O 0.237426 -0.066308 -0.252649

O 2.856557 -1.092109 -1.327588

O 2.640003 -0.777247 1.421913

$Fe_2O_4^+$

I-21.78

Fe -0.256360 -0.048861 1.291416

Fe -0.117564 -0.106233 -1.282354

O 0.160525 -1.305230 0.055296

O -0.678114 1.099888 -0.044479

O 0.776253 0.151744 -2.632062

O 0.775757 0.361920 2.454076

II-19.44

Fe -0.467840 0.882095 1.018421

Fe 1.198995 -0.882226 -1.339919

O 2.586499 0.051163 -1.408523

O -0.792195 2.371988 0.477180

O -0.066401 -0.287048 -0.253857

O -0.258199 0.368558 2.537217

III-21.24

Fe 1.191270 0.155511 0.054022

Fe -1.508354 -0.153299 0.021177

O -0.269424 1.218401 0.047486

O -0.126692 -1.327008 0.052743

O 2.984035 0.696800 0.053858

O 2.849647 -0.781134 -0.054177

$Fe_2O_5^+$

I-25.20

Fe 0.458638 0.868557 1.292433

Fe -0.114824 -0.469696 -0.885378

O 1.308415 -0.349282 0.280326

O -0.986393 0.703564 0.239785

O -0.786192 -1.934752 -0.872772

O 0.366550 0.765202 2.913413

O 0.251815 0.259570 -2.285137

II-24.92

Fe 0.060968 0.609335 1.098649

Fe 0.124469 0.009442 -1.446904

O 0.251541 1.525511 -0.489028

O -1.277123 1.091246 1.920658

O -0.262967 -0.883668 0.064891

O 1.383220 0.564004 2.036407

O 1.098579 -0.469890 -2.646604

$Fe_2O_6^+$

I-28.00

Fe 0.273132 0.603959 1.096485

Fe 0.006275 -0.328426 -1.376028

O 0.043399 1.301441 -0.567465

O -1.029187 0.807643 2.033746

O 0.264825 -1.022288 0.284183

O -1.466549 -0.681141 -1.944559

O 1.722202 0.975701 1.713022

O 1.284384 -0.564143 -2.339848

II-28.48

Fe 1.208912 0.257128 -0.019398

Fe -1.509478 0.366233 0.014980

O -0.043526 1.502507 0.265543

O -0.148407 -0.884453 -0.262122

O 3.078497 0.920610 -0.176190

O 3.064916 -0.490458 0.067710

O -3.189302 1.173249 -0.253056

O -3.285140 -0.222051 0.251315

Fe_3O^+

I-13.16

Fe 1.505325 0.370993 0.159526

Fe -0.468295 0.888334 -1.021585

Fe 0.474208 2.334120 0.980925

O -0.988084 2.436466 -0.147964

II-12.84

Fe 1.192634 -0.051537 -0.013850

Fe -1.134091 -0.060648 -0.162658

Fe -0.155214 2.034233 -0.259625

O -0.033277 0.792108 1.214815

III-12.56

Fe 1.090669 0.052450 -0.052297

Fe -1.136755 0.045080 -0.051772

Fe -0.021745 3.497537 -0.052217

O -0.035438 1.662160 -0.052141

$Fe_3O_2^+$

I-18.90

Fe 1.405546 0.085126 0.057337

Fe -1.237421 0.050452 -0.155328

Fe -0.151540 2.234134 -0.154634

O 0.045490 -1.197757 0.044796

O 1.612918 1.943554 0.045319

II-18.20

Fe 1.096202 -0.157169 0.155602

Fe -1.403295 -0.053884 0.050093

Fe -0.052979 2.035036 -0.156623

O -0.159277 0.994933 1.348520

O -0.173009 -1.312680 -0.574310

III-18.45

Fe 1.158120 0.048134 -0.047848

Fe -1.262885 0.048290 -0.047840

Fe -0.052155 2.137238 -0.102903

O -0.052281 0.782395 1.383455

O -0.052350 0.697710 -1.513739

$Fe_3O_3^+$

I-24.78

Fe 1.302862 0.013571 0.056599

Fe -1.237816 -0.052587 0.057379

Fe -0.037699 2.762113 0.167187

O 0.065026 -1.326970 -0.060511

O 1.493093 1.825363 0.142498

O -1.516283 1.746551 0.143225

II-22.32

Fe 1.161895 0.046157 0.041694

Fe -1.266038 0.046118 0.041693

Fe -0.052063 2.442555 -0.040218

O -0.052075 1.016869 1.232666

O -0.052098 -1.182839 -0.657653

O -0.052083 2.972113 -1.624301

III-22.74

Fe 0.986575 0.054050 0.013616

Fe 4.532777 -0.050418 -0.049668

Fe -2.657411 0.051857 -0.050644

O -0.757111 0.052735 -0.046873

O 2.793298 0.044133 0.043350

O -4.356844 0.051869 0.048360

$Fe_3O_4^+$

I-28.70

Fe 1.350877 0.567285 0.258606

Fe -1.439187 0.685128 0.788050

Fe -0.467986 1.736662 -1.589920

O 0.044971 -0.370213 1.104072

O 1.114829 0.785923 -1.529051

O -2.020608 0.866963 -0.989502

O -0.062966 2.094338 0.354904

II-28.56

Fe 1.472588 0.168570 -0.250892

Fe -1.608463 -0.247688 -0.087960

Fe -0.050360 2.521922 0.244582

O 0.045500 -0.928987 -0.264448

O 1.440168 1.698286 0.783817

O -1.448337 1.493061 0.479254

O 0.044742 3.701150 -0.890115

III-28.56

Fe 0.460181 -0.582580 -1.412968

Fe -0.777044 -0.598388 1.098825

Fe 0.676441 1.817529 0.049816

O 0.033842 2.026103 1.800495

O 1.103389 1.121753 -1.583526

O -0.775119 0.871926 2.259067

O -0.471106 -1.713288 -0.314664

$Fe_3O_5^+$

I-32.00

Fe 1.439962 0.261535 -0.682658

Fe -0.847132 -0.879581 0.794467

Fe -0.779565 2.033570 -0.141950

O -1.723689 0.664946 0.472832

O 0.472191 1.719721 -1.333971

O -0.684429 3.369516 0.768300

O -1.845683 -2.137811 1.180033

O 0.790979 -1.200495 0.162475

II-31.28

Fe 1.309288 0.249967 0.069063

Fe -1.321917 0.473271 0.656522

Fe -0.384496 1.517514 -1.578398

O 0.052790 -0.455625 1.381183

O 1.399843 1.301352 -1.512409

O -2.027848 1.411113 -0.780938

O -0.020557 1.815004 0.468047

O -0.345120 -0.292149 -1.086927

III-29.84

Fe 1.399553 0.567335 0.190691

Fe -0.977997 -0.399044 -0.265484

Fe -0.660281 2.237674 0.011836

O -0.392931 0.790477 1.144705

O 0.143008 1.080881 -1.186747

O -1.205519 3.742819 0.053051

O 2.686123 -0.358676 -0.284605

O -1.309780 -1.932102 0.263422

$Fe_3O_6^+$

I-35.64

Fe 1.707372 0.058088 -0.788494

Fe -1.124347 -0.992931 0.359977

Fe -0.751656 2.129441 -0.260660

O -1.721611 0.641933 -0.095844

O 0.790765 1.530577 -0.971479

O -0.763051 3.191585 0.992507

O 3.178684 -0.042341 -0.147713

O -1.510565 -1.809167 1.743704

O 0.457520 -1.122415 -0.472347

II-35.64

Fe 1.096189 0.018419 1.303463

Fe -0.665708 -0.155075 -1.349046

Fe 0.053342 2.757431 0.044912

O 1.072386 1.796955 1.204514

O 0.768821 -0.584772 -0.303721

O -0.578077 1.620446 -1.190147

O -2.024399 -0.667056 -0.569416

O 1.306691 -0.869860 2.650113

O -0.472013 -0.773627 -2.838626

III-34.56

Fe 1.246184 0.367072 0.049212

Fe -1.370368 0.354646 0.482619

Fe -0.461984 1.616954 -1.591763

O 0.028232 -0.372819 1.318098

O 1.502829 1.392729 -1.393827

O -2.135661 1.301676 -0.913971

O -0.151948 1.857398 0.352309

O -0.257727 -0.250896 -1.114690

O -0.474881 2.454555 -2.978597

$Fe_3O_7^+$

I-39.60

Fe 1.415632 -0.881605 0.365964

Fe -1.418346 -0.861426 -0.055579

Fe -0.061141 1.507312 -0.080381

O 1.515507 0.754114 -0.458460

O -1.406262 0.698423 -0.964219

O 0.033541 -1.834112 -0.386937

O -0.163160 2.970672 0.556136

O 2.772239 -1.738317 0.048657

O -2.737054 -1.510576 0.574471

O -0.266093 0.065903 1.112069

II-38.80

Fe 1.749285 0.157200 -0.894313

Fe -1.092698 -1.100994 0.369857

Fe -0.963255 1.951640 -0.483475

O -1.809696 0.413687 -0.166004

O 0.564833 1.540770 -1.214703

O -0.994069 3.176091 0.600098

O 3.489743 -0.549746 -1.095343

O -1.508292 -1.820251 1.745308

O 0.526944 -1.020894 -0.263011

O 3.480071 0.923014 -1.188983

III-38.10

Fe 1.228232 0.367064 0.170894

Fe -1.402798 0.372792 0.670353

Fe -0.496545 1.631380 -1.508276

O 0.053151 -0.407118 1.408068

O 1.328531 1.612081 -1.190228

O -2.153772 1.197238 -0.757855

O -0.261782 1.816634 0.573348

O -0.171109 -0.193584 -1.006550

O -0.771944 2.230044 -2.986068

O 2.664396 -0.355367 0.354245

$Fe_3O_8^+$

I-41.47

Fe 1.308503 0.258195 0.053575

Fe -1.369486 0.195036 0.533130

Fe -0.366556 1.506071 -1.640933

O 0.147778 -0.273950 1.406623

O 1.369211 0.881133 -1.677380

O -1.986043 1.295187 -0.782441

O 0.161473 1.764887 0.157704

O -0.380143 -0.450210 -0.898095

O -0.578775 2.655619 -2.750431

O 2.778254 0.063858 0.683814

O -2.594288 -0.673821 1.097420

II-41.91

Fe 1.728326 -1.340578 0.162934

Fe -1.664699 -1.300345 0.163401

Fe 0.045491 1.430633 0.385901

O 1.469410 0.461143 0.564808

O -1.392903 0.473675 0.575539

O 0.037065 -1.829867 0.263317

O 0.047432 2.812427 -0.483547

O 2.979080 -2.708392 -0.164727

O 3.594466 -1.389013 -0.361902

O -2.953605 -2.631981 -0.160020

O -3.409184 -1.288679 -0.579490

III-40.70

Fe 1.200121 -0.222585 0.047921

Fe -1.414713 -0.157525 -0.007041

Fe 0.045567 2.227691 -0.042737

O 0.556809 -1.917127 0.068606

O -0.903352 -1.938513 0.048542

O 2.349285 1.152950 0.052109

O 1.931482 2.557057 0.048820

O -2.400492 1.364373 -0.056240

O -1.805086 2.690041 -0.050830

O -0.044899 0.563342 1.201119

O 0.008833 0.488464 -1.200203

$Fe_3O_9^+$

I-44.40

Fe 1.218056 0.056754 0.247866

Fe -1.453483 0.255330 0.677054

Fe -0.341919 1.509077 -1.376610

O 0.047538 -0.571111 1.450608

O 1.405596 0.971587 -1.430905

O -2.021735 1.426933 -0.579500

O 0.131968 1.618016 0.480623

O -0.461614 -0.370110 -0.866812

O -0.788025 1.754413 -3.285230

O 2.759839 -0.146530 0.670321

O -2.770946 -0.370245 1.394506

O -0.466130 2.986513 -2.661964

II-44.88

Fe 1.733704 -1.402937 -0.008992

Fe -1.635149 -1.404943 -0.010231

Fe 0.048330 1.529058 0.028559

O 1.408072 0.386205 0.051367

O -1.308100 0.378777 0.051172

O 0.047319 -2.036351 -0.057629

O 0.748931 3.377703 -0.050156

O -0.692735 3.369897 -0.050313

O 2.952418 -2.873900 -0.049622

O 3.656643 -1.585432 0.049354

O -2.861614 -2.874753 -0.049451

O -3.567174 -1.591232 0.048581

III-43.32

Fe 1.718031 -1.352135 0.052505

Fe -1.620757 -1.335186 0.053179

Fe 0.058396 1.510171 0.024712

O 0.041250 3.284654 -0.054346

O 0.056055 4.648782 0.053971

O -4.350174 -2.859321 -0.059659

O -3.137475 -2.239452 0.062560

O 4.263591 -3.172202 0.049118

O 3.201268 -2.311285 0.054910

O 0.048050 -2.034405 0.051925

O 1.520447 0.444623 0.049694

O -1.416733 0.455721 0.048919

Fe_4O^+

I-16.95

Fe 1.195710 -0.157966 -0.019568

Fe -1.257138 -0.046458 0.151729

Fe 0.047351 1.196273 1.826176

Fe -0.150278 -1.255186 1.722760

O 1.610880 1.392971 0.879019

II-17.00

Fe 1.211953 0.062018 0.045687

Fe -1.211909 0.061969 0.045719

Fe 0.000032 1.142073 1.852107

Fe 0.000067 -1.199982 1.617415

O -0.000015 1.599895 -0.050827

III-16.00

Fe 1.901074 -0.177031 -0.000027

Fe -1.620765 0.057794 -0.000024

Fe -0.177033 1.900934 0.000000

Fe 0.057828 -1.620659 0.000082

O 1.636048 1.635962 -0.000063

$Fe_4O_2^+$

I-22.62

Fe 1.097202 -0.051430 -0.045001

Fe -1.201222 -0.051551 -0.045217

Fe -0.052141 1.233010 1.814030

Fe -0.052229 -1.273876 1.713226

O -0.051946 1.615282 -0.050269

O -0.052177 -0.054051 3.132619

II-22.44

Fe 1.375203 0.159763 -0.260253

Fe -1.305437 0.153788 -0.101382

Fe -0.014534 1.306810 1.728857

Fe -0.155847 -1.077054 1.601997

O -0.041154 -0.164250 -1.410398

O 1.716059 1.389647 1.084386

III-22.20

Fe 1.200189 0.010119 -0.799975

Fe -1.302551 -0.052450 -0.676014

Fe -0.056954 2.133481 0.262889

Fe 0.155250 -1.753991 0.369224

O 1.681884 1.622988 -0.036767

O -1.800658 1.560402 0.049133

$Fe_4O_3^+$

I-28.49

Fe 1.220308 -0.674720 0.163298

Fe -1.324414 -0.674714 0.163277

Fe -0.052029 1.362344 1.711985

Fe -0.052022 -0.953755 2.352585

O 1.535054 0.250240 1.818554

O -1.639248 0.250222 1.818538

O -0.052021 -1.080322 -1.103715

II-28.49

Fe 1.643119 0.166398 0.372058

Fe -0.690109 -0.563051 0.076391

Fe -0.120259 1.297583 1.925397

Fe 0.259815 -1.261669 2.242928

O -0.467589 0.067628 3.273384

O 1.298750 1.892429 0.886475

O 0.899872 -1.635942 0.440199

III-27.09

Fe 1.508751 -0.052296 -0.149560

Fe -1.293724 -0.052768 0.015933

Fe -0.050184 1.205568 1.821519

Fe -0.050010 -1.311530 1.821019

O -0.054818 -0.052070 -1.277751

O 1.497713 1.513431 0.978136

O 1.498084 -1.618490 0.977769

$Fe_4O_4^+$

I-34.56

Fe 2.147930 -0.000042 0.000000

Fe -2.148034 0.000012 0.000000

Fe -0.000125 2.361074 0.000000

Fe -0.000125 -2.361049 0.000000

O 1.677215 1.729969 0.000000

O -1.677410 1.729951 -0.000001

O -1.677482 -1.729986 0.000000

O 1.677112 -1.729904 0.000001

II-33.84

Fe 1.613553 0.108252 -0.047780

Fe -1.302031 -0.157726 -0.202539

Fe -0.148844 1.300006 1.821617

Fe -0.252141 -1.473901 1.614606

O 0.157118 0.046529 -1.199711

O 1.478147 1.640544 1.098602

O 1.407011 -1.432976 0.970216

O -1.534187 -0.019576 1.722648

III-33.76

Fe 1.308627 -0.052873 0.051038

Fe -1.416033 0.050561 -0.120101

Fe 0.053972 1.275588 1.833631

Fe -0.043497 -1.281884 1.835564

O 1.510950 -0.058609 2.026675

O -1.539525 0.054678 1.816694

O -0.150228 -1.415880 -0.164838

O -0.043582 1.416932 -0.165868

$Fe_4O_5^+$

I-39.42

Fe 1.305462 -0.783987 0.455143

Fe -0.790868 0.469203 -1.467306

Fe -0.365318 1.068885 1.564611

Fe -0.058254 -1.612564 3.128073

O 1.431973 0.898503 1.197480

O -0.785823 0.023370 2.977345

O 0.569364 -0.669721 -1.192086

O -1.288160 1.326124 0.032195

O 1.006812 -2.019094 1.740468

II-38.79

Fe 2.226121 -0.150961 0.757942

Fe 0.068653 1.950299 -0.111316

Fe 0.191627 -0.054944 2.551818

Fe -0.994735 -0.269359 -0.085142

O 1.791188 1.408324 -0.043314

O -1.096142 1.091362 -1.309703

O -0.764678 1.135042 1.503518

O 0.486267 -1.104032 0.698466

O 2.020242 0.049883 2.643326

III-38.70

Fe 2.142251 -0.195841 0.573604

Fe -2.037830 -0.242343 0.777157

Fe 0.027790 1.806572 0.479146

Fe 0.045268 -2.102432 1.195863

O -1.774879 -2.043166 0.999147

O 1.867311 1.620946 0.677044

O 1.837620 -1.819294 1.306385

O -1.731909 1.546335 0.783646

O 0.053348 -0.259818 0.237900

$Fe_4O_6^+$

I-44.00

Fe 1.593235 -0.027778 -0.265043

Fe -1.503129 0.205446 -0.260638

Fe 0.152996 1.707693 1.894297

Fe -0.054213 -1.392715 1.989222

O 0.013680 0.043527 -1.181912

O 1.640021 1.514336 0.785120

O 1.341438 -1.424543 0.881719

O -1.498242 -1.207184 0.886309

O -1.304702 1.625873 0.794346

O 0.037103 0.161432 2.859120

II-42.40

Fe 1.103760 1.296490 0.089415

Fe 1.621537 -1.402849 0.336596

Fe -1.588124 1.602454 -0.482706

Fe -1.104533 -1.092252 0.193141

O 0.375444 -0.262526 1.198684

O -0.378691 0.465408 -1.203041

O 2.491530 0.077795 -0.146137

O -2.449097 0.169227 0.178561

O -0.291408 2.650539 0.149356

O 0.233374 -2.449700 -0.067717

III-42.10

Fe -1.297426 0.665032 0.249235

Fe 1.394019 0.595968 0.266297

Fe -0.035317 -1.709006 -0.579992

Fe 0.194276 1.514894 2.449586

O -1.717711 -1.119931 0.071395

O 1.598692 -1.205579 0.133903

O 0.069424 2.028971 0.474519

O 0.048038 0.256585 -1.104265

O 1.935391 0.989031 1.954703

O -1.524128 0.893110 2.016107

$Fe_4O_7^+$

I-47.52

Fe 1.554109 0.101251 -0.330481

Fe -1.489704 0.078493 -0.036597

Fe 0.140558 1.884713 1.873447

Fe 0.023672 -1.197574 1.913347

O -0.061993 0.045234 -1.123255

O 1.498390 1.630138 0.767045

O 1.415693 -1.319413 0.904541

O -1.503508 -1.422674 1.100497

O -1.312573 1.625056 0.895224

O 0.149451 0.209944 2.851930

O 0.164789 2.972871 3.084316

II-46.09

Fe 1.322234 0.366369 -0.159882

Fe -1.352198 0.259288 -0.052722

Fe 0.051294 1.555548 1.823376

Fe 0.035395 -1.402782 1.821012

O -0.047331 -0.306114 -1.216178

O 1.835404 1.389672 1.312073

O 1.407602 -1.285894 0.797421

O -1.438071 -1.404649 0.881272

O -1.738827 1.283273 1.425185

O 0.072048 -0.045988 2.869077

O -0.049758 1.735713 -0.105965

III-46.09

Fe -1.162998 0.509977 -0.195843

Fe 1.492328 0.882735 -0.186249

Fe 0.394804 -1.713774 0.684879

Fe 0.164735 0.876323 2.099925

O -1.099444 -1.397128 -0.165806

O 1.727589 -1.011959 -0.137481

O 0.011428 1.939556 0.483580

O 0.156655 0.679761 -1.463624

O 1.948119 1.109285 1.605834

O -1.602988 0.672844 1.585329

O 0.356986 -1.020201 2.253115

$Fe_4O_8^+$

I-50.40

Fe 1.473208 0.055352 -0.368508

Fe -1.661724 0.057675 -0.044477

Fe -0.045505 1.616290 1.889930

Fe 0.055212 -1.529982 2.051483

O -0.145699 0.040404 -1.112565

O 1.371792 1.482767 0.693017

O 1.327347 -1.295343 0.805428

O -1.425367 -1.410061 1.069739

O -1.656402 1.614021 0.970643

O 0.073786 0.048281 2.876014

O 2.762696 -0.049160 -1.355568

O 0.250401 -2.861512 2.966988

II-49.80

Fe 1.278699 0.256527 -0.164503

Fe -1.302814 0.250586 -0.119415

Fe 0.018496 1.511550 1.707722

Fe 0.038050 -1.509330 1.963223

O -0.033518 -0.452261 -1.273450

O 1.809762 1.312704 1.264185

O 1.403082 -1.316785 0.846149

O -1.368625 -1.324309 0.895597

O -1.786416 1.304686 1.326634

O 0.048472 0.028006 2.852963

O -0.019079 1.741019 -0.257777

O 0.055337 -2.841127 2.863315

$Fe_4O_9^+$

I-54.34

Fe 1.428957 0.039920 -0.388501

Fe -1.723406 -0.049736 -0.106141

Fe -0.043507 1.692013 1.934340

Fe 0.054715 -1.517389 2.059649

O -0.192042 -0.046592 -1.106964

O 1.204281 1.461871 0.673148

O 1.298140 -1.302935 0.788813

