Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Content **Page**

1. Zero-Point Corrected Energies and Adiabatic Ionization Potentials

The zero-point corrected energies of each of the calculated compounds are presented (in Hartrees), calculated at the B3LYP/6-311G* level of theory. For convenience, the compounds have been divided into Table Ss of their respective families, as denoted in the main text.

The adiabatic ionization potential (IP) is calculated as the difference between the energy of the neutral compound and its respective cationic species, and is given in eV.

Table S1. Zero-Point Corrected Energies and Adiabatic Ionization Potential for compounds of Family 1.

n	Neutral (Hartree)	Cation (Hartree)	IP (eV)
PP[1]	-232.197768	-231.867317	8.99
PP[2]	-463.219436	-462.932062	7.82
PP[3]	-694.241541	-693.973574	7.29
PP[4]	-925.263705	-925.006609	7.00
PP[5]	-1156.285889	-1156.035565	6.81
PP[6]	-1387.308090	-1387.062457	6.68
PP[7]	-1618.330287	-1618.088305	6.58
PP[8]	-1849.352469	-1849.113371	6.51
PP[12]	-2773.441182	-2773.209684	6.30
PP[16]	-3697.530087	-3697.303128	6.18
PP[24]	-5545.707518	-5545.485695	6.04

Table S2. Zero-Point Corrected Energies and Adiabatic Ionization Potential for compounds of Family 2.

n	Neutral (Hartree)	Cation (Hartree)	IP (eV)
α-P[1]	-210.132611	-209.839170	7.98
α-P[2]	-419.097022	-418.853118	6.64
α-P[3]	-628.062087	-627.840201	6.04
α-P[4]	-837.027016	-836.817886	5.69
α-P[5]	-1045.992707	-1045.790863	5.49
α-P[6]	-1254.957508	-1254.761526	5.33
α-P[7]	-1463.923209	-1463.730858	5.23
α-P[8]	-1672.888405	-1672.699124	5.15
α-P[12]	-2508.749196	-2508.568012	4.93
α-P[16]	-3344.610170	-3344.433569	4.81
α-P[24]	-5016.331830	-5016.160969	4.65

Table S3. Zero-Point Corrected Energies and Adiabatic Ionization Potential for compounds of Family 3.

n	Neutral (Hartree)	Cation (Hartree)	IP (eV)
α-F[1]	-230.005697	-229.687156	8.67
α-F[2]	-458.845820	-458.578766	7.27
α-F[3]	-687.686994	-687.443183	6.63
α-F[4]	-916.528350	-916.298105	6.27
α-F[5]	-1145.369768	-1145.148355	6.02
α-F[6]	-1374.211181	-1373.995984	5.86
α-F[7]	-1603.052608	-1602.842001	5.73
α-F[8]	-1831.893986	-1831.686951	5.63
α-F[12]	-2747.259718	-2747.061427	5.40
α-F[16]	-3662.625408	-3662.432129	5.26
α-F[24]	-5493.356673	-5493.169336	5.10

Table S4. Zero-Point Corrected Energies and Adiabatic Ionization Potential for compounds of Family 4.

n	Neutral (Hartree)	Cation (Hartree)	IP (eV)
α-T[1]	-552.995629	-552.677727	8.65
α-T[2]	-1104.818113	-1104.549587	7.31
α-T[3]	-1656.641688	-1656.395315	6.70
α-T[4]	-2208.465304	-2208.231870	6.35
α-T[5]	-2760.289257	-2760.064022	6.13
α-T[6]	-3312.112948	-3311.893691	5.97
α-T[7]	-3863.936875	-3863.721836	5.85
α-T[8]	-4415.760462	-4415.548895	5.76
α-T[12]	-6623.055967	-6622.852151	5.55
α-T[16]	-8830.351259	-8830.151878	5.43
α-T[24]	-13244.941057	-13244.747137	5.28

Table S5. Zero-Point Corrected Energies and Adiabatic Ionization Potential for compounds of Family 5.

n	Neutral (Hartree)	Cation (Hartree)	IP (eV)
FP[1]	-210.132611	-209.839170	7.98
FP[2]	-341.680746	-341.429123	6.85
FP[3]	-473.228959	-473.002882	6.15
FP[4]	-604.777212	-604.569625	5.65
FP[5]	-736.325664	-736.131094	5.29
FP[6]	-867.874426	-867.689418	5.03
FP[7]	-999.422988	-999.245841	4.82
FP[8]	-1130.971539	-1130.800918	4.64
FP[12]	-1657.165242	-1657.011696	4.18
FP[16]	-2183.360034	-2183.215660	3.93
FP[24]	-3235.747679	-3235.613240	3.66

Table S6. Zero-Point Corrected Energies and Adiabatic Ionization Potential for compounds of Family 6.

n	Neutral (Hartree)	Cation (Hartree)	IP (eV)
FF[1]	-230.005697	-229.687156	8.67
FF[2]	-381.423568	-381.135483	7.84
FF[3]	-532.842373	-532.573595	7.31
FF[4]	-684.260818	-684.005582	6.95
FF[5]	-835.679234	-835.434005	6.67
FF[6]	-987.097741	-986.860223	6.46
FF[7]	-1138.515868	-1138.284900	6.28
FF[8]	-1289.934105	-1289.708477	6.14
FF[12]	-1895.607407	-1895.396094	5.75
FF[16]	-2501.280734	-2501.077695	5.52
FF[24]	-3712.627334	-3712.432455	5.30

Table S7. Zero-Point Corrected Energies and Adiabatic Ionization Potential for compounds of Family 7.

n	Neutral (Hartree)	Cation (Hartree)	IP (eV)
FT[1]	-552.995629	-552.677727	8.65
FT[2]	-1027.420208	-1027.132746	7.82
FT[3]	-1501.845616	-1501.575014	7.36
FT[4]	-1976.270933	-1976.012756	7.03
FT[5]	-2450.696219	-2450.447033	6.78
FT[6]	-2925.121475	-2924.879219	6.59
FT[7]	-3399.546834	-3399.309985	6.44
FT[8]	-3873.972141	-3873.739687	6.33
FT[12]	-5771.673400	-5771.452385	6.01
FT[16]	-7669.374646	-7669.160029	5.84
FT[24]	-11464.777120	-11464.569540	5.65

2. HOMO and LUMO Energies and HOMO-LUMO Gaps

The Kohn-Sham HOMO and LUMO energies of each of the compounds are presented (in Hartrees), calculated in the ground state at the B3LYP/6-311G* level of theory.

The HOMO-LUMO gap is calculated as the difference between these two energies, and is given in eV.

Table S8. HOMO and LUMO Energies and HOMO-LUMO Gaps for compounds of Family 1.

n	HOMO (Hartree)	LUMO (Hartree)	H-L Gap (eV)
PP[1]	-0.25551	-0.00807	6.73
PP[2]	-0.23202	-0.03432	5.38
PP[3]	-0.22204	-0.04552	4.80
PP[4]	-0.21652	-0.05208	4.47
PP[5]	-0.21438	-0.05590	4.31
PP[6]	-0.21208	-0.05857	4.18
PP[7]	-0.21064	-0.06028	4.09
PP[8]	-0.20993	-0.06128	4.04
PP[12]	-0.20839	-0.06360	3.94
PP[16]	-0.20792	-0.06426	3.91
PP[24]	-0.20728	-0.06552	3.86

Table S9. HOMO and LUMO Energies and HOMO-LUMO Gaps for compounds of Family 2.

n	HOMO (Hartree)	LUMO (Hartree)	H-L Gap (eV)
α-P[1]	-0.21098	0.03588	6.72
α-P[2]	-0.18459	0.00318	5.11
α-P[3]	-0.17252	-0.01199	4.37
α-P[4]	-0.16675	-0.01915	4.02
α-P[5]	-0.16262	-0.02511	3.74
α-P[6]	-0.16080	-0.02739	3.63
α-P[7]	-0.15887	-0.03054	3.49
α-P[8]	-0.15786	-0.03214	3.42
α-P[12]	-0.15611	-0.03503	3.29
α-P[16]	-0.15546	-0.03653	3.24
α-P[24]	-0.15497	-0.03768	3.19

Table S10. HOMO and LUMO Energies and HOMO-LUMO Gaps for compounds of Family 3.

n	HOMO (Hartree)	LUMO (Hartree)	H-L Gap (eV)
α-F[1]	-0.23385	0.00836	6.59
α-F[2]	-0.20262	-0.03202	4.64
α-F[3]	-0.18979	-0.04873	3.84
α-F[4]	-0.18313	-0.05777	3.41
α-F[5]	-0.17922	-0.06338	3.15
α-F[6]	-0.17675	-0.06713	2.98
α-F[7]	-0.17509	-0.06978	2.87
α-F[8]	-0.17394	-0.07172	2.78
α-F[12]	-0.17164	-0.07603	2.60
α-F[16]	-0.17078	**-0.07794**	2.53
α-F[24]	-0.17017	-0.07953	2.47

Table S11. HOMO and LUMO Energies and HOMO-LUMO Gaps for compounds of Family 4.

n	HOMO (Hartree)	LUMO (Hartree)	H-L Gap (eV)
α-T[1]	-0.24176	-0.01693	6.12
α-T[2]	-0.21386	-0.05020	4.45
α-T[3]	-0.20127	-0.06566	3.69
α-T[4]	-0.19504	-0.07442	3.28
α-T[5]	-0.19078	-0.07987	3.02
α-T[6]	-0.18844	-0.08362	2.85
α-T[7]	-0.18664	-0.08615	2.73
α-T[8]	-0.18571	-0.08810	2.66
α-T[12]	-0.18311	-0.09225	2.47
α-T[16]	-0.18223	-0.09402	2.40
α-T[24]	-0.18195	-0.09555	2.35

Table S12. HOMO and LUMO Energies and HOMO-LUMO Gaps for compounds of Family 5.

n	HOMO (Hartree)	LUMO (Hartree)	H-L Gap (eV)
FP[1]	-0.21098	0.03588	6.72
FP[2]	-0.17956	0.02673	5.61
FP[3]	-0.16207	0.02137	4.99
FP[4]	-0.15098	0.01397	4.49
FP[5]	-0.14345	0.00816	4.13
FP[6]	-0.13719	0.00422	3.85
FP[7]	-0.13240	0.00142	3.64
FP[8]	-0.12864	-0.00085	3.48
FP[12]	-0.11940	-0.00655	3.07
FP[16]	-0.11471	-0.01083	2.83
FP[24]	-0.11026	-0.01360	2.63

Table S13. HOMO and LUMO Energies and HOMO-LUMO Gaps for compounds of Family 6.

n	HOMO (Hartree)	LUMO (Hartree)	H-L Gap (eV)
FF[1]	-0.23385	0.00836	6.59
FF[2]	-0.21379	-0.01367	5.45
FF[3]	-0.20205	-0.02605	4.79
FF[4]	-0.19441	-0.03582	4.32
FF[5]	-0.18912	-0.04347	3.96
FF[6]	-0.18528	-0.04960	3.69
FF[7]	-0.18282	-0.05498	3.48
FF[8]	-0.18099	-0.05943	3.31
FF[12]	-0.17657	-0.07110	2.87
FF[16]	-0.17449	-0.07769	2.63
FF[24]	-0.17281	-0.08467	2.40

Table S14. HOMO and LUMO Energies and HOMO-LUMO Gaps for compounds of Family 7.

n	HOMO (Hartree)	LUMO (Hartree)	H-L Gap (eV)
FT[1]	-0.24176	-0.01693	6.12
FT[2]	-0.22316	-0.03427	5.14
FT[3]	-0.21416	-0.04732	4.54
FT[4]	-0.20713	-0.05618	4.11
FT[5]	-0.20247	-0.06291	3.80
FT[6]	-0.19900	-0.06813	3.56
FT[7]	-0.19643	-0.07225	3.38
FT[8]	-0.19444	-0.07561	3.23
FT[12]	-0.18982	-0.08431	2.87
FT[16]	-0.18770	-0.08908	2.68
FT[24]	-0.18596	-0.09395	2.50

3. Comparison with Available Experimental Data

In the main text, we show only computationally obtained HOMO-LUMO gaps and IPs. Here, we provide experimental results that were collected from the literature.