O -1.413463 -1.417548 1.069216

O -1.504145 1.421027 0.961167

O 0.044955 0.119241 2.782825

O 2.757049 0.048961 -1.290154

O 0.286625 -2.736717 3.077476

O 0.141695 2.987043 2.863668

II-52.52

Fe 1.244435 0.258972 -0.263011

Fe -1.295382 0.252559 -0.195783

Fe 0.021657 1.755865 1.671157

Fe 0.042672 -1.473929 1.932703

O -0.054083 -0.366845 -1.402219

O 1.711834 1.303726 1.225943

O 1.383144 -1.287415 0.754803

O -1.353547 -1.298765 0.818430

O -1.688373 1.294582 1.317929

O 0.053501 0.044560 2.763597

O -0.033476 1.815784 -0.268164

O 0.059848 -2.798092 2.854742

O 0.045770 3.102651 2.550241

III-52.13

Fe 1.267496 0.399655 -0.255788

Fe -1.301476 0.399738 -0.170582

Fe 0.041613 1.581757 1.698064

Fe 0.045643 -1.399304 1.819347

O -0.054043 -0.247335 -1.379633

O 1.822943 1.397320 1.207037

O 1.407787 -1.214035 0.690930

O -1.387019 -1.217597 0.781781

O -1.768464 1.399085 1.318385

O 0.065611 0.094966 2.802448

O -0.022242 1.909748 -0.265010

O 0.050479 -2.853367 3.241784

O 0.051587 -3.401562 1.930720

$Fe_4O_{10}^+$

I-57.82

Fe 1.594902 0.003797 -0.312655

Fe -1.612468 -0.005313 -0.255431

Fe 0.050931 1.696855 1.907776

Fe 0.011741 -1.512113 2.039875

O -0.023693 -0.045186 -1.074610

O 1.403016 1.419620 0.764695

O 1.350382 -1.311197 0.874313

O -1.387852 -1.319685 0.936855

O -1.322190 1.409504 0.799404

O 0.048273 0.123895 2.757049

O 2.852632 -0.158587 -1.300164

O 0.147073 -2.745625 3.061994

O -0.046866 2.989903 2.856575

O -2.903030 0.059779 -1.208541

II-57.12

Fe 1.384298 0.085046 -0.472735

Fe -1.783781 0.097570 -0.134226

Fe -0.045887 1.742483 1.928277

Fe -0.058718 -1.448939 2.025318

O -0.263352 0.052163 -1.114185

O 1.192247 1.533067 0.722005

O 1.190274 -1.210938 0.808454

O -1.505353 -1.317877 1.020835

O -1.512235 1.517195 0.951703

O -0.039852 0.143387 2.780307

O 0.160201 -2.746476 2.961226

O -0.043434 3.071203 2.853364

O 3.395028 0.053873 -0.878154

O 2.574812 -0.056620 -2.028430

III-56.70

Fe 1.148456 0.131761 -0.428065

Fe -1.893813 -0.065812 -0.363907

Fe 0.048262 1.715899 2.239001

Fe -0.167197 -1.430004 2.018690

O -0.355055 -0.156413 -1.315630

O 0.664389 1.505715 0.572103

O 1.095533 -1.189205 0.781228

O -1.621301 -1.105537 1.106688

O -1.690474 1.943570 1.754928

O 0.050973 0.107212 2.933466

O 2.559745 0.152810 -1.205974

O -0.030496 -2.843962 2.770499

O 0.784438 2.926403 2.992622

O -2.149804 1.626843 0.415426

$Fe_4O_{11}^+$

I-60.60

Fe 1.568680 0.012529 -0.341906

Fe -1.636359 0.051548 -0.236362

Fe 0.055120 1.628868 1.999079

Fe 0.030163 -1.577840 1.923824

O -0.059561 0.050459 -1.079411

O 1.409419 1.347512 0.791589

O 1.386286 -1.378733 0.773670

O -1.395854 -1.341749 0.865969

O -1.384174 1.382696 0.881948

O 0.063064 -0.014462 2.759981

O 2.775190 -0.050718 -1.397492

O 0.046859 -2.886606 2.844909

O 0.056252 3.594178 2.216976

O -2.919321 0.016518 -1.199585

O 0.051108 2.954678 3.492634

$Fe_4O_{12}^+$

I-63.20

Fe 1.555303 -0.000881 -0.335075

Fe -1.616379 0.007332 -0.249499

Fe 0.063829 1.623131 2.005037

Fe 0.051043 -1.605115 2.017288

O -0.076602 -0.054352 -1.110386

O 1.442790 1.341440 0.769015

O 1.333884 -1.369702 0.781666

O -1.410030 -1.314625 0.877931

O -1.310811 1.367525 0.811659

O 0.055659 0.016054 2.774074

O -2.978603 0.073604 -1.110675

O 2.880684 -0.162513 -1.246185

O -0.069723 2.967420 3.455248

O 0.056615 3.676803 2.237269

O -0.054486 -2.957451 3.517752

O 0.047449 -3.611730 2.271625

$Fe_4O_{13}^+$

I-65.62

Fe 1.629469 -0.061476 -0.261600

Fe -1.570026 0.030186 -0.246767

Fe 0.039438 1.665074 2.021516

Fe -0.063947 -1.601875 2.054849

O -0.015840 -0.050235 -1.084469

O 1.404764 1.326200 0.867554

O 1.312627 -1.396002 0.863436

O -1.501149 -1.328181 0.855862

O -1.371022 1.413142 0.787527

O -0.059543 0.048882 2.793038

O -2.870694 0.063656 -1.246415

O -0.048769 2.837289 3.509406

O 0.052215 3.573801 2.202005

O 0.558165 -2.781128 3.395917

O -0.619438 -3.347916 2.660952

O 2.764319 0.691154 -1.630911

O 3.374541 -0.449972 -0.871890

$Fe_4O_{14}^+$

I-65.58

Fe 1.707405 0.081345 -0.332476

Fe -1.495444 0.143316 -0.287988

Fe 0.162576 1.600045 2.029913

Fe 0.157402 -1.593534 1.920768

O 0.061112 0.159960 -1.113484

O 1.525750 1.415173 0.873817

O 1.489649 -1.313402 0.775895

O -1.214300 -1.276992 0.788640

O -1.226443 1.432766 0.886162

O 0.159734 -0.060391 2.786184

O -0.680112 2.691286 3.517131

O 0.388561 3.388772 2.902321

O -0.042827 -2.971920 3.356364

O 0.037473 -3.588531 2.076566

O 2.845948 -0.691072 -1.802313

O 3.568588 0.301106 -1.097276

O -2.853214 -0.172840 -1.719920

O -3.483731 0.053003 -0.464311

Fe_5O^+

I-20.28

Fe 2.024468 0.048541 0.112717

Fe -2.035327 0.053505 0.260866

Fe -0.046673 1.164086 -0.667180

Fe -0.048057 -1.147218 -0.572650

Fe -0.030065 0.047736 1.699225

O 1.817058 0.067635 1.927066

II-20.40

Fe 1.279226 -0.476248 -0.150988

Fe -1.463019 -0.258032 -0.050889

Fe -0.075346 1.607721 -0.030120

Fe -0.153406 -2.247459 0.569370

Fe -0.074822 -0.342065 2.009234

O 1.220097 0.894397 1.256514

$Fe_5O_2^+$

I-26.25

Fe 2.044452 0.000184 0.151623

Fe -2.044785 0.000004 0.151587

Fe -0.000218 1.158006 -0.590676

Fe -0.000124 -1.158016 -0.590402

Fe -0.000188 0.000874 1.852863

O 1.859152 0.001559 1.932892

O -1.859471 0.001151 1.932925

II-26.39

Fe -1.302444 0.685166 -0.044018

Fe 1.302104 0.779366 -0.047025

Fe 0.031225 -1.455424 -0.228844

Fe 0.192188 -0.050475 2.021019

Fe -0.050842 0.155561 -2.028794

O 1.714693 0.890536 1.789761

O -1.299632 -0.900739 1.082556

III-26.46

Fe 1.931996 -0.049178 -0.262912

Fe -2.011398 0.009649 -0.203652

Fe 0.058480 1.199069 -1.037840

Fe -0.161786 -1.273160 -0.975542

Fe -0.016578 0.038522 1.399115

O 1.083500 1.429087 0.676645

O -1.114871 -1.408018 0.786572

$Fe_5O_3^+$

I-32.48

Fe 1.724038 0.011726 0.256567

Fe -1.400388 -0.099194 -0.360471

Fe -0.166976 1.901188 -0.066684

Fe 0.050982 -2.025918 0.639774

Fe -0.266424 0.373443 1.939712

O 1.195454 1.495466 1.334405

O -1.419517 -1.065187 1.407929

O 1.754497 -1.831463 0.039653

II-32.32

Fe -1.299182 1.095391 -0.053765

Fe 1.089587 0.568051 -0.115645

Fe 0.778074 -2.028939 -0.513466

Fe -0.364123 -0.782548 1.619374

Fe -0.258362 -0.080949 -2.041695

O -1.929987 0.134774 1.392508

O 1.427462 -1.051538 0.999730

O -0.074092 -1.920056 -2.125975

III-32.08

Fe 2.226802 -0.262524 0.183420

Fe -1.920940 0.052044 -0.089891

Fe 0.365668 1.080882 -0.728941

Fe 0.163524 -1.404898 -0.579692

Fe 0.011425 -0.035498 1.618511

O 1.841180 -0.159374 1.920080

O -1.834778 0.146085 1.710790

O -0.790494 -0.140075 -1.700160

$Fe_5O_4^+$

I-39.69

Fe 1.438977 1.294531 0.046590

Fe -1.204674 1.423172 0.068142

Fe 1.269924 -1.409084 -0.073415

Fe -1.399630 -1.267345 -0.043402

Fe 0.052529 -0.042034 1.766479

O 1.929488 -0.154821 1.216618

O -1.837232 0.058178 1.273686

O 0.158438 2.336778 -0.754473

O -0.127787 -2.273009 -0.894881

II-36.54

Fe -1.095757 0.640083 0.052615

Fe 1.345108 0.676973 0.053083

Fe -0.048802 -1.569810 0.052083

Fe 0.061494 -0.084665 2.222160

Fe 0.062765 -0.081428 -2.115898

O -0.175330 -1.820611 1.846168

O 1.509205 0.902386 1.847678

O 1.509972 0.905859 -1.740978

O -0.173152 -1.818239 -1.742389

III-37.35

Fe -1.257470 0.782349 -0.053399

Fe 1.201113 0.748940 -0.059768

Fe -0.055752 -1.477061 -0.049734

Fe -0.028414 0.009535 2.106315

Fe -0.045852 0.150336 -2.125835

O -0.056991 -1.721950 1.821836

O 1.502968 0.806927 1.836843

O -1.520789 0.880244 1.846947

O -0.055111 -1.608581 -1.877038

$Fe_5O_5^+$

I-44.00

Fe -1.924241 0.784387 0.091522

Fe 2.125682 0.303835 0.453937

Fe -0.582663 -1.347823 -0.360830

Fe 0.340159 0.436895 2.238440

Fe -0.024423 0.674262 -1.817191

O 2.133803 0.891578 2.208109

O -1.279785 1.081192 1.723411

O 0.697354 -1.080541 0.910297

O 1.630423 0.883800 -1.196529

O -1.697002 -0.251266 -1.521835

II-43.20

Fe 0.447011 1.924536 -0.052082

Fe -2.764715 0.573012 -0.052083

Fe 3.114203 1.008310 -0.052083

Fe -2.046159 -1.791036 -0.052084

Fe 1.399751 -1.194782 -0.052083

O 2.160621 2.556792 -0.052084

O -1.300358 1.605775 -0.052084

O -0.255103 -1.839202 -0.052083

O 3.185783 -0.807605 -0.052083

O -3.695067 -1.000116 -0.052083

III-43.20

Fe -1.514958 0.590736 -0.804847

Fe 1.188723 0.992242 -0.287758

Fe -0.473141 -1.727223 -0.054112

Fe -0.465068 0.651710 1.716499

Fe 0.254389 -0.430547 -2.433860

O -0.871204 -1.082635 1.605846

O -1.408688 -1.213771 -1.708032

O 1.221128 -0.894972 -0.770747

O 0.982081 1.703520 1.396575

O -0.021438 1.426701 -1.724348

$Fe_5O_6^+$

I-47.96

Fe -1.295487 0.679769 -0.045101

Fe 1.411674 0.878935 -0.046181

Fe -0.045600 -1.470350 -0.051350

Fe 0.050809 0.015809 2.549048

Fe 0.048129 0.044058 -2.586979

O 1.506760 0.895893 1.754413

O -1.399545 0.789352 1.712987

O 0.045591 -1.621407 1.705601

O 1.481820 0.891517 -1.820190

O -1.439092 0.883875 -1.828398

O 0.053325 -1.670373 -1.837734

II-48.40

Fe -1.783617 1.046301 0.088898

Fe 0.785524 0.212975 1.194841

Fe 0.679516 -2.394114 -0.046578

Fe -1.408850 -1.194832 2.096248

Fe -0.326944 -0.578306 -1.618963

O 0.358326 -1.727519 1.725172

O -0.269888 1.641300 0.892482

O -0.268787 -2.416065 -1.632238

O -1.510831 0.776184 -1.723438

O -2.563835 -0.161267 1.210910

O 1.208705 -0.454695 -0.578253

III-48.40

Fe -2.340525 0.787833 0.162257

Fe 1.902055 0.065158 -0.277129

Fe -0.471265 -2.000455 0.265380

Fe 0.057909 0.378217 2.232455

Fe -0.689768 -0.060943 -1.484794

O -0.058160 -1.408397 1.906133

O 1.647243 0.878862 1.315920

O -1.531097 1.084484 1.730787

O 0.812584 -1.197531 -1.089515

O -1.605821 1.493791 -1.419966

O -2.026731 -1.087503 -0.479414

$Fe_5O_7^+$

I-53.40

Fe -1.475979 1.712696 -0.256271

Fe 1.690859 0.828798 0.196956

Fe 0.201249 -2.145102 -0.277069

Fe -0.019956 0.047478 2.035524

Fe -0.148645 -0.098662 -1.823289

O 0.045044 -1.625840 1.442696

O -1.317946 1.117671 1.449035

O -0.468078 -1.848815 -2.035038

O -1.836720 0.576422 -1.720940

O 1.493479 -0.667136 -0.885017

O 1.635830 0.798032 2.033301

O 0.387598 1.624335 -0.910298

II-53.28

Fe -1.737718 0.361406 0.020711

Fe 2.148023 1.427090 0.064256

Fe -0.573596 -1.779687 -0.070282

Fe 0.088741 -0.153590 2.342921

Fe -0.047527 0.044868 -2.096257

O 1.537735 0.775936 1.554473

O -1.413835 0.688550 1.726361

O -0.048670 -1.821796 1.624416

O 1.478147 0.782143 -1.398040

O -1.620912 0.889501 -1.706091

O -0.154612 -1.767412 -1.826850

O 2.968823 2.837548 0.042472

III-52.32

Fe -2.035651 0.369856 -0.015789

Fe 2.379976 1.305873 -0.072711

Fe -0.564981 -1.822897 -0.105188

Fe 0.251117 0.251921 2.063813

Fe 0.115513 -0.057175 -2.034580

O 0.260266 -1.455822 1.407534

O 1.806212 1.193948 1.634832

O -1.363366 0.912344 1.520375

O -0.054515 -1.884746 -1.825686

O -1.510516 0.773351 -1.682023

O 1.619918 0.783906 -1.605103

O -2.310858 -1.407593 0.047503

$Fe_5O_8^+$

I-57.46

Fe -1.460374 0.913595 -0.006209

Fe 1.486280 1.611366 -0.058463

Fe -0.820241 -2.042465 -0.140435

Fe 0.304335 -0.218072 2.159267

Fe 0.251265 -0.261675 -2.246796

O 0.049556 -1.837473 1.393933

O 1.723945 0.786929 1.548007

O -1.181267 0.683220 1.779037

O -0.146486 -1.984986 -1.826973

O -1.182048 0.691412 -1.910194

O 1.611598 0.688919 -1.603072

O -2.139586 -0.884366 -0.064691

O -0.166705 2.221980 -0.059729

II-56.55

Fe -1.141702 0.984041 0.269262

Fe 1.784814 1.090549 -0.589152

Fe 0.181674 -1.402455 0.155370

Fe -1.308701 -0.784721 2.489940

Fe -0.255727 0.049725 -2.471480

O -1.308290 0.992970 2.080351

O 0.165250 -1.711931 1.945981

O 1.303414 0.899119 -2.329618

O -1.505691 0.900778 -1.557598

O -0.151493 -1.523266 -1.674498

O 0.372946 1.954092 0.156250

O 1.799282 -0.608697 0.047093

O -1.678974 -0.885254 0.462624

III-55.90

Fe -1.403713 1.475219 0.365164

Fe 1.347380 1.318462 -0.284728

Fe -0.082116 -1.617472 -0.250024

Fe 1.402080 0.121182 1.932893

Fe -0.591213 0.047599 -2.214113

O 0.116089 1.526456 1.324231

O -1.506689 -0.237855 -0.052396

O 0.682503 -1.421690 1.370196

O -0.362307 1.771346 -1.198603

O -0.768580 -1.756878 -2.051148

O 1.160346 -0.248136 -1.189624

O 2.678290 1.080036 0.872504

O -2.664529 2.449744 0.561326

$Fe_5O_9^+$

I-60.62

Fe -1.394661 0.925439 0.043391

Fe 1.474237 0.901601 -0.001536

Fe 0.043888 -1.581595 -0.033034

Fe 0.090769 0.046946 2.457438

Fe -0.046619 0.093416 -2.439712

O 1.518494 0.877472 1.901360

O -1.349263 0.875929 1.919643

O 0.054391 -1.588773 1.842851

O 1.386966 0.897631 -1.924175

O -1.457568 0.894205 -1.874052

O -0.055369 -1.552675 -1.944179

O 0.050138 2.014690 0.027351

O 1.712931 -0.890881 -0.055206

O -1.691370 -0.905617 0.055549

II-60.06

Fe -1.547283 0.681539 0.140301

Fe 0.981109 2.213126 0.057213

Fe -0.045304 -1.832335 -0.060681

Fe 0.477072 0.082911 2.133342

Fe 0.395764 0.288105 -2.083710

O 1.403267 1.725941 1.738734

O -1.280137 0.580577 1.914529

O 0.471358 -1.710136 1.657279

O 1.299460 1.816238 -1.706229

O -1.296282 0.683615 -1.811375

O 0.364883 -1.532895 -1.826116

O -0.773728 2.398425 0.054344

O -1.723384 -1.193067 -0.045267

O 0.560388 0.141645 0.009225

$Fe_5O_{10}^+$

I-64.05

Fe -1.397574 0.805381 -0.035891

Fe 1.594146 0.991207 -0.034042

Fe -0.027217 -1.537546 -0.039658

Fe 0.069886 0.070495 2.636361

Fe 0.008153 0.057034 -2.559807

O 1.424012 0.885150 1.906723

O -1.324980 0.790685 1.838912

O 0.037154 -1.499824 1.833567

O 1.397296 0.878687 -2.027967

O -1.421333 0.799624 -1.936920

O -0.044548 -1.553353 -1.941522

O 0.036864 1.911100 -0.049281

O 1.634069 -0.813363 -0.059114

O -1.785868 -0.998463 -0.042049

O 0.035787 0.040684 4.250649

II-63.90

Fe -1.609989 0.780634 0.043853

Fe 0.944095 2.238254 0.052839

Fe -0.095119 -1.842506 -0.007135

Fe 0.367064 0.179725 2.143294

Fe 0.375129 0.274168 -2.066343

O 1.413697 1.529833 1.898578

O -1.299389 0.556770 1.940194

O 0.567371 -1.497993 1.833329

O 1.288963 1.777255 -1.704597

O -1.360476 0.666639 -1.816262

O 0.370288 -1.508210 -1.772176

O -0.882405 2.431999 0.160707

O -0.069633 -3.478418 0.056105

O -1.732336 -1.168256 0.045814

O 0.465976 0.139421 0.028348

III-63.15

Fe -1.438025 0.808971 0.078184

Fe 1.436030 1.100333 0.037392

Fe -0.237680 -1.696638 -0.040512

Fe 0.036193 -0.086921 2.461334

Fe -0.065359 0.044491 -2.322204

O 1.431006 0.837091 1.922442

O -1.404808 0.771283 1.925404

O 0.040946 -1.721385 1.755550

O 1.358782 0.890214 -1.850213

O -1.513039 0.847182 -1.832666

O -0.162535 -1.643854 -1.929155

O -0.050880 2.038663 0.065619

O 2.561118 -0.529690 -0.045540

O -1.887319 -0.979677 0.038441

O 1.820846 -1.709151 -0.160591

$Fe_5O_{11}^+$

I-67.52

Fe -1.341638 0.879293 0.053581

Fe 1.430125 0.891764 -0.039333

Fe 0.013123 -1.549017 -0.016834

Fe 0.174119 0.009011 2.676680

Fe -0.054905 0.089466 -2.672591

O 1.502248 0.779411 1.854913

O -1.200813 0.800827 1.920137

O 0.158911 -1.533012 1.872975

O 1.314128 0.884260 -1.898616

O -1.382362 0.880620 -1.844858

O -0.053674 -1.481645 -1.874068

O 0.048308 2.120168 0.037082

O 1.779531 -0.943004 -0.048474

O -1.732398 -0.944939 0.054902

O 0.060440 0.067052 4.292819

O -0.057784 0.064498 -4.288300

II-67.68

Fe -1.276227 2.044764 0.052251

Fe 1.545138 0.809689 0.005651

Fe 0.899118 -2.203752 -0.047558

Fe -0.266744 -0.163475 1.993948

Fe -0.469877 -0.168264 -2.168646

O 1.315737 0.658698 1.807595

O -1.509027 1.018185 1.500615

O -0.035227 -1.843040 1.436412

O 1.050433 0.589394 -1.811368

O -1.600765 0.873357 -1.284133

O -0.281554 -1.715098 -1.321545

O 0.443749 2.325531 -0.049284

O 2.129981 -0.969351 -0.125869

O -0.690370 -0.260611 -3.765358

O -2.135405 3.410936 0.024827

O 1.505552 -3.695579 -0.163373

III-67.52

Fe -1.296290 1.961584 -0.044957

Fe 1.713342 1.030143 0.050045

Fe 0.807845 -2.079680 -0.019396

Fe -0.384780 -0.144103 2.155297

Fe -0.293970 -0.016493 -2.329858

O 1.172130 0.678304 1.738210