Table S15. Calculated versus Experimental HOMO-LUMO Gaps.

n	Calc. H-L Gap (eV)	Exp. Bandgap (H-L Gap) (eV)
PP[1]	6.73	5.90[a]
PP[2]	5.38	4.92[a]
PP[3]	4.80	4.34[b]
PP[4]	4.47	4.11[b]
α-P[1]	6.72	5.96[a]
α-P[2]	5.11	4.92[a]
α-P[3]	4.37	4.34[a]
α-F[3]	3.84	3.75[c]
α-F[4]	3.41	3.41[c]
α-F[5]	3.15	3.20[c]
α-F[6]	2.98	3.07[c]
α-F[7]	2.87	2.97[c]
α-F[8]	2.78	2.93[c]
α-T[1]	6.12	5.37[a]
α-T[2]	4.45	4.12[a]
α-T[3]	3.69	3.52[a]

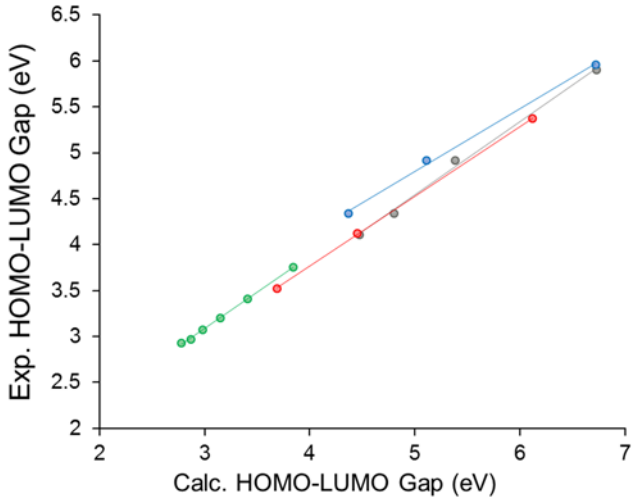

Figure S1. Correlation between computed and experimentally measured HOMO-LUMO Gaps. Gray – PP[n]; Blue – α-P[n]; Green – α-F[n]; Red – α-T[n].

Considering the (admittedly) inaccurate use of ground-state HOMO-LUMO gaps, this agreement is quite satisfactory. It also serves as further reinforcement for both our choice of methodology and the conclusions drawn.

Note: We also used this correlation as a basis for correcting all of the HOMO-LUMO gaps reported, and this afforded almost identical results.

a) Bredas, J. L.; Silbey, R.; Boudreaux, D. S.; Chance, R. R., Chain-length dependence of electronic and electrochemical properties of conjugated systems: polyacetylene, polyphenylene, polythiophene, and polypyrrole. *Journal of the American Chemical Society* **1983**, *105* (22), 6555-6559.

b) Matsuoka, S.; Fujii, H.; Yamada, T.; Pac, C.; Ishida, A.; Takamuku, S.; Kusaba, M.; Nakashima, N.; Yanagida, S., Photocatalysis of oligo (p-phenylenes): photoreductive production of hydrogen and ethanol in aqueous triethylamine. *The Journal of Physical Chemistry* **1991**, *95* (15), 5802-5808.

c) Gidron, O.; Diskin-Posner, Y.; Bendikov, M., α-Oligofurans. *Journal of the American Chemical Society* **2010**, *132* (7), 2148-2150.

4. B3LYP/6-311G* NICS(1)$_{\pi ZZ}$ Values (for all rings)

B3LYP/6-311G* NICS(1)$_{\pi ZZ}$ values were calculated for all neutral compounds with the σ-Only Model, using the Aroma software packages interfaced with Gaussian revision D.

The compounds are presented in the following tables, according to their respective families. The value of each ring within each compound is reported in ppm. Note: *n* indicates the number of the ring within the oligomer, where *n* = 1 is the outer-most ring.

Table S16. B3LYP/6-311G NICS(1)$_{\pi ZZ}$ Values for all rings in compounds in Family 1.*

n	**PP[1]**	**PP[2]**	**PP[3]**	**PP[4]**	**PP[5]**	**PP[6]**	**PP[7]**	**PP[8]**	**PP[12]**	**PP[16]**	**PP[24]**
1	-36.52	-34.09	-33.91	-33.84	-33.78	-33.80	-33.80	-33.81	-33.77	-33.84	-33.76
2		-34.10	-31.92	-31.60	-31.56	-31.53	-31.49	-31.52	-31.54	-31.60	-31.44
3			-33.92	-31.01	-31.46	-31.33	-31.32	-31.35	-31.41	-30.86	-31.25
4				-33.60	-31.56	-31.33	-31.30	-31.32	-31.38	-30.09	-31.24
5					-33.77	-31.53	-30.78	-30.79	-31.27	-30.67	-30.72
6						-33.81	-30.37	-30.14	-31.33	-31.08	-30.69
7							-33.58	-31.12	-31.36	-30.97	-31.21
8								-33.79	-31.33	-31.72	-31.22
9									-31.26	-31.07	-31.38
10									-31.41	-30.97	-30.87
11									-31.65	-31.21	-30.10
12									-33.84	-30.74	-30.70
13										-30.82	-31.22
14										-31.40	-31.23
15										-31.19	-31.25
16										-33.84	-31.26
17											-31.29
18											-31.37
19											-31.37
20											-30.89
21											-30.90
22											-31.43
23											-31.67
24											-33.84

Table S17. B3LYP/6-311G NICS(1)$_{nZZ}$ Values for all rings in compounds in Family 2.*

n	**α-P[1]**	**α-P[2]**	**α-P[3]**	**α-P[4]**	**α-P[5]**	**α-P[6]**	**α-P[7]**	**α-P[8]**	**α-P[12]**	**α-P[16]**	**α-P[24]**
1	-27.00	-24.06	-23.72	-23.77	-23.72	-23.75	-24.68	-25.49	-27.45	-29.60	-34.15
2		-24.06	-20.84	-20.82	-20.50	-20.52	-19.62	-19.65	-19.67	-20.47	-20.37
3			-23.72	-20.33	-20.25	-20.42	-19.66	-19.66	-19.76	-19.91	-19.94
4				-23.89	-20.12	-20.52	-19.15	-19.40	-19.12	-20.26	-19.94
5					-23.88	-19.79	-19.66	-19.40	-19.07	-19.92	-20.30
6						-23.67	-19.61	-19.33	-18.73	-19.88	-20.01
7							-24.68	-20.00	-19.96	-20.00	-20.30
8								-25.35	-20.34	-19.75	-20.14
9									-19.93	-18.72	-20.17
10									-19.90	-19.03	-18.79
11									-20.48	-18.88	-19.03
12									-27.45	-19.38	-18.83
13										-19.34	-19.09
14										-19.81	-18.85
15										-19.65	-19.10
16										-29.49	-18.91
17											-20.32
18											-20.45
19											-19.95
20											-20.01
21											-20.29
22											-19.92
23											-20.34
24											-35.00

Table S18. B3LYP/6-311G NICS(1)$_{nZZ}$ Values for all rings in compounds in Family 3.*

n	**α-F[1]**	**α-F[2]**	**α-F[3]**	**α-F[4]**	**α-F[5]**	**α-F[6]**	**α-F[7]**	**α-F[8]**	**α-F[12]**	**α-F[16]**	**α-F[24]**
1	-22.54	-18.71	-18.55	-18.54	-18.57	-18.75	-19.33	-19.92	-21.75	-23.82	-27.23
2		-18.70	-15.16	-14.97	-14.90	-14.87	-14.88	-14.89	-14.88	-14.87	-14.80
3			-18.55	-14.98	-14.83	-14.74	-14.66	-14.67	-14.75	-14.75	-14.75
4				-18.54	-14.90	-14.74	-14.54	-14.43	-14.58	-14.68	-14.75
5					-18.57	-14.87	-14.66	-14.43	-14.32	-14.51	-14.71
6						-18.75	-14.88	-14.67	-14.21	-14.34	-14.65
7							-19.33	-14.89	-14.21	-14.26	-14.48
8								-19.92	-14.32	-14.24	-14.42
9									-14.58	-14.24	-14.33
10									-14.75	-14.26	-14.34
11									-14.88	-14.34	-14.28
12									-21.75	-14.51	-14.31
13										-14.68	-14.27
14										-14.75	-14.32
15										-14.87	-14.29
16										-23.82	-14.36
17											-14.36
18											-14.50
19											-14.61
20											-14.72
21											-14.72
22											-14.75
23											-14.79
24											-27.23

Table S19. B3LYP/6-311G NICS(1)$_{nZZ}$ Values for all rings in compounds in Family 4.*

n	α-T[1]	α-T[2]	α-T[3]	α-T[4]	α-T[5]	α-T[6]	α-T[7]	α-T[8]	α-T[12]	α-T[16]	α-T[24]
1	-23.69	-20.01	-20.35	-20.36	-20.38	-20.44	-20.44	-20.47	-21.03	-22.34	-26.31
2		-20.00	-17.08	-17.13	-16.74	-16.81	-17.19	-16.41	-16.25	-16.16	-16.60
3			-20.36	-16.48	-16.89	-16.36	-16.35	-15.88	-15.52	-15.50	-16.76
4				-19.59	-17.13	-16.02	-16.27	-15.90	-15.87	-15.89	-15.86
5					-20.06	-16.08	-16.83	-15.43	-15.29	-15.27	-15.37
6						-19.49	-16.79	-16.04	-15.44	-15.17	-15.93
7							-20.44	-17.19	-13.36	-15.43	-15.84
8								-20.17	-13.46	-14.89	-15.89
9									-14.36	-15.37	-15.72
10									-15.17	-14.93	-15.91
11									-16.16	-15.64	-15.31
12									-19.48	-15.29	-14.85
13										-16.28	-15.17
14										-15.50	-15.27
15										-16.02	-15.88
16										-22.34	-15.65
17											-15.55
18											-15.66
19											-15.58
20											-15.93
21											-16.68
22											-16.49
23											-16.38
24											-25.71

Table S20. B3LYP/6-311G NICS(1)$_{nZZ}$ Values for all rings in compounds in Family 5.*

n	**FP[1]**	**FP[2]**	**FP[3]**	**FP[4]**	**FP[5]**	**FP[6]**	**FP[7]**	**FP[8]**	**FP[12]**	**FP[16]**	**FP[24]**
1	-27.00	-27.01	-26.19	-26.25	-26.15	-26.44	-27.67	-28.62	-30.01	-34.73	-43.83
2		-27.01	-23.74	-22.94	-21.93	-22.85	-23.92	-24.16	-22.23	-23.01	-22.62
3			-26.19	-22.77	-21.08	-20.84	-19.22	-13.77	-20.46	-21.51	-21.18
4				-25.66	-22.26	-20.84	-19.38	-18.65	-20.89	-20.87	-20.53
5					-25.97	-22.86	-19.70	-19.20	-16.40	-18.86	-19.46
6						-26.05	-20.43	-14.99	-16.79	-18.31	-18.72
7							-27.39	-25.02	-16.35	-16.17	-18.34
8								-28.62	-16.40	-15.83	-18.47
9									-20.89	-16.09	-17.87
10									-21.53	-16.75	-18.06
11									-22.23	-18.04	-17.14
12									-30.01	-17.66	-17.40
13										-19.41	-17.40
14										-20.47	-17.14
15										-22.39	-18.06
16										-34.51	-17.87
17											-18.47
18											-18.34
19											-18.72
20											-19.46
21											-20.53
22											-21.18
23											-22.62
24											-43.83

Table S21. B3LYP/6-311G NICS(1)$_{nZZ}$ Values for all rings in compounds in Family 6.*

n	**FF[1]**	**FF[2]**	**FF[3]**	**FF[4]**	**FF[5]**	**FF[6]**	**FF[7]**	**FF[8]**	**FF[12]**	**FF[16]**	**FF[24]**
1	-22.54	-21.41	-21.14	-21.10	-21.39	-22.52	-23.32	-24.35	-28.33	-29.86	-33.98
2		-21.40	-19.79	-19.59	-19.56	-20.01	-20.40	-20.60	-20.46	-20.33	-20.20
3			-21.14	-19.59	-18.80	-18.11	-17.36	-17.02	-17.98	-18.06	-19.54
4				-21.10	-19.56	-18.11	-16.66	-16.44	-17.15	-17.92	-18.64
5					-21.39	-20.01	-17.36	-16.44	-16.29	-17.14	-17.53
6						-22.52	-20.40	-17.02	-15.20	-15.88	-17.13
7							-23.32	-20.60	-15.20	-15.29	-16.50
8								-24.35	-16.29	-15.11	-16.01
9									-17.15	-15.11	-15.79
10									-17.98	-15.29	-15.73
11									-20.46	-15.88	-15.73
12									-28.33	-17.14	-15.73
13										-17.92	-15.73
14										-18.06	-15.73
15										-20.33	-15.73
16										-29.86	-15.79
17											-16.01
18											-16.50
19											-17.13
20											-17.53
21											-18.64
22											-19.54
23											-20.20
24											-33.98

Table S22. B3LYP/6-311G NICS(1)$_{nZZ}$ Values for all rings in compounds in Family 7.*

n	**FT[1]**	**FT[2]**	**FT[3]**	**FT[4]**	**FT[5]**	**FT[6]**	**FT[7]**	**FT[8]**	**FT[12]**	**FT[16]**	**FT[24]**
1	-23.69	-20.93	-20.28	-20.18	-20.19	-20.29	-20.45	-20.81	-24.45	-28.40	-36.66
2		-20.93	-18.55	-17.98	-17.96	-18.05	-18.69	-18.87	-18.11	-17.98	-17.87
3			-20.28	-17.98	-17.84	-17.76	-17.71	-17.71	-17.64	-17.64	-17.60
4				-20.18	-17.96	-17.76	-17.40	-16.95	-16.51	-17.23	-17.40
5					-20.19	-18.05	-17.71	-16.95	-14.84	-16.27	-17.12
6						-20.29	-18.68	-17.71	-13.31	-14.69	-16.54
7							-20.45	-18.87	-13.31	-13.46	-15.55
8								-20.81	-15.09	-12.91	-14.51
9									-16.84	-12.91	-13.88
10									-17.64	-13.46	-13.61
11									-18.65	-14.69	-13.52
12									-23.92	-16.27	-13.49
13										-17.23	-13.49
14										-17.64	-13.52
15										-17.98	-13.61
16										-28.40	-13.88
17											-14.51
18											-15.55
19											-16.54
20											-17.12
21											-17.40
22											-17.59
23											-17.86
24											-36.65

5. B3LYP/6-311+G* NICS(1)$_{\pi ZZ}$ Values (for rings in n = 1 – 8)

B3LYP/6-311+G* NICS(1)$_{\pi ZZ}$ values were calculated for all neutral compounds of lengths n = 1 – 8 with the σ-Only Model, using the Aroma software packages interfaced with Gaussian revision D. Previously performed B3LYP/6-311G*indicated that all of the systems are symmetrical in relation to the center of the compound (with minor numerical variations). Therefore, here we calculated only the different rings in each compound. For example, in a compound of length n = 7, rings #1, 2, 3, and 4 were calculated; rings #5, 6, and 7 are assumed to be identical to rings #3, 2, and 1, respectively.

The compounds are presented in the following tables, according to their respective families. The value of each ring within each compound is reported in ppm.

Table S23. B3LYP/6-311+G NICS(1)$_{\pi ZZ}$ Values for rings in compounds* n *= 1 – 8 in Family 1.*

n	**PP[1]**	**PP[2]**	**PP[3]**	**PP[4]**	**PP[5]**	**PP[6]**	**PP[7]**	**PP[8]**
1	-35.33	-32.83	-32.56	-32.52	-32.47	-32.50	-32.51	-32.51
2		-32.83	-30.44	-30.13	-30.10	-30.08	-30.04	-30.07
3			-32.58	-29.77	-29.97	-29.83	-29.82	-29.86
4				-32.46	-30.10	-29.82	-29.80	-29.83
5					-32.47	-30.10	-29.41	-29.42
6						-32.53	-29.15	-30.14
7							-32.41	-29.33
8								-32.48

Table S24. B3LYP/6-311+G NICS(1)$_{\pi ZZ}$ Values for rings in compounds* n *= 1 – 8 in Family 2.*

n	**α-P[1]**	**α-P[2]**	**α-P[3]**	**α-P[4]**	**α-P[5]**	**α-P[6]**	**α-P[7]**	**α-P[8]**
1	-25.48	-22.32	-22.07	-22.01	-22.05	-22.09	-22.84	-23.69
2		-22.32	-18.99	-18.96	-18.58	-18.63	-18.09	-18.09
3			-22.06	-18.96	-18.31	-18.43	-17.81	-17.81
4				-22.01	-18.58	-18.43	-17.62	-17.53
5					-22.05	-18.63	-17.81	-17.53
6						-22.09	-18.09	-17.81
7							-22.84	-18.09
8								-23.69

Table S25. B3LYP/6-311+G NICS(1)$_{\pi ZZ}$ Values for rings in compounds* n *= 1 – 8 in Family 3.*

n	**α-F[1]**	**α-F[2]**	**α-F[3]**	**α-F[4]**	**α-F[5]**	**α-F[6]**	**α-F[7]**	**α-F[8]**
1	-21.23	-17.12	-17.00	-16.97	-17.02	-17.21	-17.78	-18.39
2		-17.12	-13.23	-13.09	-13.03	-12.99	-12.99	-13.00
3			-17.00	-13.09	-12.98	-12.88	-12.80	-12.80
4				-16.97	-13.03	-12.88	-12.68	-12.55
5					-17.02	-12.99	-12.80	-12.55
6						-17.21	-12.99	-12.80
7							-17.78	-13.00
8								-18.39

Table S26. B3LYP/6-311+G NICS(1)$_{\pi ZZ}$ Values for rings in compounds* n *= 1 – 8 in Family 4.*

n	**α-T[1]**	**α-T[2]**	**α-T[3]**	**α-T[4]**	**α-T[5]**	**α-T[6]**	**α-T[7]**	**α-T[8]**
1	-21.97	-18.53	-18.62	-18.68	-18.68	-18.73	-18.75	-18.82
2		-18.52	-15.77	-15.71	-15.34	-15.43	-15.65	-14.99
3			-18.62	-14.96	-15.38	-15.02	-14.91	-14.45
4				-18.10	-15.62	-14.51	-14.81	-14.43
5					-18.52	-14.65	-15.26	-14.06
6						-18.03	-15.44	-14.57
7							-18.75	-15.74
8								-18.82

Table S27. B3LYP/6-311+G NICS(1)$_{\pi ZZ}$ Values for rings in compounds* n *= 1 – 8 in Family 5.*

n	**FP[1]**	**FP[2]**	**FP[3]**	**FP[4]**	**FP[5]**	**FP[6]**	**FP[7]**	**FP[8]**
1	-25.48	-25.23	-24.15	-23.50	-23.93	-24.20	-25.40	-27.71
2		-25.23	-22.34	-20.84	-20.09	-20.92	-21.70	-22.79
3			-24.13	-20.84	-19.12	-18.79	-17.23	-14.42
4				-23.50	-20.09	-18.79	-17.40	-16.53
5					-23.93	-20.92	-17.23	-16.53
6						-24.20	-21.70	-14.42
7							-25.40	-22.79
8								-27.71

Table S28. B3LYP/6-311+G NICS(1)$_{\pi ZZ}$ Values for rings in compounds* n *= 1 – 8 in Family 6.*

n	**FF[1]**	**FF[2]**	**FF[3]**	**FF[4]**	**FF[5]**	**FF[6]**	**FF[7]**	**FF[8]**
1	-21.23	-20.02	-19.62	-19.53	-19.74	-20.87	-21.67	-22.75
2		-20.00	-18.77	-18.37	-18.29	-18.65	-18.91	-19.01
3			-19.62	-18.37	-17.45	-16.72	-15.92	-15.57
4				-19.53	-18.29	-16.72	-15.13	-14.79
5					-19.74	-18.65	-15.92	-14.79
6						-20.87	-18.91	-15.57
7							-21.67	-19.01
8								-22.75

Table S29. B3LYP/6-311+G NICS(1)$_{\pi ZZ}$ Values for rings in compounds* n *= 1 – 8 in Family 7.*

n	**FT[1]**	**FT[2]**	**FT[3]**	**FT[4]**	**FT[5]**	**FT[6]**	**FT[7]**	**]FT[8**
1	-21.97	-19.48	-18.70	-18.56	-18.57	-18.65	-18.77	-19.11
2		-19.48	-17.38	-16.67	-16.68	-16.75	-16.92	-17.07
3			-18.70	-16.67	-15.76	-16.30	-16.31	-16.20
4				-18.56	-16.68	-16.30	-16.00	-15.44
5					-18.57	-16.75	-16.31	-15.44
6						-18.65	-16.92	-16.20
7							-18.77	-17.07
8								-19.11

6. Correlations between B3LYP/6-311G* and B3LYP/6-311+G* Values

Due to SCF convergence issues, we could not obtain NICS(1)$_{\pi ZZ}$ values at the B3LYP/6-311+G* level for oligomers of lengths n = 12, 16, 24. Therefore, we extrapolated these values using a fitting equation that ties between B3LYP/6-311G* and B3LYP/6-311+G* values. We checked various types of correlations: a) plotting all rings in all systems; b) plotting the average NICS(1)$_{\pi ZZ}$ per ring values; c) plotting the ΣNICS(1)$_{\pi ZZ}$ values. All correlations were satisfactory, but we observed that the best correlations were obtained when the ΣNICS(1)$_{\pi ZZ}$ values for each family were plotted. This is most likely because small numerical deviations between the individual rings are cancelled when the sums are taken.

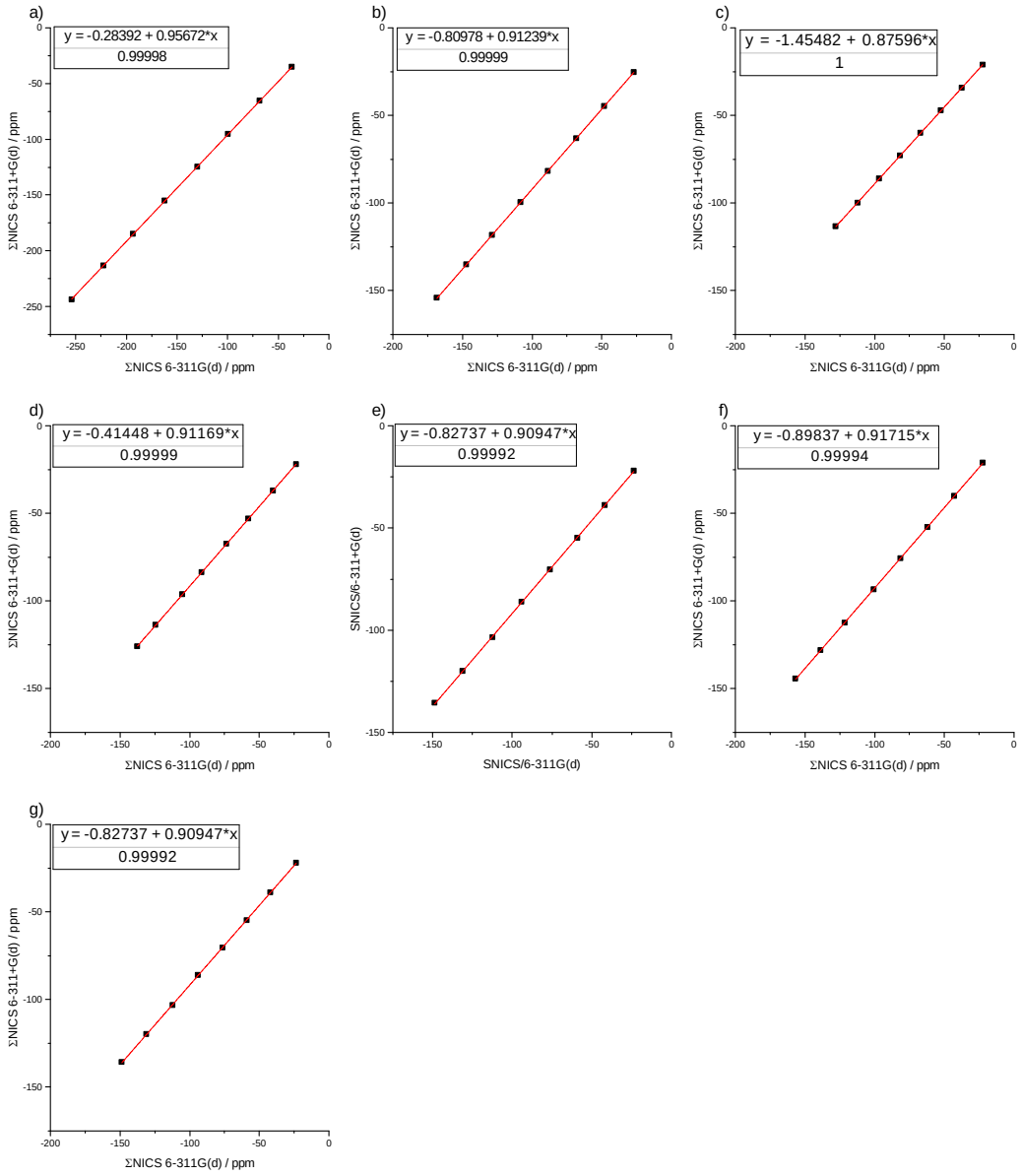

Figure S1. Correlation between 6-311G and 6-311+G* obtained values, fitting equations and the R^2 obtained for each family: a) Family 1; b) Family 2; c) Family 3; d) Family 4; e) Family 5; f) Family 6; g) Family 7.*

7. $\Sigma NICS(1)_{\pi ZZ}$ and Average $NICS(1)_{\pi ZZ}$ per Ring Values

The following tables detail the $\Sigma NICS(1)_{\pi ZZ}$ values and Average $NICS(1)_{\pi ZZ}$ per Ring for all of the neutral compounds, reported in ppm.