O -1.590397 0.964237 1.415631

O -0.069354 -1.822303 1.489404

O 1.205909 0.680326 -1.886522

O -1.502500 1.083288 -1.652842

O -0.369425 -1.385614 -1.192467

O 0.442315 2.334520 -0.077275

O 2.049175 -0.895836 -0.066306

O -0.441752 -0.375776 -3.901673

O 3.210734 1.634072 -0.266023

O 1.285685 -3.580482 -0.377377

$Fe_5O_{12}^+$

I-71.40

Fe -1.302052 1.933810 0.038492

Fe 1.719655 0.879685 -0.045075

Fe 0.796550 -2.177981 0.038360

Fe -0.165517 -0.080591 2.348678

Fe -0.330628 -0.155244 -2.264681

O 1.314605 0.677614 1.806136

O -1.406381 0.793505 1.407083

O -0.163136 -1.616236 1.432775

O 1.191963 0.604668 -1.849196

O -1.512215 0.778310 -1.308689

O -0.276407 -1.647029 -1.288342

O 0.415424 2.262639 -0.033365

O 2.079815 -0.989489 -0.033968

O -0.360057 -0.160798 3.942325

O -0.584927 -0.277997 -3.848183

O -2.245809 3.235517 0.058715

O 1.294900 -3.707207 0.047626

II-70.21

Fe -1.246356 0.992614 0.059412

Fe 1.474649 0.878714 -0.057751

Fe 0.018028 -1.770522 -0.029239

Fe 0.153590 0.056146 2.676048

Fe -0.023298 0.039317 -2.665157

O 1.491431 0.803466 1.802869

O -1.191714 0.891568 1.925758

O 0.049211 -1.509402 2.012603

O 1.392781 0.786182 -1.936608

O -1.294828 0.905793 -1.791795

O -0.042191 -1.549863 -1.945105

O 0.161220 2.165079 -0.012850

O 1.606536 -1.003536 -0.049861

O -1.506308 -0.886462 0.081620

O 0.362053 0.150077 4.279252

O -0.152803 0.046301 -4.271354

O -0.044888 -3.401224 0.042300

III-70.89

Fe -1.383068 0.917278 0.074356

Fe 1.627610 0.968030 0.025150

Fe -0.032990 -1.758346 0.063746

Fe 0.129058 0.054322 2.731693

Fe -0.054763 0.081450 -2.533062

O 1.492521 0.817860 1.940735

O -1.229818 0.868098 1.924594

O 0.049421 -1.521359 1.973634

O 1.346612 0.874999 -2.001182

O -1.420790 0.905904 -1.848853

O -0.068963 -1.516116 -1.960500

O 0.163027 1.963762 0.042754

O 1.517786 -0.833479 -0.042423

O -1.601934 -0.935351 0.067771

O 0.167944 0.050985 4.337795

O 3.067974 1.734429 -0.060135

O -0.052509 -3.392262 0.032451

$Fe_5O_{13}^+$

I-74.52

Fe -1.108057 1.834798 -0.024911

Fe 2.002880 1.034219 0.477655

Fe 0.899633 -1.926074 -0.013350

Fe -0.254727 -0.035908 2.395898

Fe -0.778145 -0.469660 -2.354655

O 1.343110 0.680061 2.120692

O -1.271725 1.184455 1.604976

O -0.263602 -1.321122 1.182130

O 0.469293 0.489413 -2.853839

O -1.600170 0.511159 -1.085524

O -0.059758 -1.875622 -1.510320

O 0.658332 1.809325 -0.356261

O 2.041302 -0.593953 -0.237413

O -0.489799 -0.462068 3.915650

O -1.825222 -0.876849 -3.524679

O 3.367362 1.818234 0.869665

O -1.726340 3.281614 -0.344754

O 1.604330 -3.313665 0.369411

II-73.80

Fe -1.495988 0.999965 0.032951

Fe 1.663393 0.884515 -0.048012

Fe -0.017548 -1.571533 -0.001096

Fe 0.125203 0.051764 2.664990

Fe -0.010956 0.047785 -2.673113

O 1.499508 0.776151 1.917064

O -1.223928 0.882147 1.980271

O 0.044491 -1.499007 1.842926

O 1.403044 0.771716 -1.999874

O -1.328888 0.874758 -1.929773

O -0.054601 -1.501346 -1.845782

O 0.118361 1.823928 -0.021623

O 1.743474 -0.884659 -0.048938

O -1.720943 -0.756417 0.046329

O 0.158172 0.072155 4.277754

O -0.053309 0.066175 -4.286037

O 3.076882 1.694476 -0.063221

O -2.846093 1.911372 0.056859

III-73.08

Fe -1.417913 1.020666 0.047795

Fe 1.655101 0.881964 -0.028509

Fe 0.002377 -1.723778 0.002317

Fe 0.143044 0.047560 2.707844

Fe 0.012689 0.065434 -2.625438

O 1.517758 0.775574 1.904128

O -1.200401 0.893108 1.964375

O 0.057104 -1.519989 1.926336

O 1.419502 0.790384 -1.990641

O -1.293182 0.907921 -1.925031

O -0.044898 -1.504843 -1.965458

O 0.160718 1.894944 0.031234

O 1.619704 -0.922736 -0.037336

O -1.538551 -0.783357 0.051275

O 0.170304 0.047371 4.313449

O 3.102259 1.627723 -0.067311

O -2.782406 1.911320 0.051099

O -0.060094 -3.351298 -0.046380

$Fe_5O_{14}^+$

I-77.33

Fe -1.299453 1.935453 0.025577

Fe 1.838961 0.921113 -0.057073

Fe 0.880086 -2.229904 -0.026812

Fe -0.247104 -0.191083 2.237348

Fe -0.364152 -0.197016 -2.234852

O 1.214149 0.576883 1.712971

O -1.460052 0.769892 1.383713

O -0.164505 -1.713985 1.342644

O 1.123508 0.570040 -1.797328

O -1.529566 0.754046 -1.305327

O -0.240797 -1.716231 -1.334828

O 0.398047 2.251812 -0.031861

O 2.115200 -1.020797 -0.059592

O -0.361385 -0.265367 3.841128

O -0.573067 -0.278475 -3.828276

O -2.247748 3.231046 0.050165

O 1.399678 -3.749464 -0.047757

O 3.478321 1.814473 -0.810042

O 3.560499 1.724926 0.603192

II-76.57

Fe -1.415534 1.047835 0.060725

Fe 1.666269 0.919424 -0.027803

Fe 0.022423 -1.721677 0.029877

Fe 0.150957 0.045090 2.704655

Fe -0.010335 0.041396 -2.660258

O 1.509603 0.776238 1.916844

O -1.185414 0.888779 1.998086

O 0.063982 -1.507597 1.954821

O 1.390464 0.784201 -1.952694

O -1.297435 0.891543 -1.876165

O -0.047889 -1.508914 -1.909790

O 0.162339 1.920362 0.035177

O 1.628720 -0.895789 -0.035891

O -1.517037 -0.765795 0.061384

O 0.240891 0.072685 4.314035

O -0.042030 0.072012 -4.271251

O 3.090424 1.694878 -0.057025

O -2.777877 1.931634 0.069830

O -0.043073 -3.346919 0.044249

III-76.57

Fe -1.618030 1.306916 0.538885

Fe 1.504811 1.024870 -0.176003

Fe -0.034724 -1.507045 -0.073843

Fe 0.284379 0.158629 2.685423

Fe 0.152652 0.121305 -2.878732

O 1.497028 0.985884 1.751549

O -1.179592 1.103228 2.265714

O -0.060348 -1.316572 1.826992

O 1.401095 0.996748 -2.017934

O -1.174387 1.067344 -2.869225

O -0.168106 -1.307616 -1.905891

O -0.154309 1.946003 -0.152029

O 1.591937 -0.776709 -0.061503

O -1.620547 -0.312852 -0.036232

O 0.570743 0.044263 4.271151

O 0.692529 -0.361732 -4.341043

O -2.973638 2.156836 0.353116

O 0.486052 -3.399354 -0.041897

O -0.648422 -4.137078 0.042223

$Fe_5O_{15}^+$

I-79.60

Fe -1.544253 1.049917 -0.011420

Fe 1.619118 0.950758 -0.033532

Fe -0.055398 -1.640282 0.064352

Fe 0.030936 0.198942 2.673089

Fe -0.010078 0.043115 -2.657250

O 1.429528 0.899588 1.916108

O -1.326668 0.997738 1.933295

O -0.047456 -1.403606 1.912303

O 1.404471 0.789560 -1.974791

O -1.354453 0.888799 -1.951042

O -0.059300 -1.510862 -1.802859

O 0.065013 1.870062 -0.049323

O 1.631673 -0.811255 0.031513

O -1.695741 -0.705025 0.045248

O 0.048690 0.258892 4.279792

O -0.041186 -0.036964 -4.262867

O 3.053315 1.725519 -0.057904

O -2.916078 1.928519 -0.043783

O 0.151236 -3.604354 -0.009882

O 0.466893 -4.297838 -1.103460

II-79.40

Fe -1.462271 1.062045 0.028097

Fe 1.640243 0.947994 -0.045680

Fe -0.016230 -1.719242 0.029436

Fe 0.131323 0.088828 2.672926

Fe -0.006547 0.041483 -2.663684

O 1.500939 0.802492 1.907973

O -1.205598 0.918911 1.966594

O 0.044562 -1.468749 1.901335

O 1.398890 0.778229 -1.982879

O -1.314010 0.886772 -1.920181

O -0.056618 -1.497116 -1.845782

O 0.125231 1.924939 -0.027523

O 1.627370 -0.834800 -0.034492

O -1.595874 -0.710900 0.054621

O 0.161761 0.163413 4.286103

O -0.048601 0.065012 -4.277670

O 3.077818 1.707956 -0.063467

O -2.839968 1.923577 0.053857

O 0.678330 -3.595356 0.047785

O -0.712107 -3.694190 0.055019

III-80.20

Fe -1.095025 1.925035 0.158519

Fe 1.936246 1.006600 -0.724099

Fe 0.770991 -2.019501 -0.050887

Fe -0.369333 -0.321224 2.443224

Fe -0.600187 -0.170813 -2.352181

O 1.147616 0.337803 2.342977

O -1.403686 0.775943 1.510487

O -0.254520 -1.765278 1.365237

O 1.010350 0.573349 -2.190581

O -1.517015 0.856096 -1.323292

O -0.328873 -1.634263 -1.414826

O 0.666113 2.012605 0.064722

O 1.827161 -0.640244 0.064157

O -0.889555 -0.663058 3.929253

O -0.997411 -0.334062 -3.899184

O 1.616205 -3.387253 -0.156335

O 3.805538 1.388196 -1.335488

O 3.683451 1.717687 0.033111

O -2.463000 3.388526 0.494515

O -1.692839 3.608642 -0.676606

$Fe_5O_{16}^+$

I-82.74

Fe -1.542097 1.087028 -0.157595

Fe 1.594705 0.903016 -0.052320

Fe 0.070839 -1.713399 0.026240

Fe 0.038186 0.127527 2.651051

Fe -0.027867 -0.002062 -2.701293

O 1.383596 0.882660 1.844667

O -1.322455 0.888612 2.017376

O -0.038840 -1.436138 1.922018

O 1.318583 0.800762 -1.961493

O -1.419608 0.825743 -2.021810

O -0.065328 -1.539515 -1.866130

O -0.024908 1.923678 -0.030311

O 1.692337 -0.899807 -0.042280

O -1.550558 -0.670620 0.063922

O 0.179041 0.164581 4.265124

O -0.039984 -0.049423 -4.314666

O 3.302947 1.841443 -0.232621

O -2.930077 1.931082 -0.060462

O 0.162181 -3.662537 -0.082713

O 0.463697 -4.354762 -1.187057

O 3.996332 2.123597 -1.335204

II-82.11

Fe -1.547404 1.092114 -0.058948

Fe 1.560891 0.940377 -0.065067

Fe 0.034168 -1.828946 -0.031879

Fe 0.055623 0.021696 2.654687

Fe -0.094665 0.049451 -2.681068

O 1.392424 0.789138 1.857594

O -1.312040 0.807499 2.048726

O -0.049727 -1.527859 1.943281

O 1.285956 0.814410 -1.940943

O -1.452787 0.878858 -1.938148

O -0.156404 -1.517372 -1.929076

O -0.027182 1.936241 0.056711

O 1.537481 -0.917784 -0.047781

O -1.465354 -0.681465 0.074616

O 0.239730 0.059535 4.263323

O -0.149806 0.065673 -4.295613

O -2.959038 1.899197 0.055566

O 0.638372 -3.717665 0.048502

O -0.775465 -3.686741 0.049265

O 3.499601 1.396204 -0.053079

O 3.919969 2.665817 -0.053903

Fe_6O^+

I-24.43

Fe 1.313192 1.408731 -0.010593

Fe 1.313191 -1.408810 -0.011471

Fe -1.107829 1.395368 -0.017977

Fe -1.108047 -1.395409 -0.018994

Fe -0.171256 -0.000978 1.714729

Fe 0.157776 0.000531 -1.617133

O 1.734855 -0.000481 1.287215

II-24.01

Fe 1.326148 1.326145 0.053813

Fe 1.089697 -1.142973 -0.052516

Fe -1.142969 1.089696 -0.052514

Fe -1.317866 -1.317865 -0.145267

Fe -0.012602 -0.012603 1.875117

Fe -0.047370 -0.047370 -1.884361

O 1.296091 1.296091 1.904354

$Fe_6O_2^+$

I-30.72

Fe 1.218615 1.671748 -0.264518

Fe -1.218192 1.672170 -0.264272

Fe 1.237883 -1.092567 0.360222

Fe -1.238271 -1.092390 0.360340

Fe -0.000050 0.569761 1.819326

Fe -0.000221 -0.053562 -1.502006

O 1.829023 0.581686 1.207970

O -1.828967 0.582012 1.207904

III-30.56

Fe 1.184997 1.375217 -0.156604

Fe -1.185031 1.375211 0.156609

Fe 1.184988 -1.375236 -0.156607

Fe -1.185038 -1.375213 0.156606

Fe -0.157548 -0.000008 1.815590

Fe 0.157538 -0.000004 -1.815588

O 1.629789 -0.000013 1.109152

O -1.629812 0.000001 -1.109166

$Fe_6O_3^+$

I-37.26

Fe 1.297194 1.300434 0.726732

Fe -1.198374 1.198976 0.889226

Fe 1.199076 -1.192365 -0.363653

Fe -1.208685 -1.266247 -0.366816

Fe -0.049329 -0.679104 2.026076

Fe -0.047775 0.524364 -1.513202

O 1.746922 -0.428291 1.414507

O -1.838028 -0.572582 1.349060

O -0.045347 2.117962 -0.368954

II-35.64

Fe 1.307035 1.516314 -0.052084

Fe -1.437463 1.488731 -0.052083

Fe 1.986184 -1.102809 -0.052083

Fe -2.040278 -1.161052 -0.052083

Fe -0.042169 -0.364036 1.167604

Fe -0.042168 -0.364037 -1.271770

O 2.865241 0.475907 -0.052083

O -2.961409 0.394296 -0.052084

O -0.076591 2.698997 -0.052084

III-36.36

Fe 1.372840 1.254134 -0.145113

Fe -1.118844 1.396168 -0.162296

Fe 1.393103 -1.238510 -0.062407

Fe -1.097758 -1.391917 -0.053851

Fe -0.051071 0.055413 1.874421

Fe -0.356669 -0.054681 -1.926750

O 1.753683 0.055027 1.445577

O -1.776898 0.048198 1.099872

O 1.517110 -0.042300 -1.622158

$Fe_6O_4^+$

I-43.60

Fe 1.304998 1.303174 -0.296457

Fe -1.407031 1.304792 -0.014977

Fe 1.305822 -1.234346 -0.254276

Fe -1.405688 -1.268416 0.043912

Fe 0.048498 -0.161730 1.725700

Fe -0.181669 0.225144 -1.997209

O 1.847176 0.060902 1.076959

O -1.829984 0.060891 1.392671

O -0.166545 -1.617106 -1.410414

O -0.163045 2.032948 -1.295935

II-43.60

Fe 1.715996 1.161700 0.055218

Fe -0.982348 1.056477 -0.108226

Fe 0.987618 -1.163913 0.015839

Fe -1.715099 -1.266918 -0.156315

Fe -0.154077 -0.048512 1.969005

Fe 0.156042 -0.056991 -2.065979

O 1.672429 0.044744 1.616896

O -1.920040 -0.151772 1.391365

O 1.922260 0.042687 -1.489234

O -1.669560 -0.148538 -1.716361

$Fe_6O_5^+$

I-48.18

Fe 1.292777 1.681264 0.159680

Fe -1.297333 1.506494 0.134120

Fe 1.189263 -1.399868 -0.147738

Fe -1.303488 -1.443048 -0.159628

Fe -0.031318 0.263515 1.854391

Fe -0.095445 -0.153853 -1.919792

O 1.817034 -0.057077 0.979701

O -1.844023 -0.176467 1.090034

O -0.022050 -2.037062 -1.512509

O 0.063842 1.630394 -1.415032

O -0.026142 2.241273 1.494908

II-48.95

Fe 1.212356 1.288382 -0.379642

Fe -1.231081 1.293146 -0.467665

Fe 1.519149 -1.195946 0.117290

Fe -1.402823 -1.192837 -0.085126

Fe -0.054015 0.006125 2.037773

Fe 0.145416 -0.264108 -2.169499

O 1.500191 -1.087867 1.925752

O -1.573109 -1.094065 1.719436

O 1.913134 -0.162988 -1.499594

O -1.689863 -0.125051 -1.726646

O -0.062580 1.724803 1.000218

III-48.51

Fe 1.818725 0.948150 -0.050873

Fe 1.608767 -1.344334 1.199859

Fe -2.443142 0.776252 -0.471798

Fe -1.319932 -1.565360 -0.398570

Fe -0.362757 0.470562 1.267202

Fe -0.269842 0.263518 -1.823580

O 1.622091 0.477689 1.787491

O -1.910589 1.500574 1.103339

O -0.254008 -1.709543 1.120778

O 1.412319 0.989758 -1.815288

O -2.032700 -0.535287 -1.839203

$Fe_6O_6^+$

I-54.12

Fe 1.692110 1.302971 0.261095

Fe -1.443240 1.261749 -0.088160

Fe 1.501032 -1.200072 0.055317

Fe -1.723995 -1.408048 -0.163930

Fe 0.159919 0.160990 1.924737

Fe -0.151523 -0.057656 -1.895239

O 2.032465 -0.198103 1.618404

O -1.584664 -0.363533 1.395556

O 1.601558 0.279555 -1.384943

O -2.059813 0.055120 -1.498002

O -0.026428 1.942025 0.893448

O -0.029591 -1.945277 -0.784620

II-53.28

Fe 0.046672 -0.187929 -0.579274

Fe 0.018595 0.058940 2.646243

Fe 1.338063 2.240465 -0.457797

Fe 1.237733 2.243075 2.764811

Fe -1.403004 2.159394 -0.378793

Fe -1.195799 2.243322 2.817939

O -0.043348 -0.824643 1.084491

O 0.046787 1.404410 4.021191

O 1.713751 2.864362 1.161323

O -1.722156 2.850016 1.223460

O 1.412543 0.662120 -1.401579

O -1.423313 0.565741 -1.298603

III-53.88

Fe 1.292467 1.297633 0.122246

Fe -1.503445 1.408245 0.189793

Fe 1.203760 -1.364031 0.061156

Fe -1.580222 -1.321211 0.142851

Fe 0.693470 -0.065464 2.160667

Fe -0.082690 0.056229 -2.024540

O 2.340534 -0.087399 0.977449

O -2.779706 0.073581 0.359515

O -0.163182 -1.650778 -1.297447

O -0.055740 1.729798 -1.218667

O -0.166815 1.527306 1.529681

O -0.256945 -1.584893 1.474184

$Fe_6O_7^+$

I-58.63

Fe 0.952523 -0.497660 1.657553

Fe -1.820388 -0.678667 1.513411

Fe -0.261639 1.617042 1.405844

Fe 1.595141 -0.900031 -1.522704

Fe -1.599863 -0.943963 -1.710850

Fe 0.048088 1.794533 -1.841923

O -0.564967 0.166898 2.633044

O 1.565532 0.806925 -2.237519

O -1.388299 0.767107 -2.226388

O 0.023190 -1.690415 -1.929857

O -0.060177 2.431066 -0.138590

O 1.906300 -0.995036 0.269160

O -2.356835 -1.192828 -0.075936

II-58.63

Fe 0.677368 -0.505284 0.562494

Fe -1.924975 -0.259403 2.063556

Fe -0.572477 1.788175 1.936010

Fe 1.511018 -0.898402 -1.856023

Fe -1.269850 -0.882791 -1.226687

Fe 0.195579 1.726306 -1.413208

O -2.151879 1.427509 2.770694

O 1.488651 0.797596 -2.336602

O -1.387605 0.880448 -1.618781

O 0.029326 -1.737274 -2.335857

O 0.573950 1.431431 0.488931

O 2.042263 -1.506213 -0.263283

O -1.208060 -1.222341 0.677913

III-59.15

Fe 1.518177 -0.392214 0.264222

Fe -1.288700 -0.576152 1.881432

Fe -1.405270 2.130767 1.615179

Fe 0.957566 -0.989306 -2.240665

Fe -1.511023 -1.071038 -1.326815

Fe 0.368110 1.617392 -1.012037

O -1.830088 0.906526 2.879798

O 0.458420 -0.986434 1.551015

O 1.910870 0.463362 -1.399606

O -0.798072 0.475937 -2.027807

O -0.465728 -2.154749 -2.341050

O -0.365592 2.654262 0.250727

O -2.146392 -0.992822 0.319774

$Fe_6O_8^+$

I-63.14

Fe 1.404560 -0.772468 1.543941

Fe -1.716354 -1.148159 1.616488

Fe -0.154441 1.473402 1.286609

Fe 1.388378 -0.850096 -1.589269

Fe -1.723420 -0.708030 -1.589775

Fe 0.255409 1.611628 -1.199582

O 1.494164 1.094389 1.838604

O -1.618388 0.675400 1.847485

O -0.055233 -1.661411 2.118325

O 1.742275 0.872154 -1.938769

O -1.384386 1.102496 -1.597560

O -0.143730 -1.415367 -2.247126

O 2.019557 -1.398567 -0.063301

O -2.242754 -1.497379 -0.070558

II-63.00

Fe 1.319402 1.369638 0.060707