Note: for oligomers of lengths n = 1 – 8, the results were obtained with a B3LYP/6-311+G* calculation. For oligomers of lengths n = 12, 16, 24, the results were extrapolated using the correlations presented in Section 5 of the Supporting Information (these are marked in **bold** and *italics*).

Table S30. $\Sigma NICS(1)_{\pi ZZ}$ and Average $NICS(1)_{\pi ZZ}$ per Ring Values for compounds of Family 1

n	ΣNICS(1)πZZ [6-311G*]	ΣNICS(1)πZZ [6-311+G*]	Average: ΣNICS(1)πZZ/n [6-311+G*]
1	-36.52	-35.33	-35.33
2	-68.19	-65.67	-32.83
3	-99.75	-95.58	-31.86
4	-130.05	-124.89	-31.22
5	-162.13	-155.11	-31.02
6	-193.33	-184.86	-30.81
7	-222.64	-213.14	-30.45
8	-253.83	-243.64	-30.45
12	-381.55	***-365.31***	***-30.44***
16	-502.05	***-480.59***	***-30.04***
24	-752.27	***-719.98***	***-30.00***

Table S31. $\Sigma NICS(1)_{\pi ZZ}$ and Average $NICS(1)_{\pi ZZ}$ per Ring Values for compounds of Family 2.

n	ΣNICS(1)πZZ [6-311G*]	ΣNICS(1)πZZ [6-311+G*]	Average: ΣNICS(1)πZZ/n [6-311+G*]
1	-27.00	-25.48	-25.48
2	-48.12	-44.64	-22.32
3	-68.27	-63.12	-21.04
4	-88.81	-81.95	-20.49
5	-108.46	-99.57	-19.91
6	-128.66	-118.29	-19.72
7	-147.06	-135.10	-19.30
8	-168.26	-154.23	-19.28
12	-251.86	***-226.13***	***-18.84***
16	-334.08	***-304.82***	***-19.05***
24	-504.19	***-459.62***	***-19.15***

Table S32. ΣNICS(1)$_{\pi ZZ}$ and Average NICS(1)$_{\pi ZZ}$ per Ring Values for compounds of Family 3.

n	ΣNICS(1)πZZ [6-311G*]	ΣNICS(1)πZZ [6-311+G*]	Average: ΣNICS(1)πZZ/n [6-311+G*]
1	-22.54	-21.23	-21.23
2	-37.41	-34.24	-17.12
3	-52.27	-47.24	-15.75
4	-67.03	-60.13	-15.03
5	-81.77	-73.07	-14.61
6	-96.74	-86.14	-14.36
7	-112.28	-99.82	-14.26
8	-127.82	-113.47	-14.18
12	-188.96	**-166.99**	**-13.92**
16	-250.94	**-221.28**	**-13.83**
24	-374.08	**-329.15**	**-13.71**

Table S33. ΣNICS(1)$_{\pi ZZ}$ and Average NICS(1)$_{\pi ZZ}$ per Ring Values for compounds of Family 4.

n	ΣNICS(1)πZZ [6-311G*]	ΣNICS(1)πZZ [6-311+G*]	Average: ΣNICS(1)πZZ/n [6-311+G*]
1	-23.69	-21.97	-21.97
2	-40.01	-37.05	-18.52
3	-57.79	-53.00	-17.67
4	-73.56	-67.45	-16.86
5	-91.19	-83.54	-16.71
6	-105.19	-96.37	-16.06
7	-124.29	-113.57	-16.22
8	-137.48	-125.89	-15.74
12	-198.81	***-181.22***	***-15.10***
16	-262.01	***-238.64***	***-14.91***
24	-400.27	***-365.34***	***-15.22***

Table S34. ΣNICS(1)$_{\pi ZZ}$ and Average NICS(1)$_{\pi ZZ}$ per Ring Values for compounds of Family 5.

n	ΣNICS(1)πZZ [6-311G*]	ΣNICS(1)πZZ [6-311+G*]	Average: ΣNICS(1)πZZ/n [6-311+G*]
1	-27.00	-25.48	-25.48
2	-54.02	-50.45	-25.23
3	-76.12	-70.62	-23.54
4	-97.62	-88.67	-22.17
5	-117.39	-107.16	-21.43
6	-139.88	-127.82	-21.30
7	-157.71	-146.07	-20.87
8	-173.03	-162.90	-20.36
12	-254.20	***-234.80***	***-19.57***
16	-334.59	***-313.59***	***-19.60***
24	-507.27	***-470.00***	***-19.58***

Table S35. $\Sigma NICS(1)_{\pi ZZ}$ and Average $NICS(1)_{\pi ZZ}$ per Ring Values for compounds of Family 6.

n	ΣNICS(1)πZZ [6-311G*]	ΣNICS(1)πZZ [6-311+G*]	Average: ΣNICS(1)πZZ/n [6-311+G*]
1	-22.54	-21.23	-21.23
2	-42.81	-40.03	-20.01
3	-62.08	-58.01	-19.34
4	-81.38	-75.81	-18.95
5	-100.70	-93.50	-18.70
6	-121.26	-112.48	-18.75
7	-138.82	-128.12	-18.30
8	-156.80	-144.23	-18.03
12	-230.83	***-216.55***	***-18.05***
16	-299.18	***-275.58***	***-17.22***
24	-445.04	***-409.52***	***-17.06***

Table S36. $\Sigma NICS(1)_{\pi ZZ}$ and Average $NICS(1)_{\pi ZZ}$ per Ring Values for compounds of Family 7.

n	ΣNICS(1)πZZ [6-311G*]	ΣNICS(1)πZZ [6-311+G*]	Average: ΣNICS(1)πZZ/n [6-311+G*]
1	-23.69	-21.97	-21.97
2	-41.85	-38.95	-19.48
3	-59.11	-54.79	-18.26
4	-76.31	-70.46	-17.62
5	-94.14	-86.27	-17.25
6	-112.20	-103.41	-17.23
7	-131.08	-119.98	-17.14
8	-148.66	-135.63	-16.95
12	-210.30	***-192.10***	***-16.01***
16	-277.14	***-252.89***	***-15.81***
24	-415.47	***-378.69***	***-15.78***

8. Correlations for Predictive Scheme

In the main text, we present a predictive scheme that allows for the calculation of HOMO-LUMO gaps and IPs using data from only 4 data points (per family): n = 2 – 5.

The scheme works by obtaining three linear fitting equations.

The first linear equation fitting serves to extrapolate $\Sigma NICS(1)_{\pi ZZ}$ values for longer oligomers, using the $\Sigma NICS(1)_{\pi ZZ}$ values of compounds n = 2 – 5.

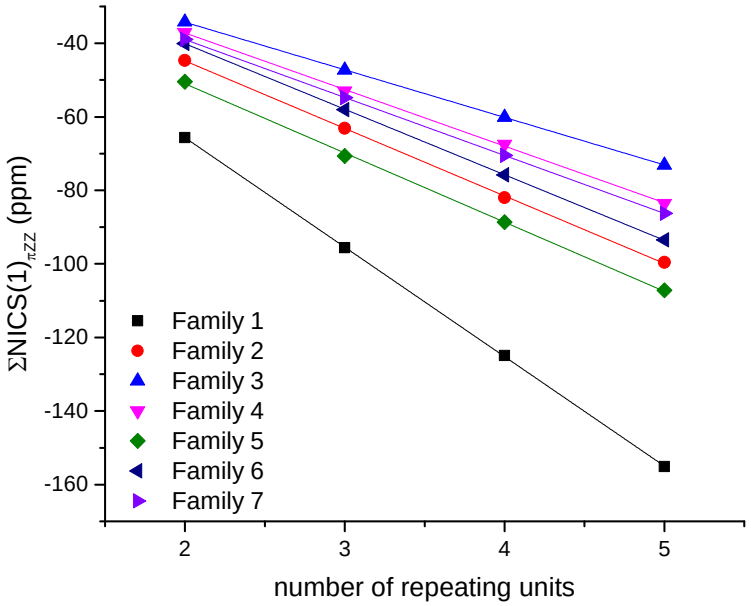

Figure S2. Correlations between $\Sigma NICS(1)_{\pi ZZ}$ and the number of repeating units, for oligomers of lengths n = 2 – 5, for all families.

Table S37. Linear fitting equation parameters for the correlation between $\Sigma NICS(1)_{\pi ZZ}$ and the number of repeating units.

	Family 1	**Family 2**	**Family 3**	**Family 4**	**Family 5**	**Family 6**	**Family 7**
slope	-29.686	-18.264	-12.939	-15.391	-18.816	-17.821	-15.763
intercept	-6.191	-8.047	-8.383	-6.390	-13.369	-4.461	-7.449
R^2	1.000	1.000	1.000	1.000	0.999	1.000	1.000

The second and third linear fitting equations are obtained from plotting the HOMO-LUMO gap and IP values against the Average NICS(1)$_{\pi ZZ}$ per ring values, for n = 2 – 5.

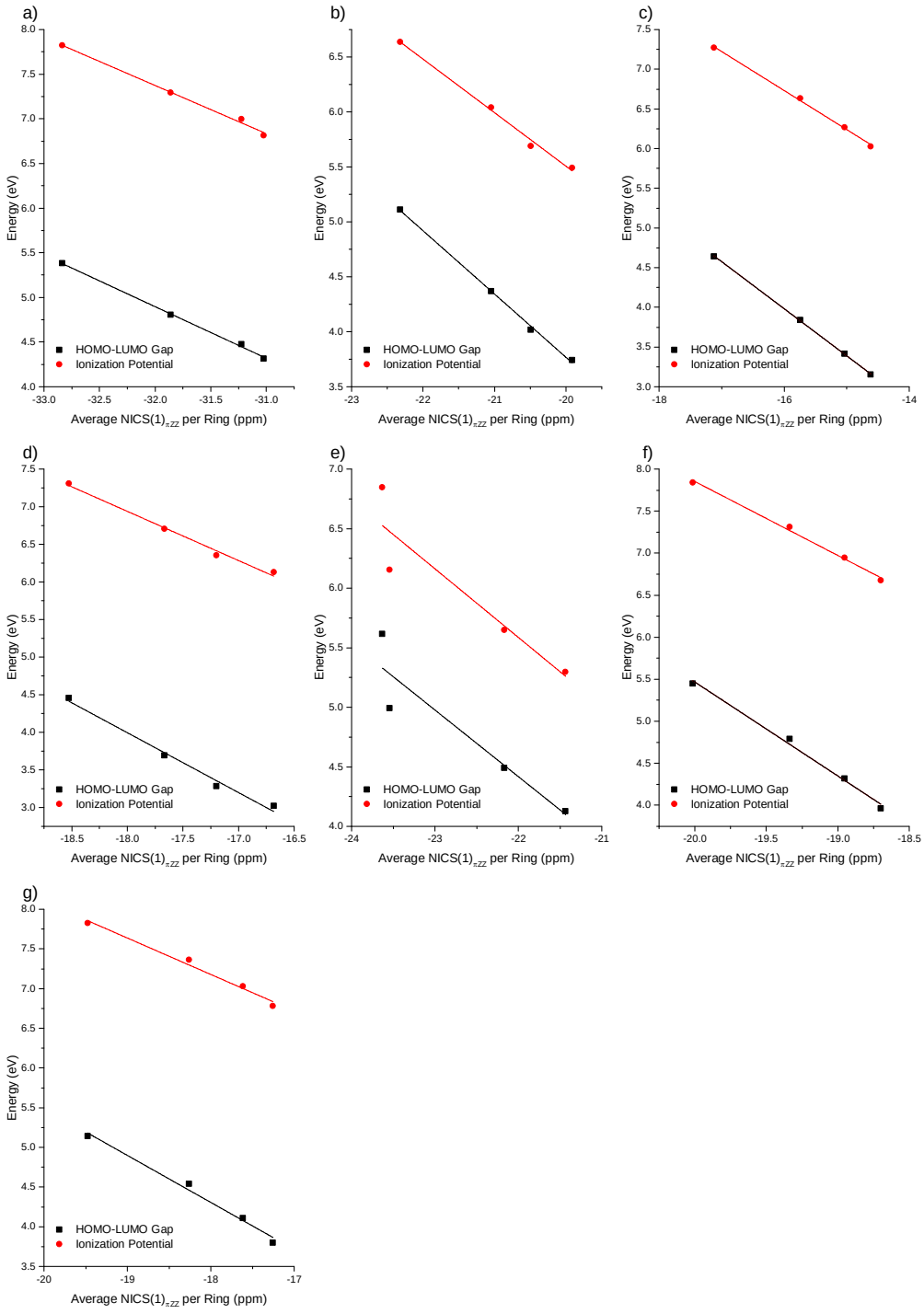

Figure S3. Correlations the HOMO-LUMO gap and IP values against the Average NICS(1)$_{\pi ZZ}$ per ring values, for oligomers of lengths n = 2 – 5, for all families: a) Family 1; b) Family 2; c) Family 3; d) Family 4; e) Family 5; f) Family 6; g) Family 7.

Table S38. Linear fitting equation parameters for HOMO-LUMO gap extrapolation.

	Family 1	Family 2	Family 3	Family 4	Family 5	Family 6	Family 7
slope	-0.578	-0.576	-0.594	-0.742	-0.386	-1.117	-0.592
intercept	-13.591	-7.752	-5.515	-9.323	-4.109	-16.882	-6.352
R^2	0.998	0.998	1.000	0.981	0.997	0.993	0.987

Table S39. Linear fitting equation parameters for Ionization Potential extrapolation.

	Family 1	Family 2	Family 3	Family 4	Family 5	Family 6	Family 7
slope	-0.539	-0.487	-0.492	-0.654	-0.576	-0.880	-0.459
intercept	-9.869	-4.237	-1.139	-4.838	-7.089	-9.744	-1.082
R^2	0.997	0.997	0.987	0.976	0.769	0.991	0.983

9. Extrapolated ΣNICS(1)$_{\pi ZZ}$, HOMO-LUMO Gaps, and Ionization Potentials

Using the linear fitting equations obtained in Section 7 of the Supporting Information, we extrapolated ΣNICS(1)$_{\pi ZZ}$ values for compounds of n = 1 – 8, 12, 16, 24. We then used these values to extrapolate HOMO-LUMO gaps and Ionization Potentials for these compounds.

Table S40. Extrapolated (predicted) values of Average NICS(1)$_{\pi ZZ}$ per Ring, HOMO-LUMO Gap, and IP for all compounds in all families. Explicitly calculated values are also presented, to facilitate easy comparison.

Series[n]	NICS	NICS^{pred}	HOMO-LUMO Gap	HOMO-LUMO Gap^{pred}	IP	IP^{pred}
PP[1]	-35.33	-35.88	6.73	7.13	8.99	9.46
PP[2]	-32.83	-32.78	5.38	5.35	7.82	7.79
PP[3]	-31.86	-31.75	4.80	4.75	7.29	7.24
PP[4]	-31.22	-31.23	4.47	4.45	7.00	6.96
PP[5]	-31.02	-30.92	4.31	4.27	6.81	6.79
PP[6]	-30.81	-30.72	4.18	4.15	6.68	6.68
PP[7]	-30.45	-30.57	4.09	4.07	6.58	6.60
PP[8]	-30.45	-30.46	4.04	4.01	6.51	6.54
PP[12]	-30.44	-30.20	3.94	3.86	6.30	6.40
PP[16]	-30.04	-30.07	3.91	3.78	6.18	6.33
PP[24]	-30.00	-29.94	3.86	3.71	6.04	6.27
α-P[1]	-25.48	-26.31	6.72	7.40	7.98	8.58
α-P[2]	-22.32	-22.29	5.11	5.09	6.64	6.62
α-P[3]	-21.04	-20.95	4.37	4.31	6.04	5.97
α-P[4]	-20.49	-20.28	4.02	3.93	5.69	5.64
α-P[5]	-19.91	-19.87	3.74	3.69	5.49	5.44
α-P[6]	-19.72	-19.61	3.63	3.54	5.33	5.31
α-P[7]	-19.30	-19.41	3.49	3.43	5.23	5.22
α-P[8]	-19.28	-19.27	3.42	3.35	5.15	5.15
α-P[12]	-19.22	-18.93	3.29	3.15	4.93	4.99
α-P[16]	-19.10	-18.77	3.24	3.06	4.81	4.91
α-P[24]	-19.20	-18.60	3.19	2.96	4.65	4.82
α-F[1]	-21.23	-21.32	6.59	7.14	8.67	9.35
α-F[2]	-17.12	-17.13	4.64	4.65	7.27	7.29
α-F[3]	-15.75	-15.73	3.84	3.82	6.63	6.60
α-F[4]	-15.03	-15.03	3.41	3.41	6.27	6.26
α-F[5]	-14.61	-14.62	3.15	3.16	6.02	6.05
α-F[6]	-14.36	-14.34	2.98	2.99	5.86	5.91
α-F[7]	-14.26	-14.14	2.87	2.88	5.73	5.81
α-F[8]	-14.18	-13.99	2.78	2.79	5.63	5.74
α-F[12]	-13.92	-13.64	2.60	2.58	5.40	5.57
α-F[16]	-13.83	-13.46	2.53	2.48	5.26	5.48
α-F[24]	-13.71	-13.29	2.47	2.37	5.10	5.40
α-T[1]	-21.97	-21.78	6.12	6.83	8.65	9.41
α-T[2]	-18.52	-18.59	4.45	4.46	7.31	7.32
α-T[3]	-17.67	-17.52	3.69	3.67	6.70	6.62
α-T[4]	-16.86	-16.99	3.28	3.28	6.35	6.28

Series[n]	NICS	NICS^{pred}	HOMO-LUMO Gap	HOMO-LUMO Gap^{pred}	IP	IP^{pred}
α-T[5]	-16.71	-16.67	3.02	3.04	6.13	6.07
α-T[6]	-16.06	-16.46	2.85	2.88	5.97	5.93
α-T[7]	-16.22	-16.30	2.73	2.77	5.85	5.83
α-T[8]	-15.74	-16.19	2.66	2.68	5.76	5.75
α-T[12]	-15.14	-15.92	2.47	2.49	5.55	5.58
α-T[16]	-14.96	-15.79	2.40	2.39	5.43	5.49
α-T[24]	-15.22	-15.66	2.35	2.29	5.28	5.41
FP[1]	-25.48	-32.19	6.72	8.31	7.98	11.45
FP[2]	-25.23	-25.50	5.61	5.73	6.85	7.60
FP[3]	-23.54	-23.27	4.99	4.87	6.15	6.32
FP[4]	-22.17	-22.16	4.49	4.44	5.65	5.68
FP[5]	-21.43	-21.49	4.13	4.19	5.29	5.29
FP[6]	-21.30	-21.04	3.85	4.01	5.03	5.04
FP[7]	-20.87	-20.73	3.64	3.89	4.82	4.85
FP[8]	-20.36	-20.49	3.48	3.80	4.64	4.72
FP[12]	-19.64	-19.93	3.07	3.58	4.18	4.39
FP[16]	-19.40	-19.65	2.83	3.48	3.93	4.23
FP[24]	-19.62	-19.37	2.63	3.37	3.66	4.07
FF[1]	-21.23	-22.28	6.59	8.02	8.67	9.86
FF[2]	-20.01	-20.05	5.45	5.52	7.84	7.90
FF[3]	-19.34	-19.31	4.79	4.69	7.31	7.24
FF[4]	-18.95	-18.94	4.32	4.28	6.95	6.92
FF[5]	-18.70	-18.71	3.96	4.03	6.67	6.72
FF[6]	-18.75	-18.56	3.69	3.86	6.46	6.59
FF[7]	-18.30	-18.46	3.48	3.74	6.28	6.50
FF[8]	-18.03	-18.38	3.31	3.65	6.14	6.43
FF[12]	-17.72	-18.19	2.87	3.45	5.75	6.26
FF[16]	-17.21	-18.10	2.63	3.34	5.52	6.18
FF[24]	-17.05	-18.01	2.40	3.24	5.30	6.10
FT[1]	-21.97	-23.21	6.12	7.39	8.65	9.57
FT[2]	-19.48	-19.49	5.14	5.19	7.82	7.86
FT[3]	-18.26	-18.25	4.54	4.45	7.36	7.29
FT[4]	-17.62	-17.63	4.11	4.08	7.03	7.01
FT[5]	-17.25	-17.25	3.80	3.86	6.78	6.84
FT[6]	-17.23	-17.00	3.56	3.72	6.59	6.72
FT[7]	-17.14	-16.83	3.38	3.61	6.44	6.64
FT[8]	-16.95	-16.69	3.23	3.53	6.33	6.58
FT[12]	-16.01	-16.38	2.87	3.35	6.01	6.44
FT[16]	-15.81	-16.23	2.68	3.26	5.84	6.37
FT[24]	-15.78	-16.07	2.50	3.17	5.65	6.29

10. Optimized Geometries

All geometries were optimized at the B3LYP/6-311G* level of theory, and frequencies analyses were performed to ensure real minima (N_{imag} = 0). The Zero-Point Corrected Energies are given in Section 1 of the Supporting Information.

In the following tables the Cartesian coordinates for all systems are presented.

PP[1]			
6	0.000000	0.000000	1.394069
6	0.000000	1.207246	-0.697013
6	0.000000	-1.207246	-0.697013
6	0.000000	1.207246	0.697013
6	0.000000	0.000000	-1.394069
6	0.000000	-1.207246	0.697013
1	0.000000	0.000000	2.479629
1	0.000000	2.147380	1.239785
1	0.000000	2.147380	-1.239785
1	0.000000	0.000000	-2.479629
1	0.000000	-2.147380	-1.239785
1	0.000000	-2.147380	1.239785

PP[1]-cation			
6	0.684332	-1.247638	0.000000
6	-1.381971	0.000038	0.000000
6	0.684332	1.247609	0.000000
6	-0.684332	-1.247609	0.000000
6	-0.684332	1.247638	0.000000
6	1.381971	-0.000038	0.000000
1	1.248035	-2.172926	0.000000
1	-1.248074	-2.172874	0.000000
1	-2.467261	0.000035	0.000000
1	-1.248035	2.172926	0.000000
1	1.248074	2.172874	0.000000
1	2.467261	-0.000035	0.000000

PP[2]			
6	1.464044	1.125637	-0.424246
6	0.742625	0.000003	-0.000009
6	1.464051	-1.125636	0.424212
6	2.855843	-1.125973	0.424588
6	3.558318	-0.000002	-0.000039
6	2.855838	1.125971	-0.424652
1	0.928109	1.998645	-0.782429
1	0.928118	-1.998641	0.782405
1	3.392853	-2.005593	0.765644
1	4.643576	-0.000004	-0.000051
1	3.392842	2.005589	-0.765721
6	-0.742625	0.000001	0.000006
6	-1.464050	-1.125635	-0.424212
6	-1.464044	1.125638	0.424245
6	-2.855845	-1.125972	-0.424588
1	-0.928121	-1.998643	-0.782406
6	-2.855836	1.125972	0.424653
1	-0.928105	1.998644	0.782429
6	-3.558318	-0.000002	0.000040
1	-3.392853	-2.005593	-0.765644
1	-3.392842	2.005588	0.765723
1	-4.643576	-0.000001	0.000055