Fe 1.319405 -1.369534 -0.060572

Fe -1.319547 1.369637 0.060701

Fe -1.319534 -1.369552 -0.060589

Fe -0.000074 0.006536 1.907686

Fe -0.000066 -0.006425 -1.907615

O 1.825424 -0.050910 1.273986

O -0.000094 1.872319 1.391796

O -1.825544 -0.050920 1.273984

O -0.000068 -1.829783 1.275882

O 1.825456 0.050953 -1.273931

O -0.000073 1.829807 -1.275820

O -1.825554 0.050945 -1.273933

O -0.000074 -1.872276 -1.391787

III-57.54

Fe 1.193514 1.626492 0.009028

Fe 1.600435 -1.614403 -0.119058

Fe -1.303687 1.648344 -0.056126

Fe -1.610337 -1.650073 -0.253860

Fe -0.042972 -0.060289 1.889724

Fe 0.021032 -0.100939 -1.674637

O 1.299382 1.291763 1.740597

O -1.395596 1.242843 1.692249

O 1.290351 -1.275491 1.611590

O -1.290440 -1.320429 1.477772

O 1.833127 0.127066 -0.984159

O 0.009197 1.830563 -1.499987

O -1.819666 0.065995 -1.105598

O 0.053637 -1.984787 -1.299367

$Fe_6O_9^+$

I-68.85

Fe 1.516888 -0.993671 1.616549

Fe -1.687998 -0.895442 1.711400

Fe -0.170772 1.939469 1.568237

Fe 1.609905 -0.890002 -1.567442

Fe -1.609838 -0.889467 -1.548941

Fe -0.028140 1.925568 -1.606819

O 1.207666 0.782394 1.702856

O -1.507966 0.877221 2.044255

O -0.069431 -1.607951 2.113742

O 1.418478 0.877280 -2.017569

O -1.434057 0.858265 -1.938936

O -0.001210 -1.600125 -1.930505

O -0.144125 2.762390 -0.012751

O 2.250032 -1.395035 0.042854

O -2.283706 -1.291444 0.064820

II-67.20

Fe 1.061409 2.034514 -0.036349

Fe 1.421315 -1.183492 -0.189587

Fe -2.276151 0.462705 -0.158556

Fe -1.120847 -2.145488 0.662037

Fe 0.586254 0.571144 1.894888

Fe 0.096358 -0.153859 -2.035144

O 1.106721 2.252413 1.933113

O 0.688013 1.511446 -1.720208

O 0.367201 -1.293045 1.531039

O -0.180206 -1.960846 -0.990197

O 2.087988 0.333234 0.577639

O 1.828321 -0.878896 -1.895711

O -2.573952 -1.088747 0.685469

O -1.638360 0.230593 -1.831064

O -0.875903 1.216439 0.762659

III-66.45

Fe 1.326208 1.300895 0.037982

Fe 1.516123 -1.515737 0.084431

Fe -1.308609 1.309060 -0.053432

Fe -1.300374 -1.325252 0.036978

Fe -0.049701 0.049425 2.146024

Fe 0.086721 -0.085036 -2.087780

O 1.711823 0.049064 1.410004

O -0.033329 1.812786 1.299170

O -1.812982 0.033616 1.298640

O -0.049752 -1.711883 1.409719

O 1.920041 -0.007942 -1.199374

O 0.047502 1.829720 -1.300721

O -1.828775 -0.046583 -1.301524

O 0.009065 -1.918885 -1.199889

O -0.062306 0.063611 3.758181

$Fe_6O_{10}^+$

I-72.32

Fe 2.451115 0.124073 -0.672154

Fe -1.895246 0.245343 0.063551

Fe 0.301090 2.455358 -0.671815

Fe 0.053141 -1.881360 0.051474

Fe -0.477911 -0.437539 2.772836

Fe 1.918616 1.791456 2.107474

O 1.729560 1.616420 -1.379711

O 1.601889 -1.451807 -0.691195

O -1.342750 1.741102 -0.691592

O -1.578322 -1.409000 -0.554172

O 0.846237 0.784582 3.045556

O -0.026476 -1.906457 1.810811

O -1.904415 0.164932 1.818521

O 2.964086 2.758413 2.876367

O 0.871603 2.724548 0.989799

O 2.762102 0.670724 0.989091

II-71.04

Fe 0.776941 1.886732 -0.056043

Fe 2.146216 -1.273846 -0.069613

Fe -1.816223 1.659002 0.362493

Fe -2.172162 -1.192713 -0.154396

Fe 0.066713 -0.051866 1.861624

Fe 0.149418 -0.483728 -1.699462

O 1.182320 1.426052 1.638220

O -1.420421 1.065452 2.020066

O 1.501258 -1.121478 1.599814

O -1.099460 -1.392891 1.197940

O 1.680502 0.467757 -0.889764

O -0.638369 1.169649 -1.287932

O 1.290250 -1.922161 -1.595498

O -1.387196 -1.488121 -1.723738

O -0.574620 3.014026 0.357899

O -3.017378 0.352323 -0.052077

III-71.20

Fe 2.344931 1.276460 0.219589

Fe 1.199959 -1.502493 -0.161901

Fe -2.244113 0.991962 -0.264271

Fe -1.806951 -1.931059 0.860649

Fe 0.070819 0.154235 2.024139

Fe 0.269175 0.989201 -2.136412

O 1.511830 1.414207 1.735681

O -1.098464 1.275250 1.118371

O 1.206977 -1.196834 1.610923

O -1.231185 -1.076671 2.316623

O 1.509848 1.921418 -1.188584

O -1.437787 1.403918 -1.816686

O 0.683761 -0.741977 -1.783352

O -0.367660 -2.526929 -0.039260

O 2.746783 -0.368604 -0.159871

O -2.762957 -0.715819 -0.034288

$Fe_6O_{11}^+$

I-75.82

Fe 1.568526 -0.886585 1.608938

Fe -1.616920 -0.886869 1.622647

Fe -0.034876 2.024131 1.815405

Fe 1.702301 -1.069483 -1.692544

Fe -1.612055 -0.886946 -1.522173

Fe 0.053636 1.819860 -1.501954

O 1.281923 0.862380 2.024628

O -1.404708 0.900071 1.809876

O -0.029311 -1.586434 2.023097

O 1.403064 0.665314 -1.900464

O -1.385554 0.838067 -1.918433

O 0.018190 -1.638047 -1.716666

O 0.051234 2.560434 0.146724

O 2.211530 -1.295989 -0.016924

O -2.358087 -1.307834 0.048748

O -0.148753 3.174516 2.942495

O 2.662898 -1.796120 -2.771254

II-75.82

Fe 1.500561 -0.948875 1.499524

Fe -1.709998 -0.777731 1.547733

Fe -0.043516 2.039483 1.625443

Fe 1.588745 -1.007795 -1.625150

Fe -1.639741 -0.885922 -1.694691

Fe -0.033555 1.969735 -1.717906

O 1.266371 0.840703 1.512119

O -1.416243 0.975622 1.904835

O -0.136192 -1.534936 1.914590

O 1.295538 0.791195 -1.710006

O -1.387804 0.891451 -2.008024

O -0.050446 -1.627452 -2.039711

O -0.258179 2.560388 -0.035060

O 2.242510 -1.511414 -0.031565

O -2.337182 -1.205245 -0.070755

O 0.250111 3.186885 2.718624

O 0.141837 3.175358 -2.784624

III-74.12

Fe 1.508810 1.543971 0.052032

Fe 2.144046 -1.154579 0.052072

Fe -1.508012 1.544467 0.051999

Fe -2.144066 -1.153193 0.052058

Fe 0.000177 -0.050267 1.930231

Fe 0.000141 -0.050109 -1.826148

O 1.288466 1.212940 1.885926

O -1.287646 1.213419 1.885869

O 1.319204 -1.424563 1.524974

O -1.319333 -1.424067 1.524848

O 1.288513 1.213026 -1.781862

O -1.287684 1.213538 -1.781935

O 1.319035 -1.424507 -1.420788

O -1.319296 -1.423966 -1.420734

O 0.000777 2.569145 0.052064

O 2.996561 0.339672 0.052154

O -2.996339 0.341318 0.052104

$Fe_6O_{12}^+$

I-79.38

Fe 1.347765 -0.916780 1.462765

Fe -1.904282 -0.772030 1.843601

Fe -0.154116 1.928240 1.621191

Fe 1.711288 -0.994443 -1.760283

Fe -1.406709 -1.203763 -0.986182

Fe -0.224741 1.708990 -1.615011

O 1.194504 0.766696 1.937695

O -1.616877 0.947387 2.038026

O -0.336052 -1.193062 0.879247

O 1.220577 0.673670 -2.038661

O -1.502377 0.458704 -1.637562

O 0.136843 -1.793516 -1.724485

O -0.155796 2.561771 -0.044460

O 2.233560 -0.971231 -0.059707

O -2.714151 -1.216245 0.363808

O 2.762661 -1.698719 -2.766328

O 1.810150 -1.994717 2.554416

O -2.037151 -1.702229 3.149226

II-77.22

Fe 1.510677 2.172374 0.365245

Fe -1.499657 2.006956 -0.068483

Fe 1.926088 -0.676579 0.163189

Fe -2.343689 -0.812376 0.249286

Fe 0.099865 -2.851813 0.463798

Fe -0.472926 0.671879 2.065242

O -0.008151 2.959378 -0.261819

O 2.887936 0.790145 0.355456

O -2.893847 0.799479 -0.258470

O 1.606913 -2.392375 -0.368167

O -1.455585 -2.353081 -0.145616

O 0.971247 1.709700 2.044262

O -1.632595 2.040798 1.739127

O 0.609003 -0.789670 1.400423

O -1.922082 -0.551116 1.938747

O 0.157032 -3.708129 1.854848

O 0.836978 0.575171 -1.013714

O -0.607215 0.467976 -1.075184

III-76.50

Fe 1.519189 1.502798 0.046743

Fe 1.505428 -1.515963 0.040206

Fe -1.500104 1.512865 -0.003586

Fe -1.508716 -1.507801 -0.005043

Fe -0.023824 -0.001404 2.161058

Fe 0.043570 -0.000469 -2.131817

O 1.287667 1.285193 1.875410

O -1.315974 1.291313 1.831236

O 1.269806 -1.297418 1.864068

O -1.318949 -1.284708 1.826354

O 1.323651 1.293636 -1.788724

O -1.245503 1.298484 -1.828058

O 1.321350 -1.302564 -1.800074

O -1.258874 -1.294316 -1.833715

O 0.015112 2.586306 0.036956

O -0.007205 -2.593374 0.036729

O 2.581653 -0.013182 0.049157

O -2.572609 0.007612 -0.038964

$Fe_6O_{13}^+$

I-87.21

Fe 1.276469 -0.876554 1.525980

Fe -1.931281 -0.790502 1.833675

Fe -0.256635 2.015765 1.710988

Fe 1.730853 -1.092073 -1.644652

Fe -1.410996 -1.272185 -0.978944

Fe -0.190416 1.624133 -1.509259

O 1.116900 0.860767 1.626581

O -1.677884 0.953909 1.919846

O -0.385861 -1.302769 0.961229

O 1.287452 0.609009 -1.837534

O -1.477939 0.390856 -1.621481

O 0.137505 -1.853453 -1.700260

O -0.271714 2.557857 0.044985

O 2.219765 -1.196251 0.053915

O -2.715842 -1.294575 0.336653

O -0.059331 3.070709 2.904101

O 2.711886 -1.733319 -2.755492

O 1.633164 -1.721686 2.842917

O -2.224409 -1.613690 3.175620

II-82.65

Fe 1.305468 -1.049975 1.527519

Fe -1.966016 -0.807203 1.778097

Fe -0.125092 1.837375 1.672199

Fe 1.855005 -0.834197 -1.643926

Fe -1.291874 -1.134278 -0.980680

Fe -0.085577 1.828131 -1.603980

O 1.168160 0.626686 2.022937

O -1.622407 0.887691 2.030594

O -0.371685 -1.297555 0.879871

O 1.419097 0.852096 -1.729244

O -1.325416 0.582507 -1.500278

O 0.244567 -1.608672 -1.710232

O -0.048762 2.531989 0.013437

O 2.280775 -1.085176 0.048991

O -2.695198 -1.195783 0.232689

O 2.759943 -1.514813 -2.788101

O -0.259457 2.829401 -2.861809

O 1.623917 -2.149298 2.648795

O -2.251038 -1.722124 3.068112

III-82.65

Fe 1.543590 -0.991234 1.700163

Fe -1.708623 -0.865479 1.711648

Fe -0.042797 1.930906 1.649029

Fe 1.516096 -1.000790 -1.547382

Fe -1.710901 -0.887702 -1.611856

Fe -0.051895 1.880150 -1.602367

O 1.220788 0.719838 1.410053

O -1.408978 0.894335 2.023066

O -0.075798 -1.576746 2.038459

O 1.154662 0.677955 -1.082328

O -1.414398 0.863160 -2.007743

O -0.073179 -1.610023 -1.943822

O -0.394598 2.547843 0.007120

O 1.893591 -1.630898 0.065808

O -2.293455 -1.187624 0.051430

O 0.341746 3.040558 2.756690

O 2.661371 -1.087575 -2.671882

O 0.506154 2.868549 -2.740230

O 2.648791 -1.289021 2.838732

$Fe_6O_{14}^+$

I-90.60

Fe 1.823535 -1.003408 1.747979

Fe -1.314733 -1.195229 1.119812

Fe -0.039131 1.742097 1.728711

Fe 1.339787 -0.977197 -1.407632

Fe -1.882255 -0.743520 -1.641784

Fe -0.065729 1.988233 -1.502769

O 1.408015 0.692453 1.619239

O -1.313288 0.555341 1.498130

O 0.188687 -1.704574 1.902890

O 1.235463 0.777162 -1.408916

O -1.538956 0.980884 -1.608668

O -0.331710 -1.401965 -0.874851

O -0.059184 2.593710 0.148673

O 2.258047 -1.344658 0.060522

O -2.643480 -1.299645 -0.143072

O -0.060849 2.480441 3.170205

O 1.711887 -1.737952 -2.770103

O 0.062235 2.982138 -2.754172

O 2.740627 -1.531655 2.965786

O -2.242676 -1.427027 -3.048522

II-84.00

Fe 1.445652 1.609111 0.156196

Fe 1.405295 -1.619712 -0.117540

Fe -1.516547 1.403801 -0.057310

Fe -1.428167 -1.594374 -0.069723

Fe 0.029410 0.249289 2.163993

Fe 0.083349 -0.180046 -2.172008

O 1.530911 0.039505 1.112170

O 0.067337 1.958284 1.396066

O -1.519094 0.066761 1.204912

O -0.020407 -1.813456 1.067651

O 1.723851 -0.232017 -1.299356

O 0.051558 1.500218 -1.014856

O -1.739276 -0.085221 -1.185126

O -0.030618 -1.911287 -1.327949

O 2.679243 2.554876 -0.136792

O 2.587248 -2.660065 0.126464

O -2.574013 2.594990 -0.043697

O -2.657689 -2.593521 0.063499

O 0.041702 -0.048331 3.717464

O -0.261128 0.347674 -3.646095

III-81.80

Fe 1.508160 1.508350 -0.000001

Fe 1.508154 -1.508258 0.000001

Fe -1.508154 1.508258 0.000001

Fe -1.508160 -1.508350 -0.000001

Fe 0.000000 0.000000 2.252648

Fe 0.000000 0.000000 -2.252644

O 1.277452 1.277444 1.800491

O -1.277478 1.277452 1.800494

O 1.277478 -1.277452 1.800495

O -1.277452 -1.277444 1.800491

O 1.277460 1.277453 -1.800493

O -1.277471 1.277445 -1.800494

O 1.277471 -1.277445 -1.800494

O -1.277460 -1.277453 -1.800493

O 0.000000 0.000000 3.893050

O 0.000000 -0.000001 -3.893052

O 2.586099 0.000048 0.000000

O -2.586099 -0.000048 0.000000

O -0.000035 2.586689 0.000000

O 0.000035 -2.586689 0.000000

$Fe_6O_{15}^+$

I-93.87

Fe 1.652290 -0.974679 1.607092

Fe -1.625887 -1.012940 1.629632

Fe -0.021244 1.848246 1.655291

Fe 1.613300 -0.963418 -1.605643

Fe -1.672550 -1.015469 -1.563715

Fe -0.080510 1.860683 -1.570067

O 1.382564 0.772805 1.506265

O -1.399517 0.737306 1.499260

O 0.016558 -1.629191 1.393743

O 1.319665 0.779238 -1.499150

O -1.438926 0.731458 -1.403816

O -0.019631 -1.630361 -1.402483

O -0.041220 2.593625 0.041766

O 2.319768 -1.300393 -0.014449

O -2.328241 -1.399455 0.045361

O -0.065488 2.751648 2.973659

O 2.342637 -1.443388 -2.950538

O -0.161774 2.777030 -2.881746

O 2.367168 -1.517636 2.930577

O -2.449128 -1.502955 -2.874498

O -2.338435 -1.506638 2.978544

II-88.41

Fe 1.653470 -1.041689 1.690226

Fe -1.614899 -1.032196 1.409836

Fe -0.069973 1.890397 1.806645

Fe 1.609265 -0.990259 -1.565688

Fe -1.668853 -0.975504 -1.697906

Fe -0.047475 1.876840 -1.509661

O 1.304283 0.663627 1.694556

O -1.420688 0.679310 1.747759

O 0.026585 -1.712465 1.699179

O 1.318725 0.746201 -1.504729

O -1.442604 0.773189 -1.511890

O -0.045739 -1.618928 -1.401933

O -0.027397 2.545236 0.089604

O 2.267679 -1.313353 0.050787

O -2.442171 -1.392420 -0.169296

O 2.333358 -1.594351 -2.862596

O -0.065401 2.882185 -2.766087

O 2.554622 -1.606698 2.894964

O -2.331681 -1.420841 -3.090754

O -0.773747 3.403342 2.760301

O 0.259870 2.664233 3.494952

III-88.62

Fe 1.502766 -0.989081 1.616012

Fe -1.757707 -0.995617 1.711956

Fe -0.127702 1.918538 1.801156

Fe 1.720809 -0.978894 -1.616954

Fe -1.536429 -1.037938 -1.371013

Fe -0.058711 1.863435 -1.504138

O 1.233300 0.736593 1.611285

O -1.532368 0.706521 1.821140

O -0.107839 -1.612352 1.283068

O 1.319971 0.736095 -1.486042

O -1.404702 0.725692 -1.611208

O 0.072655 -1.632546 -1.803297

O -0.154709 2.558285 0.097142

O 2.257264 -1.313025 0.045976

O -2.463438 -1.392785 0.144236

O 2.641930 -1.519963 -2.826170

O 0.042580 2.880518 -2.756701

O 2.141201 -1.602050 2.951403

O -2.343033 -1.742571 3.013380

O -0.842938 3.400291 2.853767

O 0.151585 2.632088 3.569137

$Fe_6O_{16}^+$

I-96.36

Fe 1.581741 -1.007774 1.602970

Fe -1.659420 -0.896563 1.626628

Fe 0.045571 1.937472 1.730147

Fe 1.579310 -1.008221 -1.607384

Fe -1.719078 -0.978578 -1.546865

Fe -0.034013 1.846962 -1.535636

O 1.380967 0.722392 1.715915

O -1.379128 0.810956 1.616428

O -0.053557 -1.586451 1.268887

O 1.339207 0.742994 -1.509185

O -1.415391 0.761729 -1.421414

O -0.077487 -1.620590 -1.500641

O 0.064013 2.611346 0.047693

O 2.276332 -1.298070 -0.001800

O -2.431196 -1.255695 0.070070

O 2.344270 -1.517249 -2.924737

O -0.073168 2.782344 -2.844935

O 2.254560 -1.721225 2.864674

O -2.553943 -1.413122 -2.850062

O -2.256276 -1.540633 2.968403

O -0.470932 3.488980 2.827183

O 0.128020 2.429862 3.593804

II-91.96

Fe 1.583503 -1.059942 1.653546

Fe -1.689210 -1.054892 1.655715

Fe -0.049230 1.817529 1.889544

Fe 1.592213 -0.909253 -1.578047

Fe -1.698664 -0.907207 -1.576583

Fe -0.051883 1.933081 -1.496355

O 1.323411 0.648493 1.933038

O -1.423547 0.653824 1.932080

O -0.053385 -1.664640 1.388355

O 1.323730 0.830301 -1.630832

O -1.429560 0.831669 -1.630288

O -0.053357 -1.520082 -1.390630

O -0.055663 2.464903 0.148775

O 2.274690 -1.187473 0.038729

O -2.381122 -1.184169 0.040395

O 2.342294 -1.506836 -2.866535

O -0.053187 3.063864 -2.657852

O 2.277288 -1.828173 2.879704

O -2.447532 -1.505658 -2.865538

O -2.380603 -1.826704 2.881485

O 0.709646 3.388310 2.874628

O -0.714333 3.384392 2.959520

O -2.475998 -1.505903 -2.780102

O -2.394821 -1.716448 2.966222

O 0.363966 2.731202 3.516117

O -0.657767 3.503054 2.745094

ANIONIC OXIDES

Fe_2O^-

I - 9.57

Fe 1.076099 -0.048445 0.000000

Fe -1.076299 -0.048698 0.000000

O -0.000702 1.509220 0.000000

II - 9.24

Fe 1.802538 0.000004 0.000018

Fe -1.802706 0.000000 0.000014

O -0.000216 -0.000001 -0.000015

III - 9.30

Fe 1.092047 -0.265790 -0.026047

Fe -1.091912 0.053350 0.021183

O 2.242901 1.001281 0.051897

$Fe_2O_2^-$

I - 15.56

Fe 1.237569 0.000003 0.000005

Fe -1.250373 0.000002 0.000010

O -0.056776 1.395778 0.000003

O -0.056775 -1.395777 0.000011

II - 15.32

Fe 0.952463 0.000000 0.000000

Fe -2.737920 0.000000 0.000000

O -0.933752 0.000001 0.000001

O 2.663851 0.000000 0.000000

III - 15.52

Fe 0.575418 0.775834 -0.052919

Fe -1.510680 -0.575868 0.052144

O 2.256728 0.895004 -0.156302

O -1.236920 1.228130 0.052887

$Fe_2O_3^-$

I - 21.35

Fe 0.309319 0.256586 1.199855

Fe 0.474640 0.466665 -1.204547