PP[2]-cation			
6	0.212220	1.461011	-1.206016
6	0.000000	0.720964	0.000000
6	-0.212220	1.461012	1.206016
6	-0.223191	2.837018	1.199214
6	0.000000	3.536015	0.000000
6	0.223191	2.837018	-1.199214
1	0.413124	0.940411	-2.132775
1	-0.413124	0.940412	2.132776
1	-0.407835	3.383459	2.116473
1	0.000000	4.620401	0.000000
1	0.407835	3.383458	-2.116473
6	0.000000	-0.720964	0.000000
6	0.212220	-1.461012	1.206016
6	-0.212220	-1.461011	-1.206016
6	0.223191	-2.837018	1.199214
1	0.413124	-0.940412	2.132776
6	-0.223191	-2.837018	-1.199214
1	-0.413124	-0.940411	-2.132775
6	0.000000	-3.536015	0.000000
1	0.407835	-3.383459	2.116473
1	-0.407835	-3.383458	-2.116473
1	0.000000	-4.620401	0.000000

PP[3]			
6	-3.627200	0.909408	0.787550
6	-2.905494	-0.000001	0.000001
6	-3.627198	-0.909408	-0.787551
6	-5.018913	-0.909277	-0.788182
6	-5.721512	-0.000001	-0.000001
6	-5.018913	0.909276	0.788180
1	-3.091747	1.604697	1.425937
1	-3.091745	-1.604696	-1.425939
1	-5.555810	-1.616411	-1.412772
1	-6.806740	-0.000001	-0.000001
1	-5.555813	1.616410	1.412768
6	-1.421605	0.000001	0.000001
6	-0.694682	-1.198961	-0.000853
6	-0.694683	1.198962	0.000853
6	0.694683	-1.198961	0.000841
1	-1.225044	-2.145591	0.016570
6	0.694684	1.198962	-0.000841
1	-1.225043	2.145593	-0.016572
6	1.421605	0.000001	0.000000
1	1.225045	-2.145591	-0.016593
1	1.225044	2.145593	0.016593
6	2.905494	0.000000	0.000000
6	3.627198	0.909415	-0.787541
6	3.627198	-0.909415	0.787543
6	5.018914	0.909282	-0.788173
1	3.091748	1.604710	-1.425924
6	5.018912	-0.909284	0.788175
1	3.091745	-1.604708	1.425926
6	5.721512	-0.000001	0.000000
1	5.555810	1.616422	-1.412756
1	5.555810	-1.616423	1.412758
1	6.806740	-0.000002	0.000001

PP[3]-cation			
6	3.612846	1.113708	-0.489890
6	2.881089	-0.000001	0.000001
6	3.612848	-1.113709	0.489891
6	4.994684	-1.106100	0.498396
6	5.693382	0.000001	0.000000
6	4.994682	1.106101	-0.498396

1	3.090573	1.966021	-0.906267
1	3.090577	-1.966023	0.906270
1	5.537512	-1.955798	0.895910
1	6.777694	0.000002	-0.000001
1	5.537508	1.955800	-0.895910
6	1.429779	-0.000001	0.000002
6	0.685580	-1.213667	0.009280
6	0.685582	1.213666	-0.009279
6	-0.685582	-1.213666	-0.009268
1	1.205397	-2.162984	-0.004763
6	-0.685580	1.213667	0.009269
1	1.205400	2.162982	0.004763
6	-1.429779	0.000001	0.000001
1	-1.205400	-2.162982	0.004782
1	-1.205397	2.162984	-0.004783
6	-2.881089	0.000001	0.000000
6	-3.612848	1.113713	0.489880
6	-3.612846	-1.113712	-0.489881
6	-4.994684	1.106104	0.498385
1	-3.090577	1.966030	0.906252
6	-4.994681	-1.106105	-0.498388
1	-3.090573	-1.966029	-0.906251
6	-5.693382	-0.000001	-0.000002
1	-5.537512	1.955806	0.895891
1	-5.537508	-1.955808	-0.895894
1	-6.777694	-0.000002	-0.000003

PP4

6	-5.791207	-0.606407	-1.039091
6	-5.069494	0.000000	-0.000001
6	-5.791211	0.606406	1.039089
6	-7.182867	0.606170	1.039579
6	-7.885347	-0.000003	-0.000003
6	-7.182864	-0.606174	-1.039584
1	-5.255696	-1.057967	-1.867885
1	-5.255701	1.057967	1.867883
1	-7.719904	1.073624	1.859015
1	-8.970580	-0.000004	-0.000004
1	-7.719897	-1.073630	-1.859021
6	-3.585691	0.000002	0.000001
6	-2.858222	1.130135	0.399830
6	-2.858221	-1.130132	-0.399828
6	-1.469071	1.130547	0.399018
1	-3.387941	2.029024	0.698154
6	-1.469070	-1.130544	-0.399015
1	-3.387939	-2.029021	-0.698153
6	-0.741211	0.000002	0.000002
1	-0.940065	2.017378	0.732507
1	-0.940062	-2.017374	-0.732503
6	0.741221	0.000002	0.000002
6	1.469076	-1.130474	0.399225
6	1.469078	1.130476	-0.399222
6	2.858227	-1.130062	0.400036
1	0.940064	-2.017240	0.732874
6	2.858228	1.130063	-0.400034
1	0.940066	2.017242	-0.732873
6	3.585691	0.000001	0.000002
1	3.387952	-2.028892	0.698529
1	3.387955	2.028892	-0.698529
6	5.069495	-0.000001	0.000001
6	5.791202	0.606220	-1.039201
6	5.791204	-0.606221	1.039201
6	7.182858	0.605984	-1.039694
1	5.255684	1.057638	-1.868069
6	7.182860	-0.605986	1.039691
1	5.255688	-1.057637	1.868071
6	7.885339	-0.000002	-0.000002
1	7.719897	1.073290	-1.859212
1	7.719900	-1.073292	1.859209
1	8.970571	-0.000002	-0.000004

PP[4]-cation

6	5.768215	0.921814	-0.787776
6	5.041415	0.000000	0.000000
6	5.768215	-0.921814	0.787775
6	7.153255	-0.913233	0.793770
6	7.852463	0.000000	-0.000001
6	7.153255	0.913233	-0.793771
1	5.242929	1.617123	-1.431812
1	5.242929	-1.617123	1.431811
1	7.694170	-1.613697	1.419920
1	8.936821	0.000000	-0.000001
1	7.694169	1.613697	-1.419922
6	3.580833	0.000000	0.000000
6	2.841856	-1.180612	0.263784
6	2.841856	1.180612	-0.263784
6	1.467063	-1.185519	0.246466
1	3.365572	-2.109986	0.450423
6	1.467063	1.185519	-0.246466
1	3.365572	2.109986	-0.450424
6	0.725188	0.000000	0.000000
1	0.949749	-2.111990	0.462031
1	0.949749	2.111990	-0.462032
6	-0.725187	0.000000	0.000000
6	-1.467063	1.185473	0.246688
6	-1.467063	-1.185473	-0.246688
6	-2.841856	1.180563	0.264004
1	-0.949749	2.111903	0.462428
6	-2.841856	-1.180563	-0.264004
1	-0.949749	-2.111903	-0.462428
6	-3.580833	0.000000	0.000000
1	-3.365572	2.109902	0.450817
1	-3.365572	-2.109902	-0.450816
6	-5.041415	0.000000	0.000000
6	-5.768215	-0.921676	-0.787937
6	-5.768215	0.921675	0.787938
6	-7.153255	-0.913093	-0.793931
1	-5.242930	-1.616873	-1.432095
6	-7.153255	0.913093	0.793932
1	-5.242930	1.616873	1.432096
6	-7.852464	0.000000	0.000001
1	-7.694169	-1.613447	-1.420204
1	-7.694169	1.613447	1.420206
1	-8.936821	0.000000	0.000001

PP5

6	7.953860	-1.202927	0.012006
6	7.231961	0.000000	0.000003
6	7.953859	1.202927	-0.011999

6	9.345512	1.203296	-0.012096
6	10.048070	0.000001	0.000004
6	9.345512	-1.203295	0.012104
1	7.418536	-2.146138	0.049576
1	7.418536	2.146138	-0.049571
1	9.882511	2.146528	-0.030479
1	11.133296	0.000000	0.000005
1	9.882513	-2.146526	0.030487
6	5.748319	0.000000	0.000002
6	5.021033	0.924409	0.763556
6	5.021034	-0.924409	-0.763551
6	3.631855	0.924691	0.763451
1	5.550850	1.630374	1.394862
6	3.631854	-0.924688	-0.763446
1	5.550848	-1.630375	-1.394857
6	2.904339	0.000001	0.000003
1	3.102495	1.630691	1.395096
1	3.102495	-1.630687	-1.395092
6	1.422122	0.000001	0.000002
6	0.694522	-1.199003	-0.000713
6	0.694519	1.199003	0.000719
6	-0.694521	-1.199005	0.000763
1	1.224233	-2.145947	0.017431
6	-0.694522	1.199001	-0.000759
1	1.224230	2.145948	-0.017421
6	-1.422123	-0.000003	0.000001
1	-1.224230	-2.145951	-0.017341
1	-1.224235	2.145945	0.017349
6	-2.904339	-0.000003	0.000001
6	-3.631853	0.924655	-0.763490
6	-3.631856	-0.924659	0.763487
6	-5.021032	0.924377	-0.763597
1	-3.102491	1.630626	-1.395165
6	-5.021036	-0.924376	0.763590
1	-3.102498	-1.630634	1.395162
6	-5.748319	0.000001	-0.000004
1	-5.550847	1.630317	-1.394932
1	-5.550854	-1.630315	1.394925
6	-7.231961	0.000001	-0.000005
6	-7.953858	-1.202926	-0.011964
6	-7.953860	1.202930	0.011952
6	-9.345512	-1.203295	-0.012062
1	-7.418535	-2.146139	-0.049499
6	-9.345511	1.203297	0.012049
1	-7.418534	2.146141	0.049487
6	-10.048069	0.000000	-0.000007
1	-9.882510	-2.146528	-0.030410
1	-9.882513	2.146528	0.030396
1	-11.133295	0.000002	-0.000008

PP[5]-cation

6	7.929733	-1.205310	0.105972
6	7.204991	0.000000	0.000004
6	7.929732	1.205310	-0.105962
6	9.316533	1.202813	-0.113716
6	10.016238	0.000001	0.000007
6	9.316534	-1.202812	0.113729
1	7.402463	-2.144979	0.224456
1	7.402461	2.144979	-0.224446
1	9.856440	2.137795	-0.214228
1	11.100689	0.000002	0.000008
1	9.856442	-2.137793	0.214242
6	5.738556	-0.000001	0.000003
6	5.001679	1.099654	0.497454
6	5.001680	-1.099656	-0.497449
6	3.623946	1.102384	0.494322
1	5.526133	1.942135	0.931860
6	3.623948	-1.102386	-0.494320
1	5.526135	-1.942136	-0.931855
6	2.884518	-0.000001	0.000001
1	3.106438	1.948766	0.929359
1	3.106441	-1.948768	-0.929359
6	1.428953	-0.000001	-0.000001
6	0.687867	-1.208188	-0.007607
6	0.687869	1.208187	0.007606
6	-0.687867	-1.208186	0.007650
1	1.206805	-2.158604	0.008078
6	-0.687865	1.208188	-0.007653
1	1.206808	2.158602	-0.008078
6	-1.428951	0.000001	-0.000002
1	-1.206807	-2.158602	-0.007999
1	-1.206803	2.158605	0.007997
6	-2.884517	0.000002	-0.000002
6	-3.623946	1.102368	-0.494365
6	-3.623946	-1.102365	0.494359
6	-5.001679	1.099638	-0.497495
1	-3.106439	1.948735	-0.929434
6	-5.001679	-1.099636	0.497489
1	-3.106438	-1.948732	0.929428
6	-5.738556	0.000001	-0.000003
1	-5.526134	1.942102	-0.931933
1	-5.526133	-1.942101	0.931926
6	-7.204992	0.000000	-0.000003
6	-7.929732	-1.205316	-0.105917
6	-7.929734	1.205315	0.105911
6	-9.316534	-1.202819	-0.113673
1	-7.402461	-2.144989	-0.224359
6	-9.316536	1.202816	0.113666
1	-7.402465	2.144989	0.224354
6	-10.016240	-0.000002	-0.000003
1	-9.856440	-2.137805	-0.214143
1	-9.856444	2.137802	0.214137
1	-11.100691	-0.000003	-0.000003