O 1.400263 -0.647857 -0.056883

O -0.578405 1.407858 -0.016206

O 0.157236 0.060120 2.877863

II - 20.60

Fe 0.362610 0.052094 -0.461276

Fe -1.367600 0.052049 -2.145807

O 1.416677 0.052084 0.869019

O -0.471557 -1.375133 -1.392119

O -0.471123 1.479269 -1.392479

III - 19.15

Fe 1.613621 -0.461042 -0.082965

Fe -1.099279 -0.398329 -0.156869

O 0.345868 0.793014 -0.260531

O 2.249623 -1.215535 -1.424487

O 2.164295 -0.892386 1.428378

$Fe_2O_4^-$

I - 27.06

Fe 0.105009 -0.045112 1.204318

Fe 0.056049 -0.054591 -1.352189

O 0.684306 -1.218875 -0.081654

O -0.689958 1.016660 -0.062418

O 0.044830 -0.055184 -3.039039

O 0.050049 -0.070639 2.874198

II - 25.56

Fe -0.439220 0.788366 0.895728

Fe 1.364005 -0.466897 -0.890773

O 2.881298 -0.162500 -1.613798

O -0.681853 2.421348 0.665181

O -0.475733 -0.350284 -0.457295

O -0.155334 0.249721 2.447731

III - 24.72

Fe 1.118342 0.000000 0.000000

Fe -1.209516 0.000000 0.000000

O -0.141823 1.472956 0.000000

O -0.141823 -1.472956 0.000000

O 2.851627 0.771909 -0.000001

O 2.851627 -0.771909 0.000000

$Fe_2O_5^-$

I - 31.43

Fe 0.359793 0.565723 1.442465

Fe -0.054304 -0.458363 -0.977501

O 1.307772 -0.475143 0.269525

O -0.996738 0.589766 0.218396

O -0.760196 -1.942209 -1.209455

O 0.595409 1.208666 2.980204

O 0.357191 0.354790 -2.364289

II - 31.36

Fe 0.036331 0.670644 1.124989

Fe 0.364199 -0.058674 -1.409125

O 0.375521 1.520169 -0.478030

O -1.411435 1.098307 1.814155

O -0.051473 -0.901885 0.157301

O 1.335491 0.689633 2.156774

O 0.668980 -0.562266 -2.986340

$Fe_2O_6^-$

I - 34.80

Fe 0.271269 0.569015 1.132715

Fe -0.028979 -0.336001 -1.293752

O 0.036955 1.325286 -0.518139

O -1.017641 0.793414 2.144265

O 0.260268 -1.091706 0.350761

O -1.516062 -0.686569 -1.926678

O 1.724606 0.965917 1.818154

O 1.218181 -0.585150 -2.352175

II - 35.84

Fe 1.374233 0.000001 -0.000001

Fe -1.477238 0.000000 0.000023

O -0.014115 1.224755 -0.000011

O -0.014114 -1.224756 -0.000011

O 2.828788 1.097234 -0.000018

O 2.828789 -1.097235 -0.000018

O -2.764237 1.204113 -0.000001

O -2.764239 -1.204113 -0.000001

Fe_3O^-

I - 13.12

Fe 1.401134 0.369045 0.157653

Fe -0.439596 0.879107 -0.997238

Fe 0.504604 2.239749 0.988314

O -0.985835 2.448611 -0.133260

II - 12.44

Fe 1.088421 0.056002 -0.053616

Fe -1.194750 -0.155237 -0.155768

Fe 0.057810 2.104795 -0.164252

O -0.167012 0.768102 1.320044

III - 11.88

Fe 1.079459 -0.045582 0.000000

Fe -1.079451 -0.045579 0.000000

Fe -0.000002 3.518085 0.000000

O 0.000010 1.602288 0.000000

$Fe_3O_2^-$

I - 19.80

Fe 1.405546 0.085126 0.057337

Fe -1.237421 0.050452 -0.155328

Fe -0.151540 2.234134 -0.154634

O 0.045490 -1.197757 0.044796

O 1.612918 1.943554 0.045319

II - 19.85

Fe 1.096202 -0.157169 0.155602

Fe -1.403295 -0.053884 0.050093

Fe -0.052979 2.035036 -0.156623

O -0.159277 0.994933 1.348520

O -0.173009 -1.312680 -0.574310

III - 18.15

Fe 1.483305 0.882568 0.580475

Fe -1.190811 -0.003103 -0.166865

Fe 0.570866 2.027029 -1.306886

O 0.161147 -0.260534 1.007068

O -1.018843 1.208516 -1.501368

$Fe_3O_3^-$

I - 26.58

Fe 1.151843 0.156452 0.051498

Fe -1.201008 -0.047365 0.049616

Fe -0.020748 2.221199 0.163051

O 0.067385 -1.394189 -0.046690

O 1.809860 1.928665 0.150300

O -1.824818 1.719148 0.154349

II - 24.54

Fe 1.068151 0.035889 0.150445

Fe -1.172318 0.035887 0.150439

Fe -0.052086 2.293406 -0.163209

O -0.052080 1.107961 1.434693

O -0.052083 -1.197206 -0.776544

O -0.052083 3.190396 -1.609139

III - 24.06

Fe 0.997161 0.049297 0.049197

Fe 4.576550 -0.049840 -0.049905

Fe -2.660873 0.057503 0.056952

O -0.787219 -0.065763 -0.063945

O 2.778145 0.052345 0.051476

O -4.364793 0.052637 0.053150

$Fe_3O_4^-$

I - 31.01

Fe 1.200262 0.469861 0.189535

Fe -1.325622 0.618702 0.638438

Fe -0.448493 1.594808 -1.428813

O 0.043094 -0.480200 1.304752

O 1.283834 0.888886 -1.627229

O -2.222793 1.096853 -0.966667

O 0.030517 2.152163 0.478877

II - 31.36

Fe 1.298414 0.063153 -0.103363

Fe -1.245623 -0.055964 0.056664

Fe -0.002637 2.341093 0.146003

O 0.059106 -1.263879 -0.362736

O 1.696884 1.701831 0.569905

O -1.716889 1.688842 0.260053

O -0.141965 3.819407 -0.651478

III - 31.22

Fe 0.504635 -0.576213 -1.305275

Fe -0.475032 -0.443140 0.994572

Fe 0.579214 1.513316 0.093467

O 0.043000 2.094419 1.804684

O 1.198063 1.095976 -1.619653

O -0.678194 0.816982 2.377597

O -0.363623 -1.819021 -0.268743

$Fe_3O_5^-$

I - 36.08

Fe 1.197402 0.264850 -0.675947

Fe -0.788661 -0.923346 0.568712

Fe -0.697324 2.073465 -0.121381

O -1.692887 0.646538 0.252014

O 0.574130 1.818671 -1.409883

O -0.677473 3.491595 0.785455

O -1.795571 -2.120910 1.206384

O 0.971459 -1.311253 0.157917

II - 34.80

Fe 1.095809 0.255013 0.104794

Fe -1.302538 0.262977 0.506562

Fe -0.390847 1.500752 -1.451828

O 0.091101 -0.579221 1.504718

O 1.433324 1.303570 -1.494765

O -2.132431 1.319873 -0.887243

O -0.063643 1.932734 0.454896

O -0.358609 -0.465542 -1.188241

III - 35.12

Fe 1.413849 0.680748 -0.260380

Fe -0.999077 -0.455981 -0.057656

Fe -0.690659 2.147507 0.024310

O -0.146121 0.876568 1.208109

O -0.282795 0.867504 -1.314016

O -1.201339 3.715909 0.272930

O 3.000112 0.124114 -0.046082

O -1.508525 -2.050324 0.162261

$Fe_3O_6^-$

I - 41.22

Fe 1.616197 0.123723 -0.569453

Fe -0.984983 -1.028742 0.472538

Fe -0.580605 2.101324 0.047400

O -1.620289 0.669524 0.444245

O 0.720769 1.609590 -1.082266

O -0.878116 3.692479 0.480384

O 3.278362 -0.052965 -0.379924

O -1.624721 -2.332001 1.309218

O 0.373571 -1.185664 -0.684157

II - 40.32

Fe 1.161615 0.151877 1.202506

Fe -0.788148 -0.082393 -1.319149

Fe 0.049550 2.244328 0.325113

O 1.576833 1.899896 1.298510

O 0.895575 -0.569475 -0.327424

O -0.760051 1.728092 -1.199025

O -2.039948 -0.793680 -0.488129

O 0.791111 -0.671586 2.583734

O -0.477887 -0.670626 -2.842700

III - 37.62

Fe 1.181004 0.253386 0.050081

Fe -1.389341 0.300658 0.512967

Fe -0.376222 1.517234 -1.583045

O 0.049866 -0.471331 1.408002

O 1.545288 1.211398 -1.525743

O -2.150857 1.295161 -0.858472

O -0.053975 1.835948 0.330063

O -0.361375 -0.387990 -1.106362

O -0.553452 2.436718 -2.965342

$Fe_3O_7^-$

I - 45.30

Fe 1.407080 -0.909069 0.172451

Fe -1.374019 -0.889314 -0.057316

Fe -0.030747 1.544827 0.058073

O 1.593866 0.806805 -0.372532

O -1.427835 0.773478 -0.782995

O 0.058153 -1.723338 -0.755396

O 0.048601 3.184741 0.265376

O 2.771902 -1.831251 0.361504

O -2.696812 -1.718600 0.467332

O -0.147146 -0.152877 1.180364

II - 44.00

Fe 1.182995 0.331026 0.182196

Fe -1.471006 0.363968 0.562026

Fe -0.343593 1.570958 -1.553451

O -0.061118 -0.366755 1.499215

O 1.537134 1.303612 -1.415439

O -2.141531 1.314947 -0.870277

O -0.047257 1.838793 0.359286

O -0.256590 -0.289898 -0.978467

O -0.475497 2.451536 -2.959347

O 2.701124 -0.144104 0.669721

III - 43.80

Fe 1.182995 0.331026 0.182196

Fe -1.471006 0.363968 0.562026

Fe -0.343593 1.570958 -1.553451

O -0.061118 -0.366755 1.499215

O 1.537134 1.303612 -1.415439

O -2.141531 1.314947 -0.870277

O -0.047257 1.838793 0.359286

O -0.256590 -0.289898 -0.978467

O -0.475497 2.451536 -2.959347

O 2.701124 -0.144104 0.669721

$Fe_3O_8^-$

I - 48.29

Fe 1.303599 0.270698 0.054653

Fe -1.295367 0.193812 0.474161

Fe -0.349042 1.510224 -1.603971

O 0.199552 -0.467902 1.404030

O 1.535876 1.197234 -1.609532

O -2.081402 1.224006 -0.883322

O 0.030204 1.709009 0.277557

O -0.230831 -0.386718 -1.019109

O -0.581744 2.546173 -2.881315

O 2.853458 -0.053867 0.558592

O -2.583794 -0.460908 1.292103

II - 47.08

Fe 1.725821 -1.296156 0.151843

Fe -1.629045 -1.400342 0.123112

Fe -0.053857 1.457385 0.154135

O 1.418589 0.470917 0.454378

O -1.414371 0.350697 0.477023

O 0.067358 -1.948122 0.274569

O -0.044342 3.084086 -0.251221

O 3.065080 -2.635957 0.061812

O 3.484856 -1.311886 -0.576470

O -2.868947 -2.857852 0.173879

O -3.372959 -1.637242 -0.587179

III - 45.21

Fe 1.407471 -0.260225 0.019392

Fe -1.248138 -0.149891 0.047812

Fe 0.046344 2.093884 0.038654

O 0.648544 -1.936253 0.054127

O -0.892911 -2.024452 0.052467

O 2.549700 1.177481 0.050992

O 1.877551 2.575812 0.056122

O -2.579908 1.224302 -0.053948

O -1.814711 2.544874 -0.043953

O 0.067242 0.571562 1.319227

O 0.156901 0.532260 -1.249051

$Fe_3O_9^-$

I - 51.12

Fe 1.227762 0.157286 0.168414

Fe -1.352061 0.257120 0.675030

Fe -0.363337 1.515460 -1.440141

O 0.081020 -0.566307 1.513924

O 1.507018 1.094828 -1.444795

O -2.043659 1.398565 -0.657053

O 0.077730 1.673411 0.466281

O -0.374760 -0.367231 -0.896846

O -0.658352 1.816854 -3.289813

O 2.756191 -0.268806 0.657726

O -2.679494 -0.254116 1.525420

O -0.478337 3.075614 -2.491908

II - 50.16

Fe 1.616295 -1.413054 0.056804

Fe -1.717156 -1.373692 -0.044430

Fe -0.056211 1.521783 0.009671

O 1.336770 0.373306 0.050449

O -1.437134 0.397305 -0.155756

O -0.058491 -2.038202 0.146090

O 0.639393 3.277911 -0.265114

O -0.742741 3.258452 0.366859

O 2.766953 -2.885425 -0.273323

O 3.475663 -1.708165 0.376762

O -2.955330 -2.760751 -0.563838

O -3.567780 -1.734005 0.376706

III - 48.00

Fe 1.706247 -1.378094 0.037998

Fe -1.617662 -1.341184 0.048837

Fe 0.053665 1.514972 0.051533

O 0.042567 3.300046 -0.058117

O 0.054913 4.689111 0.054751

O -4.420704 -2.860917 -0.052728

O -3.178335 -2.240863 0.053499

O 4.402716 -3.065054 0.050969

O 3.212260 -2.341095 0.055682

O 0.037992 -2.048242 0.057735

O 1.522211 0.436002 0.061648

O -1.392052 0.443415 0.054509

Fe_4O^-

II - 16.60

Fe 1.441983 -0.367384 -0.364744

Fe -0.886479 0.230453 -0.675584

Fe 0.477919 1.204752 1.206822

Fe -0.156893 -1.131902 1.195130

O -0.897446 1.929020 0.145019

III - 15.95

Fe 1.855086 -0.220704 -0.000008

Fe -1.589050 0.006733 -0.000002

Fe -0.220861 1.855293 -0.000002

Fe 0.006782 -1.589230 0.000017

O 1.605357 1.605484 -0.000022

$Fe_4O_2^-$

I - 22.98

Fe 1.153530 -0.055827 -0.044260

Fe -1.257352 -0.055875 -0.044347

Fe -0.052055 1.192960 1.760972

Fe -0.052063 -1.265159 1.707248

O -0.052092 1.648647 -0.057831

O -0.052046 -0.034473 3.148201

II - 22.98

Fe 1.200931 0.262382 -0.153927

Fe -1.308035 0.257473 -0.061583

Fe -0.150810 1.261499 1.721801

Fe -0.154295 -1.192166 1.544312

O -0.057508 -0.261476 -1.403803

O 1.705463 1.293520 1.298522

III - 23.10

Fe 1.289910 0.002539 -0.256780

Fe -1.258333 -0.057057 -0.258570

Fe -0.046748 2.089403 -0.052208

Fe 0.055122 -1.892344 -0.158999

O 1.761359 1.841435 -0.158226

O -1.842060 1.740967 -0.054103

$Fe_4O_3^-$

II - 29.61

Fe 1.508668 0.199376 0.361817

Fe -0.860015 -0.478657 0.041465

Fe 0.020517 1.188535 1.937650

Fe 0.146654 -1.185794 2.197893

O -0.465962 0.047652 3.406914

O 1.426932 1.955712 0.878429

O 0.893424 -1.631244 0.469746

III - 28.91

Fe 1.285933 -0.051983 0.002313

Fe -1.288060 -0.052540 0.122917

Fe -0.051424 1.161988 1.824301

Fe -0.050758 -1.267283 1.823773

O -0.159993 -0.051980 -1.315519

O 1.516452 1.613016 0.996778

O 1.517649 -1.716986 0.996103

$Fe_4O_4^-$

I - 36.16

Fe 2.147930 -0.000042 0.000000

Fe -2.148034 0.000012 0.000000

Fe -0.000125 2.361074 0.000000

Fe -0.000125 -2.361049 0.000000

O 1.677215 1.729969 0.000000

O -1.677410 1.729951 -0.000001

O -1.677482 -1.729986 0.000000

O 1.677112 -1.729904 0.000001

II - 35.76

Fe 1.302044 0.147053 0.055033

Fe -1.294627 -0.048316 -0.084359

Fe -0.071564 1.202577 1.711859

Fe -0.110605 -1.298492 1.714567

O -0.056904 0.052185 -1.399735

O 1.519585 1.821861 1.087511

O 1.514867 -1.606488 0.986060

O -1.630060 -0.071584 1.841115

III - 34.08

Fe 1.199244 -0.048779 0.088720

Fe -1.195401 0.048697 -0.160342

Fe 0.054572 1.295287 1.726093

Fe -0.046230 -1.296260 1.724892

O 1.513600 -0.055553 2.140201

O -1.543947 0.056373 1.830559

O -0.066655 -1.643229 -0.274974

O 0.052072 1.645754 -0.271958

$Fe_4O_5^-$

I - 41.40

Fe 1.509499 -0.596940 0.444859

Fe -0.993149 -0.258653 -0.504889

Fe -0.135647 1.173431 1.618097

Fe -0.480046 -1.470373 2.035324

O 1.717344 1.119422 1.215973

O -0.884249 0.046521 2.925370

O 0.585024 -0.805784 -1.182277

O -1.421604 1.319251 0.254820

O 1.113275 -2.113809 1.491587

II - 41.13

Fe 2.134833 -0.015401 0.886725

Fe -0.052312 1.826768 0.052635

Fe 0.305216 0.055866 2.435238

Fe -0.679611 -0.487901 -0.468824

O 1.786844 1.508795 -0.050609

O -1.284944 1.100357 -1.191021

O -0.468566 1.604859 1.866179

O 0.451571 -1.229811 0.779175

O 2.144765 -0.246334 2.770311

III - 41.31

Fe 1.938364 -0.154957 0.819902

Fe -1.862127 -0.154485 0.792043

Fe 0.068371 1.732884 0.561091

Fe 0.015985 -2.034420 1.090108

O -1.849092 -1.999807 1.092743

O 1.934152 1.699449 0.582676

O 1.832004 -1.908929 1.390221

O -1.748717 1.687571 0.873802

O 0.045061 -0.270477 -0.032983

$Fe_4O_6^-$

I - 47.20

Fe 1.413911 0.164221 -0.100202

Fe -1.434096 -0.052072 0.045171

Fe 0.251593 1.506638 1.765865

Fe -0.057141 -1.343025 1.829314

O -0.110430 0.053525 -1.176885

O 1.818201 1.787407 0.767499

O 1.479090 -1.420869 0.877563

O -1.706854 -1.624643 0.997724

O -1.401299 1.539966 0.890106

O 0.161870 0.063456 2.944438

II - 45.70

Fe 0.970828 1.232725 0.164562

Fe 1.543474 -1.404120 0.259920

Fe -1.508422 1.547035 -0.366544

Fe -0.975254 -1.010627 0.129170

O 0.263249 -0.172045 1.387051

O -0.381184 0.464583 -1.307121

O 2.461316 0.149816 -0.163326

O -2.532551 0.164377 0.156456

O -0.251674 2.748604 0.164726

O 0.109711 -2.542680 -0.132639

III - 45.20

Fe -1.312816 0.605889 0.265256

Fe 1.334425 0.574153 0.355539

Fe -0.117195 -1.616544 -0.155913

Fe 0.064090 1.409011 2.411404

O -1.936104 -1.113952 0.038939

O 1.653108 -1.244328 0.269941

O 0.021858 2.036268 0.467395

O 0.050881 0.189598 -1.090454

O 1.897389 1.080727 2.038726

O -1.708140 0.998220 2.029866

$Fe_4O_7^-$

I - 51.15

Fe 1.503585 0.048136 -0.298767

Fe -1.393725 0.002009 0.054854

Fe 0.229420 1.741357 1.950809

Fe 0.013196 -1.301168 1.812299

O -0.075906 0.057100 -1.208957

O 1.561216 1.618723 0.782142

O 1.523768 -1.411532 0.796671

O -1.632870 -1.602771 0.989633

O -1.285204 1.600780 0.926668

O 0.270188 0.148164 2.872950

O 0.147004 2.980114 3.050383

II - 50.27

Fe 1.267740 0.266917 -0.056504

Fe -1.306750 0.219326 0.046999

Fe 0.114473 1.420020 1.826626

Fe -0.072661 -1.348304 1.763586

O -0.059827 -0.375056 -1.216235

O 1.925597 1.390631 1.307547

O 1.517421 -1.330566 0.779000

O -1.711371 -1.412952 0.796055

O -1.733090 1.296983 1.515142

O 0.155440 0.033654 3.004494

O -0.036235 1.740271 -0.107610

III - 50.27

Fe -1.284223 0.596007 -0.082279

Fe 1.287036 0.788194 -0.183131

Fe 0.050799 -1.522943 0.719628

Fe 0.149200 0.918832 2.033280

O -1.614277 -1.213612 -0.149496

O 1.614228 -1.002486 -0.164888

O -0.058194 2.072795 0.455903

O -0.054574 0.682661 -1.492021

O 1.945058 1.193572 1.535532

O -1.703655 0.880441 1.717495

O 0.261629 -0.850232 2.451869

$Fe_4O_8^-$

I - 55.20

Fe 1.541995 0.058351 -0.348503

Fe -1.616413 0.062188 -0.153939

Fe -0.043088 1.570695 1.924966

Fe -0.002985 -1.586609 1.996344

O -0.091582 0.130403 -1.112397

O 1.401076 1.430376 0.771032

O 1.302066 -1.300528 0.798492

O -1.426587 -1.411470 0.951953

O -1.534913 1.521869 0.907522

O -0.049698 0.014175 2.836421

O 2.694490 -0.050683 -1.506807

O 0.160728 -2.792437 3.091051

II - 54.48

Fe 1.227111 0.267300 -0.166970

Fe -1.304216 0.228280 -0.149777

Fe -0.000470 1.424423 1.667170

Fe 0.052493 -1.407277 1.788098

O -0.053195 -0.371927 -1.380877

O 1.833563 1.396832 1.218057

O 1.520767 -1.313472 0.682019

O -1.425621 -1.402909 0.785328

O -1.827855 1.292770 1.282630

O 0.051165 0.070094 2.881765

O -0.054361 1.750775 -0.266473

O 0.159807 -2.765057 2.735286

III - 54.00

$Fe_4O_9^-$

I - 59.80

Fe 1.452409 -0.042883 -0.330962

Fe -1.514128 -0.044818 -0.044807

Fe -0.055795 1.540243 2.012422

Fe -0.027713 -1.680338 2.026918