PP6

6	10.117932	-1.146724	-0.363705
6	9.396104	0.000000	-0.000003
6	10.117931	1.146725	0.363698
6	11.509595	1.147110	0.363687
6	12.212123	0.000001	-0.000006
6	11.509595	-1.147107	-0.363697
1	9.582583	-2.054647	-0.621986
1	9.582583	2.054647	0.621981
1	12.046577	2.049084	0.640253
1	13.297353	0.000002	-0.000007
1	12.046577	-2.049082	-0.640264
6	7.912420	0.000000	-0.000001
6	7.185319	0.635128	1.017003
6	7.185317	-0.635128	-1.017004
6	5.796187	0.634892	1.017295

1	7.715579	1.104978	1.839008
6	5.796185	-0.634893	-1.017293
1	7.715576	-1.104978	-1.839011
6	5.068558	-0.000001	0.000001
1	5.266908	1.103751	1.840435
1	5.266904	-1.103752	-1.840433
6	3.586356	0.000000	0.000003
6	2.858204	-1.131494	-0.395981
6	2.858205	1.131493	0.395988
6	1.469259	-1.131738	-0.395475
1	3.387108	-2.032034	-0.690632
6	1.469260	1.131738	0.395484
1	3.387110	2.032033	0.690638
6	0.741091	0.000000	0.000005
1	0.940566	-2.019690	-0.726379
1	0.940568	2.019690	0.726390
6	-0.741091	0.000000	0.000006
6	-1.469261	1.131747	-0.395448
6	-1.469259	-1.131748	0.395458
6	-2.858206	1.131501	-0.395953
1	-0.940568	2.019707	-0.726332
6	-2.858205	-1.131504	0.395962
1	-0.940565	-2.019708	0.726340
6	-3.586356	-0.000002	0.000006
1	-3.387111	2.032047	-0.690583
1	-3.387108	-2.032052	0.690590
6	-5.068558	-0.000002	0.000003
6	-5.796187	-0.634914	1.017284
6	-5.796183	0.634911	-1.017279
6	-7.185319	-0.635149	1.016991
1	-5.266909	-1.103787	1.840416
6	-7.185315	0.635148	-1.016991
1	-5.266902	1.103786	-1.840408
6	-7.912419	-0.000001	-0.000001
1	-7.715582	-1.105014	1.838987
1	-7.715575	1.105014	-1.838988
6	-9.396103	0.000000	-0.000004
6	-10.117930	1.146732	-0.363685
6	-10.117933	-1.146730	0.363676
6	-11.509594	1.147117	-0.363678
1	-9.582580	2.054659	-0.621950
6	-11.509597	-1.147113	0.363664
1	-9.582585	-2.054658	0.621942
6	-12.212123	0.000003	-0.000008
1	-12.046574	2.049098	-0.640228
1	-12.046579	-2.049093	0.640213
1	-13.297352	0.000003	-0.000010

PP[6]-cation

6	10.089006	1.190958	0.205310
6	9.365653	0.000000	0.000000
6	10.089006	-1.190958	-0.205311
6	11.476898	-1.190756	-0.198276
6	12.177004	0.000000	0.000000
6	11.476898	1.190756	0.198275
1	9.559934	2.128837	0.332035
1	9.559934	-2.128837	-0.332036
1	12.016212	-2.120701	-0.341532
1	13.261540	0.000000	0.000000
1	12.016212	2.120702	0.341531
6	7.895291	0.000000	0.000000
6	7.160577	-0.905086	-0.795771
6	7.160577	0.905086	0.795771
6	5.780405	-0.909072	-0.792965
1	7.685932	-1.584668	-1.456376
6	5.780405	0.909072	0.792965
1	7.685932	1.584669	1.456376
6	5.044167	0.000000	0.000000
1	5.260930	-1.592001	-1.454908
1	5.260930	1.592001	1.454908
6	3.583214	0.000000	0.000000
6	2.845377	1.169329	0.297536
6	2.845377	-1.169329	-0.297537
6	1.467247	1.173426	0.282708
1	3.367115	2.094315	0.511467
6	1.467247	-1.173426	-0.282708
1	3.367115	-2.094315	-0.511467
6	0.729515	0.000000	0.000000
1	0.947180	2.091737	0.527506
1	0.947180	-2.091738	-0.527507
6	-0.729515	0.000000	0.000000
6	-1.467247	-1.173432	0.282683
6	-1.467247	1.173432	-0.282683
6	-2.845377	-1.169335	0.297512
1	-0.947180	-2.091749	0.527463
6	-2.845377	1.169335	-0.297512
1	-0.947180	2.091749	-0.527462
6	-3.583214	0.000000	0.000000
1	-3.367116	-2.094326	0.511423
1	-3.367115	2.094326	-0.511423
6	-5.044167	0.000000	0.000000
6	-5.780405	0.909087	-0.792948
6	-5.780405	-0.909086	0.792948
6	-7.160577	0.905101	-0.795754
1	-5.260930	1.592027	-1.454879
6	-7.160577	-0.905100	0.795754
1	-5.260930	-1.592027	1.454879
6	-7.895291	0.000000	0.000000
1	-7.685932	1.584695	-1.456347
1	-7.685932	-1.584695	1.456347
6	-9.365652	0.000000	0.000000
6	-10.089006	-1.190962	0.205285
6	-10.089006	1.190962	-0.205284
6	-11.476898	-1.190760	0.198250
1	-9.559933	-2.128844	0.331990
6	-11.476898	1.190760	-0.198248
1	-9.559934	2.128845	-0.331989
6	-12.177004	0.000000	0.000001
1	-12.016211	-2.120709	0.341486
1	-12.016211	2.120709	-0.341484
1	-13.261539	0.000000	0.000001

PP7

6	12.282253	-0.967276	-0.715304
6	11.560541	0.000000	0.000005
6	12.282254	0.967274	0.715315
6	13.673927	0.967645	0.715469
6	14.376387	-0.000004	0.000008
6	13.673926	-0.967651	-0.715455
1	11.746714	-1.742690	-1.253373

1	11.746716	1.742690	1.253382
1	14.211013	1.731459	1.269106
1	15.461619	-0.000005	0.000009
1	14.211011	-1.731465	-1.269092
6	10.076893	0.000000	0.000003
6	9.349523	0.270877	1.167910
6	9.349528	-0.270877	-1.167907
6	7.960402	0.270243	1.168157
1	9.879303	0.448773	2.098179
6	7.960407	-0.270243	-1.168159
1	9.879312	-0.448773	-2.098173
6	7.232389	0.000000	-0.000002
1	7.431766	0.446322	2.099339
1	7.431775	-0.446321	-2.099344
6	5.750238	-0.000001	-0.000003
6	5.021938	-0.935968	-0.748913
6	5.021939	0.935967	0.748907
6	3.632994	-0.936215	-0.748775
1	5.550580	-1.688073	-1.325429
6	3.632995	0.936216	0.748767
1	5.550583	1.688070	1.325424
6	2.904844	0.000002	-0.000005
1	3.104295	-1.663908	-1.355725
1	3.104298	1.663910	1.355718
6	1.422718	0.000003	-0.000007
6	0.694460	1.198800	0.000240
6	0.694461	-1.198795	-0.000255
6	-0.694459	1.198799	-0.000458
1	1.223105	2.146253	-0.018912
6	-0.694457	-1.198796	0.000444
1	1.223109	-2.146248	0.018896
6	-1.422718	0.000001	-0.000007
1	-1.223103	2.146256	0.018538
1	-1.223099	-2.146255	-0.018553
6	-2.904844	0.000002	-0.000004
6	-3.632998	-0.936109	0.748896
6	-3.632996	0.936114	-0.748903
6	-5.021940	-0.935861	0.749035
1	-3.104305	-1.663713	1.355957
6	-5.021940	0.935868	-0.749040
1	-3.104303	1.663717	-1.355964
6	-5.750241	0.000004	-0.000002
1	-5.550584	-1.687886	1.325653
1	-5.550582	1.687895	-1.325657
6	-7.232390	0.000002	-0.000001
6	-7.960410	0.270068	-1.168198
6	-7.960405	-0.270065	1.168198
6	-9.349532	0.270701	-1.167946
1	-7.431782	0.446006	-2.099412
6	-9.349526	-0.270702	1.167952
1	-7.431772	-0.446002	2.099409
6	-10.076895	-0.000001	0.000003
1	-9.879318	0.448465	-2.098238
1	-9.879308	-0.448466	2.098245
6	-11.560542	-0.000003	0.000004
6	-12.282249	-0.967231	0.715382
6	-12.282249	0.967223	-0.715372
6	-13.673923	-0.967604	0.715534
1	-11.746702	-1.742601	1.253509
6	-13.673924	0.967597	-0.715522
1	-11.746702	1.742592	-1.253501
6	-14.376382	-0.000003	0.000007
1	-14.211010	-1.731379	1.269223
1	-14.211010	1.731373	-1.269211
1	-15.461614	-0.000002	0.000008

PP[7]-cation

6	-12.249122	-1.083979	0.532271
6	-11.526267	-0.000002	-0.000002
6	-12.249122	1.083974	-0.532277
6	-13.637687	1.085551	-0.526453
6	-14.338133	-0.000004	-0.000006
6	-13.637688	-1.085558	0.526444
1	-11.719308	-1.947494	0.919094
1	-11.719308	1.947490	-0.919099
1	-14.176603	1.937258	-0.927242
1	-15.422747	-0.000005	-0.000007
1	-14.176603	-1.937265	0.927230
6	-10.053331	-0.000001	-0.000001
6	-9.320221	0.622463	-1.030739
6	-9.320221	-0.622463	1.030739
6	-7.938455	0.627101	-1.029200
1	-9.846877	1.071754	-1.864581
6	-7.938455	-0.627098	1.029201
1	-9.846877	-1.071755	1.864580
6	-7.204471	0.000002	0.000001
1	-7.416836	1.078947	-1.865046
1	-7.416836	-1.078944	1.865047
6	-5.739620	0.000003	0.000002
6	-5.004052	-1.048098	0.595388
6	-5.004051	1.048103	-0.595383
6	-3.624006	-1.055258	0.583410
1	-5.527487	-1.883105	1.045882
6	-3.624005	1.055263	-0.583404
1	-5.527486	1.883112	-1.045876
6	-2.888729	0.000002	0.000003
1	-3.102280	-1.875485	1.062434
1	-3.102278	1.875490	-1.062426
6	-1.425847	0.000002	0.000003
6	-0.689814	1.205716	-0.007153
6	-0.689815	-1.205712	0.007158
6	0.689813	1.205716	0.007045
1	-1.211818	2.155152	0.008993
6	0.689812	-1.205713	-0.007041
1	-1.211820	-2.155148	-0.008989
6	1.425845	0.000001	0.000002
1	1.211817	2.155151	-0.009191
1	1.211816	-2.155148	0.009194
6	2.888726	0.000001	0.000002
6	3.624004	-1.055319	-0.583298
6	3.624005	1.055320	0.583302
6	5.004050	-1.048161	-0.595278
1	3.102278	-1.875596	-1.062236
6	5.004051	1.048161	0.595280
1	3.102280	1.875596	1.062242
6	5.739620	0.000000	0.000001
1	5.527482	-1.883216	-1.045687
1	5.527484	1.883216	1.045690
6	7.204470	0.000000	0.000000
6	7.938456	0.627220	1.029126
6	7.938455	-0.627220	-1.029127

6	9.320222	0.622584	1.030664
1	7.416838	1.079164	1.864921
6	9.320221	-0.622585	-1.030666
1	7.416837	-1.079163	-1.864921
6	10.053332	0.000000	-0.000001
1	9.846878	1.071975	1.864454
1	9.846876	-1.071975	-1.864456
6	11.526269	-0.000001	-0.000002
6	12.249122	-1.084042	-0.532146
6	12.249125	1.084039	0.532141
6	13.637688	-1.085621	-0.526320
1	11.719308	-1.947604	-0.918865
6	13.637690	1.085616	0.526314
1	11.719312	1.947602	0.918861
6	14.338135	-0.000003	-0.000003
1	14.176603	-1.937377	-0.927004
1	14.176607	1.937371	0.926998
1	15.422749	-0.000004	-0.000004