O -0.267994 -0.026882 -1.223755

O 1.260067 1.383938 0.769410

O 1.284550 -1.430346 0.793484

O -1.499197 -1.498994 0.961623

O -1.613491 1.408553 0.864409

O -0.043167 -0.060062 2.836642

O 2.543073 0.149144 -1.582510

O 0.369812 -2.903519 3.091619

O -0.168630 3.070236 2.676192

II - 58.37

Fe 1.299132 0.260261 -0.188247

Fe -1.236018 0.173140 -0.171847

Fe -0.059644 1.611438 1.612629

Fe 0.055355 -1.387539 1.822582

O 0.031278 -0.465795 -1.377002

O 1.836369 1.396676 1.128730

O 1.499841 -1.314740 0.783689

O -1.403412 -1.426582 0.770850

O -1.839069 1.292008 1.162738

O 0.048826 0.062617 2.789775

O -0.044233 1.685428 -0.351483

O -0.028341 -2.754485 2.759184

O 0.063666 2.884977 2.707074

III - 43.94

Fe 1.223102 0.362577 -0.149396

Fe -1.302129 0.362835 -0.166435

Fe 0.001467 1.487918 1.668589

Fe -0.055708 -1.524504 1.824503

O -0.054514 -0.233258 -1.400478

O 1.815830 1.440283 1.276491

O 1.422636 -1.206207 0.659488

O -1.515387 -1.239268 0.678269

O -1.839515 1.412633 1.258245

O -0.043761 0.069597 2.782042

O -0.033619 1.890582 -0.256497

O 0.653833 -2.778764 3.090346

O -0.418759 -3.398325 2.248222

$Fe_4O_{10}^-$

I - 64.12

Fe 1.604382 0.020579 -0.358291

Fe -1.612591 0.017991 -0.270260

Fe 0.052760 1.691817 1.915447

Fe 0.053512 -1.529972 2.012744

O -0.027361 -0.032020 -1.109003

O 1.400186 1.413454 0.760238

O 1.400260 -1.306821 0.837349

O -1.343955 -1.316614 0.896938

O -1.339312 1.420686 0.813331

O 0.062176 0.108143 2.761239

O 2.892423 0.040951 -1.388717

O 0.060345 -2.864410 2.989366

O 0.056102 3.085004 2.796284

O -2.975279 0.038397 -1.195524

II - 62.44

Fe 1.452433 0.058152 -0.483006

Fe -1.509033 0.051437 0.048045

Fe 0.034723 1.731837 1.931574

Fe 0.043806 -1.498648 2.023959

O -0.299929 0.040664 -1.196901

O 1.290395 1.495980 0.715467

O 1.300118 -1.309038 0.802706

O -1.483818 -1.399195 1.007130

O -1.506662 1.532792 0.956151

O 0.053209 0.141096 2.779945

O -0.037684 -2.858061 2.962865

O -0.047906 3.158017 2.766348

O 3.293094 0.050374 -0.873498

O 2.432239 -0.050568 -2.123559

III - 61.88

Fe 1.176179 -0.056046 -0.494004

Fe -1.718078 0.018826 -0.361651

Fe 0.067308 1.668382 2.125672

Fe -0.254777 -1.524772 1.942048

O -0.346930 -0.161490 -1.497823

O 0.973788 1.403886 0.614260

O 1.010546 -1.412344 0.668034

O -1.740734 -1.208505 0.994471

O -1.688056 2.145614 1.642553

O 0.049501 0.066181 2.840075

O 2.567097 0.168644 -1.383563

O -0.178414 -2.649170 3.158840

O 0.361719 2.986322 3.088055

O -2.143723 1.693830 0.302954

$Fe_4O_{11}^-$

I - 66.75

Fe 1.536079 -0.035965 -0.338035

Fe -1.626860 -0.037784 -0.227104

Fe 0.036734 1.570138 2.004311

Fe 0.037700 -1.614220 1.954198

O -0.074718 -0.056286 -1.131286

O 1.395987 1.319225 0.798711

O 1.397272 -1.432253 0.784129

O -1.401141 -1.431563 0.882203

O -1.398213 1.321621 0.891266

O 0.059811 -0.069379 2.841578

O 2.775700 0.052987 -1.421489

O 0.060719 -2.904052 2.981319

O 0.051288 3.483590 2.233450

O -2.951802 0.048308 -1.207007

O 0.054494 2.671160 3.512283

$Fe_4O_{12}^-$

I - 65.10

Fe 1.613976 0.044898 -0.257440

Fe -1.580105 0.042018 -0.263984

Fe 0.055412 1.697814 2.025036

Fe 0.056501 -1.589615 2.024100

O -0.030247 -0.036576 -1.100895

O 1.496683 1.438771 0.772386

O 1.419460 -1.362345 0.805891

O -1.426394 -1.302458 0.821719

O -1.304351 1.408627 0.801162

O 0.135073 0.048651 2.759838

O -2.923587 0.163578 -1.199491

O 2.960252 -0.063534 -1.211055

O -0.047782 2.857335 3.537113

O 0.050724 3.592952 2.223471

O -0.478055 -2.748084 3.439022

O 0.070618 -3.495325 2.258486

$Fe_4O_{13}^-$

I - 67.84

Fe 1.638798 -0.069505 -0.257331

Fe -1.564502 0.039986 -0.249636

Fe 0.033150 1.670677 2.026913

Fe -0.084889 -1.600796 2.081585

O -0.032095 -0.051731 -1.106594

O 1.411511 1.310743 0.868558

O 1.296003 -1.374763 0.855697

O -1.508150 -1.316260 0.855834

O -1.383064 1.428619 0.763280

O -0.116107 0.051539 2.788709

O -2.840880 0.048276 -1.278963

O -0.053205 2.880752 3.484091

O 0.052867 3.577035 2.150467

O 0.377360 -2.753474 3.506253

O -0.284815 -3.481604 2.365564

O 2.641682 0.075443 -1.875140

O 3.491323 -0.069464 -0.641301

$Fe_4O_{14}^-$

I - 66.24

Fe 1.584807 0.047491 -0.341639

Fe -1.633659 0.063492 -0.256049

Fe 0.047689 1.612031 2.034067

Fe 0.057184 -1.605186 1.988016

O -0.030560 0.069537 -1.118899

O 1.407489 1.412183 0.846252

O 1.377743 -1.314638 0.804311

O -1.354749 -1.325334 0.878642

O -1.324945 1.401064 0.900002

O 0.072183 0.009230 2.840155

O -0.055353 2.728849 3.556475

O 0.063161 3.569319 2.341639

O -0.057851 -2.732911 3.534790

O 0.054041 -3.488841 2.244549

O 2.665823 -0.055563 -1.886569

O 3.527292 0.062004 -0.682932

O -2.760254 -0.060355 -1.801259

O -3.516039 0.054785 -0.510336

Fe_5O^-

I - 20.46

Fe 1.920572 0.012167 0.159360

Fe -1.952274 0.043761 0.246660

Fe -0.045133 1.212381 -0.648958

Fe -0.056232 -1.236623 -0.565997

Fe -0.003814 0.050442 1.612672

O 1.842973 0.056736 2.017447

II - 20.10

Fe 1.205532 -0.520340 -0.270713

Fe -1.515107 -0.265820 0.056639

Fe -0.048565 1.511860 -0.056908

Fe -0.158466 -2.237230 0.538459

Fe -0.073124 -0.370372 1.949987

O 1.205780 0.898588 1.320612

III - 19.92

Fe -1.224266 0.787512 0.049139

Fe 1.313214 0.788754 0.050326

Fe 0.051792 -1.479366 0.053024

Fe 0.047340 -0.165171 1.903104

Fe 0.049298 -0.158036 -1.805813

O 0.048826 2.198257 -0.053786

$Fe_5O_2^-$

I - 26.88

Fe 1.860872 -0.256100 0.149055

Fe -1.934301 0.255863 0.108511

Fe 0.087762 1.193911 -0.670186

Fe -0.155089 -1.255858 -0.573277

Fe -0.049178 0.050902 1.743725

O 1.809933 0.047419 1.950930

O -1.910025 0.066889 1.927994

II - 26.60

Fe -1.338013 0.777975 0.051436

Fe 1.484295 0.466469 -0.043473

Fe 0.050593 -1.465920 -0.150108

Fe 0.150172 0.003181 1.917529

Fe -0.107289 0.264033 -1.819557

O 1.747706 0.889276 1.803143

O -1.352837 -0.895087 1.198427

III - 26.53

Fe 1.963249 -0.047577 -0.465910

Fe -1.925965 0.162626 -0.399239

Fe 0.047081 1.394361 -0.819289

Fe 0.058197 -1.362114 -0.683383

Fe -0.155415 0.151183 1.304368

O 1.303624 1.296661 0.782193

O -1.307656 -1.293405 0.803202

$Fe_5O_3^-$

I - 33.20

Fe 1.813756 -0.120041 0.474168

Fe -1.576107 -0.040424 -0.265979

Fe 0.046069 1.595696 -0.260625

Fe 0.123413 -1.819234 0.474666

Fe -0.150720 0.147431 1.924764

O 1.108225 1.516515 1.369999

O -1.515622 -1.113296 1.357762

O 1.927914 -1.925295 0.052246

II - 30.24

Fe -1.164876 0.773807 -0.149311

Fe 1.193263 0.432602 -0.052560

Fe 0.366867 -1.820307 -0.407672

Fe -0.365188 -0.575245 1.755671

Fe -0.154906 -0.157573 -2.137540

O -1.971442 0.273786 1.496522

O 1.322192 -1.205821 1.191351

O 0.045976 -2.006897 -2.228653

III - 33.12

Fe 2.147809 -0.372682 0.261076

Fe -1.828945 -0.018529 -0.044672

Fe 0.360304 0.993659 -0.680017

Fe 0.162589 -1.399049 -0.638285

Fe 0.049751 0.148110 1.680407

O 1.880249 0.051810 2.035829

O -1.825723 0.165059 1.776212

O -0.988864 -0.066023 -1.731956

$Fe_5O_4^-$

I - 40.23

Fe 1.404280 1.272294 0.060808

Fe -1.200427 1.473656 0.063021

Fe 1.199470 -1.405676 0.017868

Fe -1.402994 -1.202923 0.016146

Fe -0.000878 0.010600 1.542548

O 2.044125 -0.143586 1.180999

O -2.045447 0.169952 1.183238

O 0.175679 2.359982 -0.794862

O -0.173603 -2.253348 -0.884687

II - 33.97

Fe -0.880047 0.461213 0.057701

Fe 1.356638 1.379289 0.110498

Fe -0.634126 -1.948416 -0.008910

Fe 0.367050 -0.365146 1.979639

Fe 0.380996 -0.239796 -1.894202

O -0.478392 -1.999348 1.828092

O 1.496340 1.094726 1.925392

O 1.399534 1.294854 -1.732211

O -0.370964 -1.922209 -1.833510

III - 38.34

Fe -1.270535 0.784261 -0.059180

Fe 1.165825 0.784214 -0.059543

Fe -0.052041 -1.500005 0.009779

Fe -0.052051 0.048850 2.052704

Fe -0.052323 0.003162 -2.020870

O -0.051962 -1.785442 1.848417

O 1.625327 0.766215 1.777248

O -1.729656 0.766107 1.777670

O -0.052544 -1.829832 -1.829386

$Fe_5O_5^-$

I - 45.50

Fe -1.714425 0.573079 -0.052634

Fe 1.828959 0.666869 0.090905

Fe -0.055782 -1.306510 -0.151993

Fe 0.153504 0.156151 2.071435

Fe -0.034859 0.483460 -1.926780

O 1.925293 0.803199 1.906512

O -1.468922 0.986078 1.696180

O -0.055882 -1.670933 1.611331

O 1.721571 0.902586 -1.720892

O -1.861921 0.571099 -1.914064

II - 45.60

Fe 0.510669 1.608754 -0.052095

Fe -2.681476 0.570476 -0.052201

Fe 3.024784 0.984208 -0.052076

Fe -2.028635 -1.716268 -0.051981

Fe 1.214595 -0.867641 -0.052089

O 2.113762 2.567284 -0.052087

O -1.300063 1.704896 -0.051993

O -0.255698 -1.928280 -0.052191

O 3.080888 -0.843184 -0.052097

O -3.719523 -0.965338 -0.052094

III - 44.80

Fe -1.401975 0.679112 -0.746809

Fe 1.056954 0.982984 -0.272016

Fe -0.436755 -1.469679 0.130279

Fe -0.481986 0.552486 1.740241

Fe 0.065180 -0.466093 -2.265085

O -0.998309 -1.196200 1.931653

O -1.628892 -1.198175 -1.498700

O 1.306981 -0.965070 -0.768600

O 0.796276 1.826273 1.417556

O 0.018681 1.510346 -1.941218

$Fe_5O_6^-$

I - 51.37

Fe -1.345949 0.785288 -0.049128

Fe 1.346435 0.785245 0.048982

Fe 0.000538 -1.559002 -0.000241

Fe 0.051456 -0.028840 2.206174

Fe -0.051220 -0.028565 -2.206483

O 1.538372 0.880333 1.878327

O -1.412733 0.868021 1.790031

O 0.152323 -1.753402 1.825541

O 1.413024 0.868113 -1.790155

O -1.538111 0.880509 -1.878413

O -0.151983 -1.753145 -1.826100

II - 51.04

Fe -1.814422 1.093154 0.048474

Fe 0.671027 0.275854 1.061290

Fe 0.672277 -2.243246 -0.052816

Fe -1.299775 -1.131470 1.619274

Fe -0.561590 -0.638867 -1.618073

O 0.482652 -1.726190 1.792852

O -0.287076 1.796692 0.888237

O -0.257233 -2.549553 -1.605569

O -1.733688 0.787144 -1.811037

O -2.669874 -0.023486 1.305567

O 1.193213 -0.375992 -0.663935

III - 50.71

Fe -1.965428 0.776387 0.163727

Fe 1.559500 -0.104455 -0.283761

Fe -0.141072 -1.723028 0.268256

Fe 0.092103 0.160536 2.029883

Fe -0.529273 0.059347 -1.717518

O 0.054435 -1.714148 2.130635

O 1.736051 0.771774 1.314171

O -1.523307 1.097458 1.922496

O 0.871633 -1.303644 -1.563814

O -1.710809 1.506248 -1.533673

O -1.831768 -1.043110 -0.475321

$Fe_5O_7^-$

I - 56.52

Fe -1.470741 1.415758 -0.250956

Fe 1.683494 0.884861 0.252481

Fe 0.267038 -1.969365 -0.252631

Fe 0.037217 0.043432 2.050495

Fe -0.186935 -0.059632 -1.717018

O 0.022801 -1.722508 1.523660

O -1.411876 1.053155 1.521523

O -0.552292 -1.838051 -1.961987

O -1.830959 0.704750 -1.976321

O 1.595893 -0.636822 -0.894810

O 1.725571 0.898352 2.110745

O 0.394542 1.709713 -0.887328

II - 56.28

Fe -0.983964 0.756560 0.053301

Fe 1.620766 1.196616 0.050948

Fe -0.466892 -1.777854 0.069102

Fe 0.154791 -0.185695 2.227634

Fe 0.059217 -0.124310 -2.043593

O 1.826141 0.474578 1.720838

O -1.310694 0.895487 1.817315

O -0.363659 -1.927228 1.863478

O 1.702024 0.577122 -1.634907

O -1.295507 1.108021 -1.713775

O -0.163704 -1.950566 -1.732050

O 1.804110 2.853597 0.173771

III - 55.56

Fe -1.933035 0.326801 -0.049847

Fe 1.991865 1.198385 0.052159

Fe -0.463247 -1.794462 -0.171034

Fe 0.374787 0.293437 1.820803

Fe 0.149862 -0.019874 -2.019734

O 0.300824 -1.520872 1.414248

O 2.024038 1.196205 1.884746

O -1.302322 0.992119 1.498581

O 0.047228 -1.928595 -1.906816

O -1.497961 0.887325 -1.749830

O 1.715282 0.884716 -1.701546

O -2.256699 -1.509931 -0.053443

$Fe_5O_8^-$

I - 61.10

Fe -1.504870 0.884857 -0.018249

Fe 1.396409 1.389027 0.085333

Fe -0.678080 -1.817502 -0.185008

Fe 0.222163 0.017935 1.996455

Fe 0.068127 -0.218520 -2.130670

O 0.169823 -1.724742 1.393283

O 1.836269 0.981376 1.813803

O -1.417244 0.809473 1.803810

O -0.156110 -2.073751 -1.913733

O -1.425265 0.819918 -1.920804

O 1.612856 0.581559 -1.509941

O -2.197445 -0.911279 -0.048507

O -0.176473 2.200304 -0.055098

II - 59.54

Fe -1.097397 0.886555 0.161775

Fe 1.726672 1.023774 -0.573622

Fe 0.257011 -1.407548 0.130693

Fe -1.263124 -0.780492 2.333554

Fe -0.110648 -0.051979 -2.357348

O -1.515381 0.997341 1.979647

O 0.176257 -1.842198 1.944625

O 1.411890 0.874292 -2.400377

O -1.521426 0.799207 -1.696617

O -0.048271 -1.713644 -1.726372

O 0.354962 1.990202 0.149089

O 1.924738 -0.670902 0.086826

O -1.658159 -0.995481 0.370168

III - 59.28

Fe -1.301609 1.704160 0.328990

Fe 1.335018 1.261400 -0.322863

Fe -0.076151 -1.498196 -0.269559

Fe 0.890472 0.053059 1.754932

Fe -0.674679 0.152943 -2.034301

O 0.306762 2.040363 1.191294

O -0.983734 -0.100524 0.886261

O 0.875754 -1.740866 1.310321

O -0.283302 1.919703 -1.294110

O -1.122840 -1.623480 -1.856415

O 1.228801 -0.236974 -1.397510

O 2.550038 0.799524 0.890545

O -2.924132 1.940918 0.582276

$Fe_5O_9^-$

I - 64.82

Fe -1.344728 0.824238 0.052760

Fe 1.409239 0.827313 0.049757

Fe -0.008624 -1.532408 0.011992

Fe 0.100029 0.050080 2.342418

Fe -0.050597 0.044224 -2.245051

O 1.603653 0.896203 1.947191

O -1.398902 0.888341 1.950005

O 0.050269 -1.655048 1.909765

O 1.429647 0.884756 -1.927879

O -1.519002 0.894578 -1.893688

O -0.061127 -1.662200 -1.936705

O 0.035327 2.023959 0.037940

O 1.727487 -0.965776 -0.030694

O -1.787306 -0.984570 0.054553

II - 64.82

Fe -1.519667 0.764069 0.146044

Fe 0.948757 2.227351 0.068551

Fe -0.043384 -1.774106 -0.035767

Fe 0.481921 0.134923 2.100559

Fe 0.403912 0.270663 -2.021466

O 1.500246 1.707723 1.809178

O -1.308709 0.575163 1.952874

O 0.554853 -1.715064 1.693397

O 1.323142 1.828211 -1.738722

O -1.328564 0.673939 -1.830468

O 0.466549 -1.601310 -1.829601

O -0.884557 2.477271 0.140088

O -1.736384 -1.214085 -0.030259

O 0.586896 0.176204 0.022651

$Fe_5O_{10}^-$

I - 69.45

Fe -1.270881 0.803400 0.005670

Fe 1.340450 0.784514 -0.064075

Fe 0.016436 -1.469636 -0.015421

Fe 0.103726 0.052928 2.542832

Fe -0.025711 0.026928 -2.097380

O 1.505011 0.862196 1.825078

O -1.321914 0.883295 1.905052

O 0.060983 -1.587374 1.879411

O 1.494207 0.885226 -1.985559

O -1.524023 0.904628 -1.906985

O -0.041827 -1.713414 -1.927635

O 0.045363 2.118083 -0.028495

O 1.818063 -1.011364 -0.047092

O -1.777406 -0.984137 0.053306

O 0.153461 0.056515 4.184196

II - 68.70

Fe -1.503047 0.772506 0.128449

Fe 0.988847 2.128033 0.113697

Fe -0.049393 -1.846865 -0.056331

Fe 0.400674 0.121795 2.102920

Fe 0.360732 0.319805 -2.023795

O 1.491524 1.526870 1.912295

O -1.307679 0.581612 2.007556

O 0.571294 -1.590760 1.850006

O 1.329703 1.822639 -1.720880

O -1.365838 0.683770 -1.821566

O 0.361813 -1.493548 -1.884555

O -0.838733 2.453520 0.169285

O 0.060590 -3.503036 -0.058026

O -1.690050 -1.194563 0.056011

O 0.643354 0.048266 0.036985

III - 67.65

Fe -1.418262 0.754902 0.136911

Fe 1.414141 0.953917 0.263733

Fe -0.190483 -1.624638 -0.055834

Fe 0.118810 0.055790 2.345533

Fe -0.053436 0.053010 -2.186119

O 1.610339 1.111383 2.136012

O -1.500080 0.795126 1.965462

O 0.079122 -1.653331 1.728090

O 1.409886 0.821154 -1.711446

O -1.495153 0.924596 -1.814707

O -0.263306 -1.650486 -2.012260

O -0.053868 2.007057 0.150855

O 2.419229 -0.667574 0.373215

O -1.932065 -1.003942 0.037470

O 1.704191 -1.712935 -0.406543

$\mathbf{Fe_5O_{11}^-}$

I - 73.28

Fe -1.242128 0.783176 0.049827

Fe 1.322768 0.786371 -0.024106

Fe -0.023541 -1.477908 0.011559

Fe 0.061419 0.044025 2.531733

Fe -0.061778 0.053403 -2.507645

O 1.512253 0.811751 1.853737

O -1.377773 0.886350 1.941790

O 0.052334 -1.615344 1.897793

O 1.410843 0.843913 -1.911572

O -1.465074 0.893324 -1.835702

O -0.046238 -1.606839 -1.877634

O 0.044904 2.114389 0.028573

O 1.774049 -1.014319 -0.045451

O -1.799660 -0.982712 0.055563

O 0.145651 0.042481 4.173040

O -0.069487 0.047314 -4.150772

II - 72.96

Fe -1.180368 2.037770 -0.021398

Fe 1.395522 0.771496 -0.063049

Fe 0.966249 -2.072807 -0.027887

Fe -0.260425 -0.099607 1.826602

Fe -0.365794 -0.153748 -2.238672

O 1.304597 0.705517 1.827005

O -1.528520 1.083784 1.520995

O -0.034794 -1.816830 1.506819

O 1.168804 0.661411 -1.900438

O -1.526550 0.918693 -1.422624

O -0.141776 -1.726651 -1.437690

O 0.545079 2.436026 -0.049367

O 2.271818 -0.880819 -0.057580

O -0.777137 -0.363461 -3.821571

O -2.240913 3.299174 -0.160334

O 1.409037 -3.660861 -0.160137

III - 72.48

Fe -1.180321 1.631439 0.152034

Fe 1.638631 0.863176 -0.055594

Fe 0.827287 -2.138642 -0.047106

Fe -0.271492 0.031082 1.996724

Fe -0.256881 -0.118340 -2.330599

O 1.361808 0.688353 1.837908

O -1.745376 1.110322 1.824390

O -0.162768 -1.659088 1.383346

O 1.248820 0.679879 -1.917007

O -1.512577 0.793353 -1.411633

O -0.242389 -1.639583 -1.391993

O 0.426029 2.352105 -0.047124

O 2.142666 -0.978138 -0.058709

O -0.477584 -0.366441 -3.936837

O 3.135875 1.612227 -0.075002

O 1.302620 -3.705759 -0.170815

$Fe_5O_{12}^-$

I - 77.52

Fe -1.239932 1.952805 -0.000802

Fe 1.510671 0.778743 -0.063926

Fe 0.790613 -2.127869 -0.026884

Fe -0.158640 -0.074336 2.260124

Fe -0.289810 -0.103361 -2.285943

O 1.364549 0.686202 1.795183

O -1.428778 0.881288 1.427312

O -0.159502 -1.665905 1.425704

O 1.253810 0.666772 -1.912657

O -1.516385 0.881204 -1.416171

O -0.253592 -1.674863 -1.415048

O 0.481691 2.338247 -0.048589

O 2.132767 -0.981213 -0.067082

O -0.357311 -0.164904 3.892852

O -0.568770 -0.250917 -3.902400

O -2.207857 3.285102 0.042512

O 1.295204 -3.695323 -0.043651

II - 76.33

Fe -1.158554 0.915106 0.043392

Fe 1.394861 0.805446 -0.064372

Fe 0.041091 -1.840440 -0.059208

Fe 0.148694 0.042990 2.569746

Fe -0.015389 0.023081 -2.628498

O 1.573678 0.798617 1.810802

O -1.229883 0.965668 1.925568

O 0.057307 -1.590618 2.014067

O 1.442657 0.783274 -1.941008

O -1.341140 0.893534 -1.875799

O -0.067488 -1.619029 -2.010849

O 0.181112 2.144032 -0.046351

O 1.612395 -1.021243 -0.045733

O -1.493932 -0.875384 0.052492

O 0.264394 0.136853 4.209164

O -0.049551 0.047072 -4.268007

O -0.034727 -3.494897 -0.044196

III - 77.01

Fe -1.078120 0.884934 0.057189

Fe 1.704376 1.006325 -0.022343

Fe 0.061586 -1.772291 0.052595

Fe 0.159283 0.007094 2.666079

Fe -0.054000 0.059912 -2.386110

O 1.540008 0.795599 2.046215

O -1.201138 0.871268 1.906673

O 0.147126 -1.620190 1.994904

O 1.396655 0.873349 -2.133178

O -1.414908 0.989610 -1.843215

O -0.040214 -1.598014 -2.013440

O 0.291082 2.113896 0.031361

O 1.606027 -0.792030 -0.054028

O -1.510215 -0.940276 0.056874

O 0.053826 -0.058334 4.314399

O 3.148625 1.825104 -0.054315

O 0.034712 -3.432883 0.049313

$Fe_5O_{13}^-$

I - 81.00

Fe -1.302600 1.930509 -0.006266

Fe 1.810766 1.002848 -0.083568

Fe 0.812748 -2.129812 0.051292

Fe -0.130774 -0.027307 2.309756

Fe -0.370433 -0.158877 -2.269607

O 1.313009 0.765957 1.778557

O -1.413088 0.823673 1.396546

O -0.073793 -1.642540 1.518427

O 1.112646 0.634301 -1.813414

O -1.574324 0.831328 -1.407414

O -0.269103 -1.658179 -1.297691

O 0.382782 2.320140 -0.056564

O 2.026017 -0.881094 -0.047048

O -0.362519 -0.157503 3.932745

O -0.665157 -0.371508 -3.874057

O 3.175860 1.936082 0.046822

O -2.358162 3.191127 -0.039140

O 1.312355 -3.697281 0.035320

II - 80.46

Fe -1.494259 0.960484 0.038645

Fe 1.649310 0.876845 -0.046545

Fe 0.012242 -1.479594 -0.000200

Fe 0.121344 0.064304 2.667340

Fe -0.017105 0.062049 -2.671415

O 1.512874 0.796384 1.933918

O -1.261091 0.884567 2.008130

O 0.055191 -1.523649 1.855428

O 1.415087 0.793566 -2.017945

O -1.362328 0.880775 -1.940052

O -0.046408 -1.524927 -1.855430

O 0.104297 1.828396 -0.013526

O 1.782109 -0.910628 -0.050213

O -1.724358 -0.816326 0.048973

O 0.159683 -0.043353 4.309820

O -0.060063 -0.046413 -4.313700

O 3.160064 1.577896 -0.065183

O -2.971404 1.728227 0.063196

III - 79.56

Fe -1.492695 1.064173 0.033192

Fe 1.622872 0.906502 -0.076400

Fe 0.035126 -1.755267 -0.007540

Fe 0.120517 0.057423 2.651950

Fe -0.051433 0.019209 -2.477565

O 1.497934 0.790875 1.857277

O -1.246600 0.903785 1.966125

O 0.058480 -1.530275 1.951031

O 1.410530 0.787789 -2.026509

O -1.416751 0.903246 -1.950278

O -0.064036 -1.618655 -1.985591

O 0.073740 1.915101 -0.039353

O 1.634197 -0.976951 -0.055862

O -1.487509 -0.770268 0.037179

O 0.162186 0.072580 4.287714

O 2.944561 1.924299 -0.135327

O -2.862526 2.009046 0.066035

O -0.072502 -3.404471 0.044664

$Fe_5O_{14}^-$

I - 83.60

Fe -1.350556 1.957242 -0.019068

Fe 1.744547 0.970621 -0.077296

Fe 0.778617 -2.136086 -0.050434

Fe -0.265684 -0.121147 2.247988

Fe -0.376429 -0.084090 -2.328032

O 1.178677 0.672508 1.780296

O -1.507410 0.797101 1.319376

O -0.171157 -1.706809 1.392356

O 1.107567 0.666831 -1.914683

O -1.595257 0.901430 -1.429537

O -0.279008 -1.622319 -1.385063

O 0.357877 2.333756 -0.045605

O 2.055237 -0.945222 -0.078327

O -0.579393 -0.270332 3.854052

O -0.765303 -0.266498 -3.915136

O -2.332887 3.273317 0.040020

O 1.300840 -3.694922 -0.065831

O 3.460292 1.827115 -0.810695

O 3.499758 1.738853 0.625639

II - 83.79

Fe -1.559041 1.024272 0.024591

Fe 1.715361 0.919183 -0.051948

Fe -0.003548 -1.862151 0.013590

Fe 0.107864 0.040853 2.568983

Fe -0.018651 0.012334 -2.581883

O 1.535301 0.804432 1.908406

O -1.297308 0.898617 1.974748

O 0.051509 -1.601973 1.959798

O 1.441326 0.786784 -2.001804

O -1.396894 0.878087 -1.931300

O -0.052447 -1.618781 -1.946096

O 0.102027 1.717655 -0.027193

O 1.497505 -0.869365 -0.042412

O -1.435342 -0.773328 0.041588

O 0.150829 0.050729 4.202112

O -0.055745 0.009590 -4.215222

O 3.180925 1.715801 -0.072319

O -2.970470 1.914290 0.054339

O -0.053486 -3.529327 0.037755

III - 83.22

Fe -1.436754 1.080712 0.042819

Fe 1.414393 0.750742 -0.052860

Fe 0.024438 -1.678138 -0.005430

Fe 0.126569 0.060840 2.660638

Fe -0.046708 0.059024 -2.670559

O 1.516846 0.779742 1.805964

O -1.201517 0.980067 2.033614

O 0.058865 -1.519325 1.939222

O 1.402012 0.775607 -1.914604

O -1.328311 0.975998 -1.956679

O -0.058881 -1.521703 -1.946042

O 0.060159 2.039046 -0.015371

O 1.733381 -1.061429 -0.056491

O -1.561186 -0.676456 0.049535

O 0.251692 0.067266 4.300707

O -0.047564 0.066391 -4.315172

O -2.846765 1.933485 0.067540

O 0.486482 -3.492792 -0.043428

O -0.937938 -3.601292 0.048377

$Fe_5O_{15}^-$

I - 86.40

Fe -1.511371 1.015467 -0.036778

Fe 1.586979 0.887370 -0.051014

Fe -0.034559 -1.516892 0.080047

Fe 0.028364 0.216258 2.671687

Fe -0.018559 0.043421 -2.677147

O 1.436189 0.901660 1.928752

O -1.334252 1.007054 1.946775

O -0.042346 -1.406818 1.943045

O 1.408278 0.782394 -1.997351

O -1.376422 0.888199 -1.986393

O -0.055929 -1.497094 -1.832313

O 0.069098 1.890509 -0.051249

O 1.720296 -0.889483 0.036424

O -1.733263 -0.746282 0.046596

O 0.045271 0.247779 4.316544

O -0.040359 -0.061272 -4.319271

O 3.082247 1.607081 -0.061435

O -2.909341 1.904542 -0.045658

O 0.152898 -3.441645 -0.046803

O 0.466761 -4.087084 -1.208895

II - 86.40

Fe -1.412859 1.090059 0.011011

Fe 1.726817 0.957699 0.056566

Fe 0.032829 -1.640457 0.023966

Fe 0.151702 0.071182 2.640820

Fe 0.049659 0.065514 -2.626643

O 1.613853 0.802736 1.994652

O -1.160899 0.996213 2.002223

O 0.062719 -1.532531 1.941774

O 1.485277 0.774100 -2.019185

O -1.261743 0.992460 -1.918175

O -0.049373 -1.531740 -1.915037

O 0.245153 1.915304 0.026519

O 1.639727 -0.829522 -0.044656

O -1.516843 -0.681386 0.046636

O 0.175391 0.050225 4.278218

O -0.054575 0.051875 -4.260288

O 3.180321 1.729617 -0.028074

O -2.872362 1.864744 0.052276

O 0.662716 -3.601939 0.034375

O -0.741286 -3.482951 0.057671

III - 86.20

Fe -1.293105 2.071583 -0.054256

Fe 1.808505 0.983406 -0.163270

Fe 0.753230 -2.138329 -0.059301

Fe -0.249412 -0.056966 2.246063

Fe -0.327046 -0.155304 -2.359521

O 1.228976 0.641774 1.729352

O -1.415689 0.896075 1.363093

O -0.256669 -1.592423 1.348686

O 1.201747 0.544355 -2.039881

O -1.448375 0.844628 -1.483115

O -0.256638 -1.721956 -1.513557

O 0.491822 2.242549 -0.147769

O 2.011696 -0.972919 -0.053873

O -0.483176 -0.154909 3.863159

O -0.666024 -0.358168 -3.953007

O 1.205912 -3.715348 -0.255213

O 3.588618 1.830556 -1.023755

O 3.693135 1.716989 0.397102

O -2.239280 3.522184 0.703408

O -2.340658 3.483886 -0.792575

$Fe_5O_{16}^-$

I - 89.25

Fe -1.504039 1.053574 -0.070669

Fe 1.483832 0.770894 -0.037755

Fe 0.050973 -1.570670 0.070176

Fe 0.020656 0.150698 2.651540

Fe 0.007535 0.031333 -2.595461

O 1.410951 0.876986 1.877237

O -1.338720 0.984881 2.022511

O -0.037270 -1.467176 1.962239

O 1.442482 0.798966 -1.939532

O -1.406536 0.887291 -1.995074

O -0.049322 -1.551698 -1.853862

O 0.014388 1.934471 -0.022644

O 1.782757 -0.993473 0.033504

O -1.611520 -0.722543 0.050971

O 0.145212 0.161390 4.284126

O -0.049312 -0.047976 -4.231117

O 3.118699 1.728863 -0.049590

O -2.905350 1.926938 -0.046877

O 0.148216 -3.470838 -0.013897

O 0.458766 -4.121220 -1.176186

O 3.728592 2.117221 -1.210702

II - 89.04

Fe -1.469823 0.976624 0.042532

Fe 1.605997 0.827690 -0.038643

Fe -0.027322 -1.760849 0.007450

Fe 0.121618 0.053897 2.667316

Fe -0.011415 0.048295 -2.660952

O 1.506529 0.788128 1.896838

O -1.259549 0.883070 2.005188

O 0.043277 -1.523595 1.922360

O 1.412763 0.783428 -1.962799

O -1.356733 0.875940 -1.932877

O -0.058963 -1.530033 -1.907913

O 0.056966 1.859311 -0.007620

O 1.640231 -0.972385 -0.044933

O -1.616735 -0.792393 0.050567

O 0.155266 0.062933 4.308198

O -0.056337 0.056434 -4.301410

O -2.864769 1.845811 0.061400

O 0.593563 -3.672996 0.049129

O -0.845655 -3.518845 0.047475

O 3.502066 1.088166 -0.057540

O 2.974384 2.419244 -0.052251

Fe_6O^-

I - 24.15

Fe 1.298101 1.387078 -0.048605

Fe 1.298094 -1.387272 -0.048616

Fe -1.089915 1.251145 0.048279

Fe -1.089920 -1.251276 0.048274

Fe -0.161339 -0.000078 1.853362

Fe 0.228849 -0.000064 -1.672285

O 1.720345 -0.000101 1.283393

II - 24.08

Fe 1.335070 1.335069 0.054949

Fe 1.053592 -1.097383 -0.056231

Fe -1.097383 1.053592 -0.056231

Fe -1.324205 -1.324205 -0.255240

Fe 0.059603 0.059603 1.867669

Fe -0.153979 -0.153979 -1.903287

O 1.392685 1.392684 1.935582

III - 23.80

Fe 0.787699 -0.541795 -0.882660

Fe -1.535135 -0.159176 -0.975956

Fe 0.050137 1.690391 -0.768615

Fe 1.626027 0.459607 1.084079

Fe -0.815214 0.161523 1.184088

Fe 0.156243 2.340508 1.514311

O 0.461418 0.692867 2.634123

$Fe_6O_2^-$

I - 30.40

Fe 1.224204 1.629198 -0.276908

Fe -1.224372 1.629121 -0.276926

Fe 1.228745 -1.099860 0.364187

Fe -1.228950 -1.099807 0.364217

Fe 0.000092 0.473689 1.721320

Fe -0.000182 -0.018220 -1.430645

O 1.863369 0.563206 1.217368

O -1.863288 0.563284 1.217553

II - 30.32

Fe -1.722378 -0.154301 -0.055087

Fe 1.725790 0.366445 0.296513

Fe 0.327849 -1.501579 0.055145

Fe 0.050944 0.324037 2.022432

Fe 0.023474 0.254288 -1.615163

Fe -0.153279 1.886575 0.372145

O -1.090756 -1.096174 1.510532

O -1.843753 0.357505 -1.825411

III - 30.24

Fe 1.161353 1.376548 -0.190110

Fe -1.161414 1.376554 0.190105

Fe 1.161343 -1.376567 -0.190124

Fe -1.161413 -1.376570 0.190108

Fe -0.143736 -0.000010 1.806644

Fe 0.143715 -0.000002 -1.806659

O 1.707441 0.000008 1.109753

O -1.707466 0.000018 -1.109748

$Fe_6O_3^-$

I - 37.08

Fe 1.200718 1.210796 0.780333

Fe -1.197300 1.201675 0.856084

Fe 1.151724 -1.309364 -0.472576

Fe -1.196417 -1.316114 -0.401903

Fe 0.045985 -0.683295 1.825672

Fe -0.054875 0.586308 -1.271701

O 1.881400 -0.565960 1.201761

O -1.826731 -0.581379 1.315917

O -0.036701 2.356568 -0.171759

II - 36.99

Fe 1.266754 1.396573 -0.052083

Fe -1.370005 1.397726 -0.052084

Fe 1.827592 -1.144330 -0.052085

Fe -1.932652 -1.141972 -0.052081

Fe -0.052229 -0.362464 1.192032

Fe -0.052231 -0.362466 -1.296197

O 2.841041 0.369380 -0.052082

O -2.945409 0.371805 -0.052084

O -0.051006 2.681846 -0.052083

III - 36.36

Fe 1.188805 1.229351 -0.075224

Fe -1.192033 1.415442 -0.115543

Fe 1.192455 -1.238639 -0.028864

Fe -1.184534 -1.418210 -0.030637

Fe -0.061620 0.049535 1.881865

Fe -0.408938 -0.049538 -1.829581

O 1.755517 0.035129 1.516431

O -1.816225 0.041044 1.192630

O 1.511112 -0.039162 -1.626052

$Fe_6O_4^-$

I - 43.90

Fe 1.319100 1.310650 -0.023351

Fe -1.407657 1.249860 0.165382

Fe 1.390018 -1.068859 -0.368954

Fe -1.098027 -1.128015 -0.056142

Fe 0.123648 0.152457 1.716625

Fe -0.144986 0.023205 -1.935738

O 2.014593 -0.033154 1.185820

O -1.816594 -0.048951 1.506831

O 0.051428 -1.840943 -1.574981

O -0.152960 1.819278 -1.200244

II - 44.20

Fe 1.473607 0.987313 -0.153009

Fe -1.402015 1.092699 -0.013401

Fe 1.196484 -1.397380 0.012252

Fe -1.299520 -1.305560 -0.051266

Fe -0.212480 0.160875 1.823799

Fe 0.220876 0.050050 -1.936898

O 1.625863 0.050400 1.565806

O -2.047992 -0.067465 1.502630

O 2.035856 -0.292137 -1.602400

O -1.622256 0.065908 -1.677532

$Fe_6O_5^-$

I - 50.38

Fe 1.269115 1.488436 -0.011659

Fe -1.292175 1.382760 0.075655

Fe 1.292839 -1.308582 -0.161280

Fe -1.092553 -1.197157 -0.156850

Fe -0.034447 0.168157 1.760542

Fe -0.054140 -0.034022 -1.951382

O 1.921289 -0.068805 1.087377

O -1.956154 -0.176124 1.199525

O 0.174003 -1.909764 -1.602491

O -0.039921 1.786722 -1.519233

O 0.045668 2.163697 1.396603

II - 49.39

Fe 1.280990 1.361219 -0.468531

Fe -1.296097 1.309434 -0.469840

Fe 1.626923 -0.991244 0.095794

Fe -1.826176 -1.001378 0.019853

Fe -0.074720 -0.066418 1.719017

Fe 0.157327 -0.154780 -1.895487

O 1.521377 -1.109378 1.917236

O -1.729756 -1.072718 1.824257

O 2.047221 -0.049496 -1.598501

O -1.756045 -0.155583 -1.707814

O -0.045868 1.842643 0.865222

III - 49.28

Fe 1.888404 0.841742 -0.132420

Fe 0.722683 -1.200234 1.096223

Fe -2.334979 0.730255 -0.369899

Fe -1.199277 -1.658407 -0.478938

Fe -0.295593 1.094786 1.196186

Fe -0.149284 0.324805 -1.615842

O 1.500512 0.474019 1.690324

O -2.042357 1.735821 1.117282

O -0.237239 -2.717561 0.677071

O 1.577734 0.983550 -1.917124

O -1.950308 -0.463332 -1.796980

$Fe_6O_6^-$

I - 55.92

Fe 1.404537 1.298630 0.155248

Fe -1.482570 1.197475 -0.052065

Fe 1.486150 -1.197032 0.051710

Fe -1.403706 -1.298486 -0.156009

Fe 0.047773 0.159524 1.885785

Fe -0.045885 -0.159517 -1.885601

O 1.934939 -0.159383 1.620371

O -1.760069 -0.268181 1.438466

O 1.762914 0.268092 -1.438773

O -1.933131 0.159594 -1.620268

O -0.151004 2.075227 0.995795

O 0.153148 -2.074082 -0.995310

II - 55.68

Fe -0.052182 -0.049305 -0.573526

Fe -0.051247 0.054955 2.552150

Fe 1.398111 2.066344 -0.366600

Fe 1.164931 2.224247 2.705322

Fe -1.501451 2.067137 -0.366807

Fe -1.259588 2.226855 2.704120

O -0.051879 -0.904931 1.058786

O -0.049347 1.395205 3.970516

O 1.843921 2.883239 1.195555

O -1.941062 2.886593 1.195546

O 1.489727 0.664642 -1.503264

O -1.594459 0.664796 -1.502483

III - 55.32

Fe 1.473854 1.097382 0.047615

Fe -1.134392 1.516768 0.476121

Fe 1.198683 -1.489779 -0.153172

Fe -1.620797 -0.880354 0.534948

Fe 0.615647 -0.167621 1.929452

Fe -0.769071 -0.170282 -1.653882

O 2.419991 -0.371067 0.899462

O -2.433917 0.416355 -0.572938

O 0.457621 -1.511680 -1.848013

O 0.137944 1.529771 -1.208738

O 0.260777 1.738256 1.714697

O -0.242301 -1.840039 1.315803

$Fe_6O_7^-$

I - 60.84

Fe 0.569689 -0.720829 1.047466

Fe -1.922214 -0.676482 1.715351

Fe -0.294022 1.515712 1.309474

Fe 1.514486 -0.782030 -1.711041

Fe -1.307257 -0.888862 -0.921545

Fe 0.379975 1.557834 -1.598551

O -1.517908 0.896167 2.527391

O 1.718597 0.801236 -2.677926

O -1.322540 0.790623 -1.593724

O -0.065909 -1.722567 -1.936323

O 0.571077 2.416407 0.031627

O 2.035587 -0.991431 0.055590

O -2.234039 -1.829406 0.374516

II - 60.19

Fe 0.681959 -0.357141 0.583108

Fe -1.864765 -0.150850 1.935449

Fe -0.580051 1.817898 1.890361

Fe 1.505516 -0.878045 -1.791056

Fe -1.206080 -0.885368 -1.201533

Fe 0.161880 1.659947 -1.420031

O -2.014494 1.390332 2.961870

O 1.523541 0.872009 -2.348668

O -1.483853 0.879982 -1.618268

O -0.055880 -1.819295 -2.339291

O 0.635391 1.616682 0.486083

O 2.149971 -1.311244 -0.061300

O -1.201051 -1.308629 0.686341

III - 60.71

Fe 0.881245 -0.354133 0.299381

Fe -1.433372 -0.671906 1.818271

Fe -0.670802 1.828361 1.505696

Fe 0.883680 -0.998481 -2.171640

Fe -1.353799 -1.105175 -1.134962

Fe 0.060063 1.600224 -1.191395

O -1.615161 0.959536 2.794422

O 0.340239 -1.302490 1.711032

O 1.731535 0.478871 -1.213110

O -0.885519 0.417458 -2.315437

O -0.336153 -2.346010 -2.242317

O -0.372460 2.865432 0.050483

O -2.357654 -1.316992 0.376000

$Fe_6O_8^-$

I - 66.08

Fe 1.624541 -0.892885 1.868798

Fe -1.113929 -0.891936 0.887728

Fe 0.873604 1.409133 1.020893

Fe 1.088770 -0.848445 -0.992223

Fe -1.612208 -1.200748 -1.923893

Fe -0.864576 1.269873 -0.971547

O 2.029563 0.902933 2.360963

O -1.045077 1.107201 0.982271

O -0.041415 -1.602644 2.173648

O 1.101946 1.152335 -0.887816

O -1.932308 0.590386 -2.262097

O 0.121808 -1.714490 -2.269619

O 2.229066 -1.522589 0.253556

O -2.238531 -1.728361 -0.275518

II - 65.52

Fe 1.269051 1.269132 0.000011

Fe 1.269057 -1.269132 0.000010

Fe -1.269064 1.269124 0.000012

Fe -1.269066 -1.269128 0.000012

Fe -0.000007 0.000001 1.788083

Fe -0.000008 0.000001 -1.788077

O 1.904159 0.000000 1.337470

O -0.000008 1.904273 1.337682

O -1.904172 -0.000002 1.337477

O -0.000005 -1.904272 1.337680

O 1.904154 0.000000 -1.337454

O -0.000010 1.904270 -1.337663

O -1.904168 -0.000002 -1.337457

O -0.000007 -1.904268 -1.337661

III - 65.10

Fe 1.258196 1.607249 0.012319

Fe 1.275548 -1.550068 -0.158254

Fe -1.308043 1.611239 0.011975

Fe -1.298727 -1.566772 -0.157749

Fe -0.023039 0.060412 1.909354

Fe -0.021525 -0.051589 -1.707578

O 1.326636 1.416038 1.826887

O -1.396547 1.397643 1.821715

O 1.300075 -1.203299 1.621658

O -1.323601 -1.219757 1.621372

O 1.821898 0.071781 -1.116758

O -0.032490 1.906761 -1.486712

O -1.857762 0.058617 -1.105810

O -0.015029 -2.002514 -1.605244

$Fe_6O_9^-$

I - 71.85

Fe 1.433317 -0.884966 1.320443

Fe -1.433259 -0.884937 1.320600

Fe -0.000020 1.603026 1.321326

Fe 1.433312 -0.884996 -1.320556

Fe -1.433383 -0.885032 -1.320391

Fe 0.000023 1.602747 -1.321934

O 1.605508 0.872326 1.821776

O -1.605538 0.872267 1.821814

O -0.000056 -1.915732 1.820847

O 1.605539 0.872364 -1.821883

O -1.605497 0.872418 -1.821855

O 0.000045 -1.915864 -1.820866

O -0.000109 2.889975 -0.000718

O 2.557810 -1.521830 -0.000097

O -2.557812 -1.521841 0.000361

II - 69.90

Fe 1.422773 1.422711 0.000000

Fe 1.422777 -1.422714 0.000000

Fe -1.422775 1.422716 0.000000

Fe -1.422771 -1.422711 0.000000

Fe 0.000001 0.000000 2.008049

Fe 0.000001 0.000000 -2.008054

O 0.000001 1.958568 1.401034

O 0.000001 1.958577 -1.401032

O -0.000005 -1.958567 1.401032

O -0.000005 -1.958575 -1.401030

O 1.958558 0.000002 1.401060

O 1.958567 0.000002 -1.401058

O -1.958559 -0.000004 1.401058

O -1.958568 -0.000004 -1.401056

O 0.000002 0.000000 -0.000002

III - 69.75

Fe 1.292982 1.278615 -0.050978

Fe 1.209371 -1.239370 0.048557

Fe -1.204816 1.344289 -0.048781

Fe -1.290378 -1.171443 0.050413

Fe 0.016975 0.146438 2.475628

Fe -0.001984 -0.028522 -2.086644

O 1.855728 0.050081 1.284432

O 0.062672 2.037415 1.170532

O -1.843850 0.157627 1.288456

O -0.054830 -1.836522 1.317398

O 1.930618 -0.053518 -1.296785

O 0.057454 1.917606 -1.403601

O -1.932045 0.057910 -1.295076

O -0.058427 -1.915116 -1.252435

O 0.049256 0.167834 4.213041

$Fe_6O_{10}^-$

I - 75.84

Fe 2.181530 0.145119 -0.371373

Fe -1.862564 0.088618 0.014238

Fe 0.263674 2.188287 -0.368595

Fe -0.043527 -1.836931 0.012178

Fe -0.253752 -0.223173 2.345810

Fe 2.031916 1.921741 2.246132

O 1.617942 1.535889 -1.388033

O 1.617072 -1.517483 -0.671671

O -1.431542 1.725477 -0.665137

O -1.739646 -1.618406 -0.689061

O 0.939030 0.894351 3.175676

O 0.135030 -1.918824 1.817308

O -1.927353 0.254989 1.821570

O 3.081419 2.899776 3.044836

O 0.964530 2.874038 1.109432

O 2.909723 0.786716 1.109615

II - 75.20

Fe 0.777731 1.814377 0.019564

Fe 1.882570 -1.299301 -0.048786

Fe -1.652588 1.616980 0.377986

Fe -1.974592 -1.111289 -0.089948

Fe 0.058562 -0.058224 1.892610

Fe 0.125277 -0.485486 -1.624609

O 1.272305 1.397833 1.707349

O -1.388400 1.103733 2.107724

O 1.510645 -1.178260 1.709526

O -1.092584 -1.457232 1.439326

O 1.749614 0.488027 -0.886066

O -0.567586 1.252052 -1.329318

O 1.292120 -1.925778 -1.705904

O -1.441628 -1.411287 -1.823881

O -0.491880 3.085180 0.383789

O -2.940158 0.414648 -0.064787

III - 74.88

Fe 2.075978 1.188444 0.256492

Fe 1.198310 -1.425602 -0.094528

Fe -1.920840 0.992994 -0.203338

Fe -1.501619 -1.769182 0.681518

Fe 0.041063 0.192218 1.929425

Fe 0.255174 0.681468 -1.996939

O 1.499767 1.430132 1.917570

O -1.208262 1.491561 1.409092

O 1.197723 -1.202015 1.714916

O -1.314935 -1.068988 2.297950

O 1.498790 1.838058 -1.293233

O -1.402365 1.403508 -1.889021

O 0.790729 -1.066046 -1.890893

O -0.170154 -2.757859 0.048498

O 2.771618 -0.384904 -0.166302

O -2.645042 -0.694688 -0.154493

$Fe_6O_{11}^-$

I - 79.73

Fe 1.407727 -0.634932 1.303927

Fe -1.548813 -0.462357 1.198886

Fe -0.030559 2.121635 2.013291

Fe 1.723304 -1.114302 -1.693798

Fe -1.575787 -0.988935 -1.604041

Fe -0.168931 1.423141 -0.979571

O 1.383314 1.038832 2.126316

O -1.498094 1.084289 2.146144

O -0.143461 -1.415623 1.788524

O 1.385880 0.659323 -1.520949

O -1.489986 0.790624 -2.007908

O 0.055525 -1.728362 -1.935574

O -0.058653 2.683927 0.265029

O 2.342915 -1.424038 -0.025961

O -2.515102 -1.299383 -0.076625

O -0.060726 3.387639 3.064934

O 2.757231 -1.696465 -2.838692

II - 79.39

Fe 1.528304 -0.987513 1.470897

Fe -1.514323 -0.882713 1.369529

Fe -0.029870 2.010681 1.609924

Fe 1.359304 -0.993508 -1.404358

Fe -1.712331 -0.870716 -1.602162

Fe -0.060212 1.935725 -1.732274

O 1.303999 0.827965 1.611871

O -1.380914 0.891638 1.800025

O -0.060740 -1.708541 2.007412

O 1.293106 0.761490 -1.905698

O -1.480378 0.876868 -2.024163

O -0.161937 -1.709094 -2.038771

O -0.156918 2.633224 -0.016835

O 2.339453 -1.626203 -0.026878

O -2.500153 -1.395964 -0.048479

O 0.133117 3.155347 2.775736

O 0.139286 3.303474 -2.663332

III - 78.71

Fe 1.440238 1.513805 0.048158

Fe 2.039485 -1.089098 0.097949

Fe -1.404497 1.514923 0.089162

Fe -2.038025 -1.087789 0.025270

Fe 0.040135 -0.046171 1.916478

Fe -0.007932 -0.182164 -1.769398

O 1.306586 1.255184 1.899303

O -1.298026 1.216722 1.906442

O 1.346055 -1.415362 1.656787

O -1.237219 -1.431185 1.506518

O 1.281123 1.106810 -1.728995

O -1.266039 1.117582 -1.718376

O 1.308443 -1.543545 -1.418323

O -1.362336 -1.533213 -1.499015

O 0.005495 2.695524 0.057563

O 3.005360 0.356470 0.056296

O -3.002705 0.335236 0.058876

$Fe_6O_{12}^-$

I - 83.70

Fe 1.509842 -0.892003 1.444829

Fe -1.955711 -0.684825 1.811436

Fe -0.051100 1.828207 1.461681

Fe 1.811944 -0.915301 -1.826280

Fe -1.186801 -1.090423 -0.847034

Fe -0.046732 1.668680 -1.411715

O 1.294490 0.746183 2.113288

O -1.628897 1.053886 1.937536

O -0.195508 -1.197612 0.925445

O 1.333928 0.788883 -2.142784

O -1.417233 0.578536 -1.583941

O 0.230329 -1.722149 -1.813132

O -0.039320 2.830189 -0.059561

O 2.348639 -0.769238 -0.085421

O -2.646672 -1.308926 0.285453

O 2.972349 -1.711994 -2.708825

O 2.126783 -2.025054 2.445906

O -2.138554 -1.410679 3.282213

II - 82.08

Fe 1.348057 1.907975 0.367649

Fe -1.502720 2.032893 0.040640

Fe 1.917599 -0.732129 0.148544

Fe -2.034089 -0.598754 0.075475

Fe 0.212348 -2.730180 0.622826

Fe -0.569021 0.496383 1.941906

O 0.004796 2.978898 -0.278768

O 2.876460 0.897851 0.156220

O -2.966810 0.967166 -0.249319

O 1.697346 -2.548432 -0.359037

O -1.298344 -2.230051 -0.180886

O 0.965511 1.621113 2.083978

O -1.600937 2.068863 1.838312

O 0.572745 -0.908956 1.536829

O -2.071830 -0.579086 1.906900

O 0.166833 -3.842733 1.825271

O 0.711666 0.474626 -1.085975

O -0.792675 0.478839 -1.219465

III - 82.44

Fe 1.413492 1.390698 0.052321

Fe 1.382863 -1.419566 0.052389

Fe -1.397259 1.419151 0.051962

Fe -1.427731 -1.391455 0.051974

Fe -0.008587 -0.000913 2.040826

Fe -0.007620 -0.000858 -1.936599

O 1.318572 1.301229 1.913027

O -1.308573 1.326347 1.912883

O 1.295470 -1.325746 1.913259

O -1.334309 -1.303027 1.912949

O 1.319362 1.301362 -1.808439

O -1.308155 1.325900 -1.808880

O 1.296704 -1.325343 -1.808549

O -1.333261 -1.303140 -1.808957

O 0.024386 2.630354 0.052089

O -0.037040 -2.630582 0.052056

O 2.623709 -0.030885 0.052786

O -2.637523 0.030218 0.051909

$Fe_6O_{13}^-$

I - 92.53

Fe 1.296311 -0.880218 1.560339

Fe -1.980032 -0.734659 1.777212

Fe -0.228130 2.017536 1.710444

Fe 1.719149 -1.151004 -1.624331

Fe -1.340312 -1.226148 -0.913759

Fe -0.154826 1.509646 -1.407843

O 1.150173 0.862437 1.729199

O -1.726481 1.004461 1.839092

O -0.373113 -1.284097 0.965581

O 1.306475 0.550420 -1.927316

O -1.506618 0.385941 -1.705819

O 0.116981 -1.935758 -1.717154

O -0.254940 2.582112 0.035242

O 2.239950 -1.187299 0.074486

O -2.755806 -1.318871 0.279777

O -0.167686 3.074866 2.956004

O 2.782838 -1.829264 -2.675797

O 1.710133 -1.750305 2.871642

O -2.223818 -1.513094 3.192896

II - 87.97

Fe 1.473316 -0.999315 1.491639

Fe -2.338091 -0.811186 1.789678

Fe -0.189063 1.239784 1.534733

Fe 1.824745 -0.996096 -1.714152

Fe -1.196756 -1.185670 -0.939414

Fe -0.148295 1.737632 -1.608783

O 1.417675 0.580160 2.305640

O -1.930292 0.859165 2.134176

O -0.229904 -0.766292 0.777359

O 1.294167 0.689830 -1.934048

O -1.417341 0.489110 -1.607504

O 0.254211 -1.836801 -1.789860

O -0.056494 2.312241 0.070589

O 2.427188 -1.088011 0.037151

O -2.671992 -1.421303 0.168209

O 3.002888 -1.719702 -2.637565

O -0.459640 2.865976 -2.766877

O 1.498243 -2.320624 2.444275

O -2.541835 -1.818302 3.082721

III - 87.59

Fe 1.367330 1.508291 -0.040113

Fe 1.330523 -1.505789 0.032285

Fe -1.319466 1.518834 0.030178

Fe -1.384997 -1.425926 0.073687

Fe 0.062195 0.160040 2.071860

Fe -0.046471 -0.119881 -2.334512

O 1.398985 1.391931 1.824295

O -1.266353 1.415195 1.886815

O 1.299493 -1.238224 1.820056

O -1.219222 -1.200438 1.855058

O 1.106686 1.376492 -1.852927

O -1.105827 1.397000 -1.815890

O 1.306873 -1.268696 -1.849766

O -1.332857 -1.280191 -1.836783

O -0.051965 -0.176649 -3.988655

O 2.446132 -0.017152 -0.152790

O -2.457859 0.065394 -0.079971

O 0.044402 2.771563 0.061455

O -0.048030 -2.699305 -0.048658

$Fe_6O_{14}^-$

I - 96.40

Fe 1.844977 -1.133449 1.742402

Fe -1.210993 -1.152198 1.183014

Fe -0.020294 1.715091 1.727314

Fe 1.405714 -0.956897 -1.409024

Fe -1.820996 -0.813869 -1.619454

Fe -0.058787 1.933196 -1.602026

O 1.383839 0.588136 1.822309

O -1.295150 0.491511 1.935079

O 0.262694 -1.911574 1.933201

O 1.305937 0.759265 -1.717403

O -1.537460 0.899859 -1.827106

O -0.240495 -1.294905 -0.747692

O -0.137824 2.451861 0.092589

O 2.371381 -1.304752 0.040491

O -2.590992 -1.199953 -0.068864

O -0.053554 2.907837 2.862547

O 1.736703 -1.928086 -2.673255

O 0.041147 2.966093 -2.885679

O 2.984183 -1.737516 2.774236

O -2.147024 -1.733817 -2.917921

II - 89.40

Fe 1.409546 1.512699 0.004590

Fe 1.415966 -1.500031 -0.176760

Fe -1.505975 1.401217 -0.016844

Fe -1.436450 -1.459933 -0.054108

Fe 0.030039 0.123518 2.057913

Fe 0.010262 -0.128193 -2.197260

O 1.685724 0.052455 1.109245

O 0.047271 1.859142 1.303910

O -1.768892 0.058078 1.207514

O -0.046257 -1.727579 1.087726

O 1.728166 -0.110777 -1.396175

O -0.044196 1.610398 -1.139282

O -1.829506 -0.059726 -1.222904

O -0.043157 -1.869803 -1.387618

O 2.626219 2.547511 -0.273604

O 2.549204 -2.560069 0.348664

O -2.516764 2.675091 0.050796

O -2.648030 -2.551010 0.044951

O -0.363760 -0.263585 3.594710

O -0.379611 0.368164 -3.706505

III - 88.20

Fe 1.404402 1.404461 0.000000

Fe 1.404403 -1.404462 0.000000

Fe -1.404403 1.404462 0.000000

Fe -1.404402 -1.404461 0.000000

Fe 0.000000 0.000000 2.255949

Fe 0.000000 0.000000 -2.255949

O 1.296262 1.296256 1.838257

O -1.296362 1.296356 1.838318

O 1.296362 -1.296356 1.838318

O -1.296262 -1.296256 1.838257

O 1.296262 1.296256 -1.838257

O -1.296362 1.296356 -1.838318

O 1.296362 -1.296356 -1.838318

O -1.296262 -1.296256 -1.838257

O 0.000000 0.000000 3.917841

O 0.000000 0.000000 -3.917841

O 2.629237 -0.000010 0.000000

O -2.629236 0.000009 0.000000

O -0.000009 2.629212 0.000000

O 0.000009 -2.629212 0.000000

$Fe_6O_{15}^-$

I - 99.96

Fe 1.597974 -0.966574 1.660144

Fe -1.703732 -0.976500 1.665844

Fe -0.054442 1.916231 1.674540

Fe 1.595732 -0.959376 -1.560331

Fe -1.703283 -0.961905 -1.557021

Fe -0.052969 1.926351 -1.562180

O 1.309704 0.779216 1.707058

O -1.414786 0.769727 1.715997

O -0.049516 -1.614318 1.712488

O 1.309544 0.786004 -1.602267

O -1.413385 0.783419 -1.603605

O -0.053117 -1.606397 -1.610514

O -0.055245 2.660366 0.058100

O 2.249512 -1.337066 0.049091

O -2.354936 -1.339898 0.051819

O -0.054526 2.920981 2.964427

O 2.565760 -1.527956 -2.760188

O -0.052577 2.941411 -2.844921

O 2.570360 -1.529939 2.859863

O -2.670531 -1.527090 -2.760035

O -2.662653 -1.582974 2.857117

II - 94.29

Fe 1.700551 -0.977238 1.707228

Fe -1.404440 -0.982785 1.163594

Fe -0.072583 1.899733 1.748214

Fe 1.595205 -0.955506 -1.515089

Fe -1.666563 -0.963995 -1.801269

Fe -0.053686 1.895152 -1.524769

O 1.318100 0.722699 1.490621

O -1.425527 0.647166 1.818063

O 0.101080 -1.721455 1.842861

O 1.338445 0.796587 -1.398795

O -1.457901 0.795342 -1.624619

O -0.059476 -1.626868 -1.387219

O -0.160572 2.643220 0.046292

O 2.268636 -1.418523 0.076423

O -2.451947 -1.407202 -0.256605

O 2.334359 -1.401786 -2.900993

O 0.052067 2.860778 -2.837964

O 2.664172 -1.310812 2.979061

O -2.326427 -1.501347 -3.184542

O -0.717076 3.385173 2.739744

O 0.403310 2.664028 3.430732

III - 94.50

Fe 1.389457 -0.910101 1.543964

Fe -1.857421 -0.779831 1.718366

Fe -0.083191 2.042214 1.828289

Fe 1.952253 -0.956994 -1.640463

Fe -1.123598 -1.092055 -0.983444

Fe 0.052518 1.801413 -1.516416

O 1.261947 0.773964 1.928276

O -1.614052 0.901832 1.907649

O -0.263579 -1.304243 0.886699

O 1.517429 0.749991 -1.723041

O -1.224683 0.579381 -1.628698

O 0.339401 -1.732407 -1.761208

O 0.058616 2.534592 0.091713

O 2.368130 -1.174825 0.066816

O -2.582896 -1.201419 0.145356

O 2.963636 -1.595871 -2.760130

O -0.049724 2.886588 -2.746716

O 1.732230 -1.933197 2.762056

O -2.234821 -1.713425 2.995372

O -0.680289 3.667344 2.658591

O 0.054735 2.757866 3.587639

$Fe_6O_{16}^-$

I - 102.74

Fe 1.591433 -1.022030 1.615956

Fe -1.679666 -1.013368 1.611332

Fe -0.049898 1.889572 1.716497

Fe 1.608631 -1.039954 -1.613216

Fe -1.662187 -0.994598 -1.608543

Fe -0.035091 1.850672 -1.519992

O 1.321225 0.702369 1.508958

O -1.449743 0.708051 1.603607

O -0.022587 -1.709108 1.513836

O 1.318272 0.710955 -1.604514

O -1.434759 0.752804 -1.416940

O -0.042246 -1.704461 -1.515013

O -0.040120 2.649178 0.041123

O 2.249000 -1.412930 0.001235

O -2.343618 -1.404056 -0.032747

O 2.392878 -1.513483 -2.971534

O -0.062372 2.788179 -2.860101

O 2.441672 -1.498878 2.915976

O -2.467128 -1.397806 -2.964787

O -2.441880 -1.513802 2.979829

O -0.684400 3.366871 2.749543

O 0.210583 2.446534 3.512392

II - 98.12

Fe 1.550083 -0.979015 1.625970

Fe -1.705839 -0.928132 1.713730

Fe -0.000818 1.966698 1.811396

Fe 1.545112 -0.971705 -1.593719

Fe -1.715534 -0.851423 -1.502315

Fe 0.007337 1.943153 -1.500917

O 1.338787 0.756481 1.600968

O -1.441306 0.763296 1.911351

O -0.076619 -1.611861 1.406630

O 1.350574 0.789999 -1.613947

O -1.440859 0.886846 -1.521673

O -0.098403 -1.547728 -1.290559

O -0.039022 2.654325 0.085414

O 2.271817 -1.303441 0.002047

O -2.454538 -1.098411 0.117553

O 2.224932 -1.532397 -2.975853

O 0.045147 2.958013 -2.782837

O 2.329784 -1.521718 2.950818

O -2.475998 -1.505903 -2.780102

O -2.394821 -1.716448 2.966222

O 0.363966 2.731202 3.516117

O -0.657767 3.503054 2.745094