PP8

6	-14.445241	-0.982698	0.694025
6	-13.723620	0.000000	0.000000
6	-14.445241	0.982698	-0.694025
6	-15.836917	0.983118	-0.694098
6	-16.539336	0.000000	0.000000
6	-15.836917	-0.983118	0.694099
1	-13.909543	-1.769518	1.215113
1	-13.909544	1.769518	-1.215113
1	-16.374043	1.758865	-1.230849
1	-17.624569	0.000000	0.000000
1	-16.374043	-1.758865	1.230849
6	-12.239950	0.000000	0.000000
6	-11.512612	0.294350	-1.162229
6	-11.512612	-0.294350	1.162228
6	-10.123471	0.293849	-1.162472
1	-12.042416	0.490801	-2.088741
6	-10.123471	-0.293849	1.162471
1	-12.042416	-0.490801	2.088741
6	-9.395532	0.000000	0.000000
1	-9.594767	0.488726	-2.089876
1	-9.594766	-0.488726	2.089875
6	-7.913352	0.000000	-0.000001
6	-7.185221	-0.954780	0.724867
6	-7.185221	0.954780	-0.724868
6	-5.796257	-0.955084	0.724637
1	-7.714152	-1.721137	1.282013
6	-5.796257	0.955083	-0.724638
1	-7.714151	1.721137	-1.282015
6	-5.068224	0.000000	0.000000
1	-5.267423	-1.697900	1.312841
1	-5.267423	1.697899	-1.312842
6	-3.586049	0.000000	0.000000
6	-2.857898	1.198408	0.033374
6	-2.857898	-1.198409	-0.033375
6	-1.468952	1.198373	0.034418
1	-3.386647	2.144908	0.079042
6	-1.468952	-1.198373	-0.034419
1	-3.386646	-2.144909	-0.079042
6	-0.740956	0.000000	0.000000
1	-0.939922	2.145787	0.042612
1	-0.939922	-2.145787	-0.042612
6	0.741164	0.000000	0.000000
6	1.469130	-0.908757	-0.781977
6	1.469130	0.908757	0.781976
6	2.858091	-0.908062	-0.782643
1	0.940171	-1.614525	-1.414157
6	2.858091	0.908062	0.782642
1	0.940171	1.614526	1.414157
6	3.586280	0.000000	0.000000
1	3.386782	-1.638386	-1.386539
1	3.386783	1.638386	1.386539
6	5.068298	0.000000	0.000000
6	5.796386	0.224731	1.177727
6	5.796386	-0.224731	-1.177727
6	7.185328	0.224893	1.177689
1	5.267604	0.364812	2.114918
6	7.185328	-0.224893	-1.177689
1	5.267605	-0.364813	-2.114918
6	7.913320	0.000000	0.000000
1	7.714342	0.365379	2.114702
1	7.714343	-0.365379	-2.114702
6	9.395466	0.000000	0.000000
6	10.123228	-0.914183	-0.775686
6	10.123228	0.914182	0.775686
6	11.512396	-0.914937	-0.774704
1	9.594159	-1.649027	-1.373783
6	11.512396	0.914937	0.774705
1	9.594159	1.649027	1.373784
6	12.239608	0.000000	0.000000
1	12.042425	-1.625913	-1.400184
1	12.042425	1.625913	1.400184
6	13.723354	0.000000	0.000000
6	14.445176	1.203025	-0.005963
6	14.445176	-1.203025	0.005964
6	15.836840	1.203326	-0.006298
1	13.909897	2.146433	-0.038748
6	15.836840	-1.203326	0.006299
1	13.909898	-2.146432	0.038749
6	16.539415	0.000001	0.000001
1	16.373803	2.146655	-0.020167
1	16.373804	-2.146654	0.020168
1	17.624638	0.000001	0.000001

PP[8]-cation

6	-14.411992	1.085340	-0.527942
6	-13.689534	0.000000	0.000000
6	-14.411992	-1.085340	0.527942
6	-15.801041	-1.086784	0.522824
6	-16.501737	0.000000	0.000000
6	-15.801041	1.086784	-0.522824
1	-13.881270	1.949670	-0.912033
1	-13.881270	-1.949670	0.912033
1	-16.339681	-1.939897	0.921272
1	-17.586413	0.000000	0.000000
1	-16.339681	1.939897	-0.921272
6	-12.214895	0.000000	0.000000
6	-11.482744	-0.607416	1.038759
6	-11.482744	0.607416	-1.038759
6	-10.099883	-0.611367	1.037577
1	-12.010003	-1.046099	1.878097

6	-10.099883	0.611367	-1.037577
1	-12.010003	1.046099	-1.878097
6	-9.366949	0.000000	0.000000
1	-9.577389	-1.051831	1.879151
1	-9.577389	1.051831	-1.879151
6	-7.899408	0.000000	0.000000
6	-7.164943	1.048499	-0.592523
6	-7.164943	-1.048499	0.592523
6	-5.783554	1.054574	-0.582408
1	-7.689115	1.884325	-1.041050
6	-5.783554	-1.054574	0.582408
1	-7.689115	-1.884325	1.041050
6	-5.049551	0.000000	0.000000
1	-5.261071	1.874879	-1.060922
1	-5.261071	-1.874879	1.060922
6	-3.583609	0.000000	0.000000
6	-2.848734	-1.204480	-0.014743
6	-2.848734	1.204480	0.014743
6	-1.467687	-1.204332	-0.026854
1	-3.371546	-2.153210	-0.048029
6	-1.467687	1.204332	0.026854
1	-3.371546	2.153210	0.048029
6	-0.733081	0.000000	0.000000
1	-0.945361	-2.153972	-0.026093
1	-0.945361	2.153972	0.026093
6	0.732683	0.000000	0.000000
6	1.467126	1.034349	0.617574
6	1.467126	-1.034349	-0.617574
6	2.848197	1.027844	0.628023
1	0.944675	1.838038	1.123244
6	2.848197	-1.027844	-0.628023
1	0.944675	-1.838038	-1.123244
6	3.582969	0.000000	0.000000
1	3.371064	1.848829	1.104505
1	3.371064	-1.848829	-1.104505
6	5.048761	0.000000	0.000000
6	5.783652	-0.594680	-1.047614
6	5.783652	0.594680	1.047614
6	7.164811	-0.592825	-1.048332
1	5.262122	-1.020357	-1.897058
6	7.164811	0.592825	1.048332
1	5.262122	1.020357	1.897058
6	7.900194	0.000000	0.000000
1	7.687950	-1.017259	-1.897190
1	7.687950	1.017259	1.897190
6	9.367693	0.000000	0.000000
6	10.100248	1.034352	0.616511
6	10.100248	-1.034352	-0.616511
6	11.483248	1.038464	0.607891
1	9.577466	1.861758	1.082714
6	11.483248	-1.038464	-0.607891
1	9.577466	-1.861758	-1.082714
6	12.214902	0.000000	0.000000
1	12.010904	1.845963	1.102514
1	12.010904	-1.845963	-1.102514
6	13.689522	0.000000	0.000000
6	14.412152	-1.204188	0.082061
6	14.412152	1.204188	-0.082061
6	15.801172	-1.202850	0.086857
1	13.881472	-2.144944	0.180003
6	15.801172	1.202850	-0.086858
1	13.881472	2.144944	-0.180003
6	16.501951	0.000000	0.000000
1	16.339775	-2.141142	0.165754
1	16.339775	2.141142	-0.165754
1	17.586618	0.000000	0.000000

P12

6	-14.450037	-0.930861	0.755566
6	-13.722168	-0.000002	0.000000
6	-14.450035	0.930860	-0.755566
6	-15.839061	0.931659	-0.754683
6	-16.566732	0.000001	0.000000
6	-15.839063	-0.931657	0.754683
1	-13.920945	-1.678520	1.337499
1	-13.920941	1.678518	-1.337499
1	-16.368475	1.655732	-1.365399
1	-16.368478	-1.655729	1.365399
6	-12.240101	-0.000003	0.000000
6	-11.512093	0.249690	-1.172705
6	-11.512094	-0.249697	1.172704
6	-10.123153	0.249484	-1.172743
1	-12.041025	0.409817	-2.106615
6	-10.123154	-0.249493	1.172743
1	-12.041026	-0.409822	2.106615
6	-9.395061	-0.000005	0.000000
1	-9.594423	0.409208	-2.106822
1	-9.594424	-0.409217	2.106822
6	-7.913042	-0.000006	0.000000
6	-7.184921	-0.925347	0.762176
6	-7.184920	0.925334	-0.762176
6	-5.795956	-0.925941	0.761602
1	-7.713708	-1.669014	1.349446
6	-5.795955	0.925927	-0.761601
1	-7.713706	1.669002	-1.349446
6	-5.068051	-0.000007	0.000000
1	-5.266937	-1.645391	1.378076
1	-5.266936	1.645377	-1.378075
6	-3.585904	-0.000007	0.000001
6	-2.857936	1.198882	-0.006672
6	-2.857937	-1.198897	0.006674
6	-1.468977	1.198890	-0.005469
1	-3.386944	2.146243	0.007114
6	-1.468978	-1.198905	0.005471
1	-3.386945	-2.146258	-0.007113
6	-0.740989	-0.000008	0.000001
1	-0.940020	2.146092	-0.028921
1	-0.940020	-2.146108	0.028923
6	0.741163	-0.000008	0.000002
6	1.469078	-0.934098	-0.751574
6	1.469078	0.934081	0.751577
6	2.858041	-0.933553	-0.752111
1	0.940073	-1.660098	-1.360310
6	2.858041	0.933536	0.752115
1	0.940073	1.660082	1.360313
6	3.586135	-0.000008	0.000002
1	3.386875	-1.683546	-1.331222
1	3.386874	1.683530	1.331225
6	5.068171	-0.000008	0.000002
6	5.796260	0.260371	1.170383
6	5.796261	-0.260386	-1.170380

6	7.185199	0.260542	1.170354
1	5.267534	0.428703	2.102949
6	7.185199	-0.260556	-1.170351
1	5.267534	-0.428719	-2.102945
6	7.913205	-0.000007	0.000002
1	7.714096	0.429228	2.102774
1	7.714096	-0.429242	-2.102771
6	9.395254	-0.000005	0.000001
6	10.123168	-0.937842	-0.746860
6	10.123167	0.937832	0.746862
6	11.512166	-0.938565	-0.746074
1	9.594088	-1.690895	-1.321787
6	11.512165	0.938558	0.746076
1	9.594086	1.690885	1.321789
6	12.239928	-0.000003	0.000001
1	12.041422	-1.668143	-1.350315
1	12.041419	1.668137	1.350316
6	13.722137	-0.000001	0.000000
6	14.449886	1.198865	-0.019303
6	14.449889	-1.198866	0.019303
6	15.838886	1.198753	-0.020675
1	13.920625	2.145591	-0.053599
6	15.838889	-1.198751	0.020674
1	13.920630	-2.145593	0.053599
6	16.566642	0.000002	-0.000001
1	16.368461	2.145924	-0.018287
1	16.368466	-2.145920	0.018285
6	18.048798	0.000004	-0.000001
6	18.776395	-0.914931	0.775104
6	18.776392	0.914942	-0.775107
6	20.165567	-0.914745	0.775081
1	18.247184	-1.612949	1.415693
6	20.165563	0.914760	-0.775084
1	18.247178	1.612958	-1.415695
6	20.892835	0.000008	-0.000002
1	20.695398	-1.612896	1.415036
1	20.695392	1.612913	-1.415039
6	22.376447	0.000011	-0.000002
6	23.098292	-1.202980	0.001446
6	23.098289	1.203002	-0.001450
6	24.489953	-1.203353	0.001295
1	22.562921	-2.146533	-0.025523
6	24.489950	1.203379	-0.001298
1	22.562916	2.146555	0.025519
6	25.192503	0.000014	-0.000001
1	25.026935	-2.146739	-0.006557
1	25.026930	2.146766	0.006555
1	26.277726	0.000015	-0.000001
6	-18.049088	0.000004	0.000000
6	-18.776577	-1.199002	-0.012409
6	-18.776573	1.199011	0.012408
6	-20.165759	-1.198833	-0.014011
1	-18.247133	-2.145821	-0.041210
6	-20.165755	1.198846	0.014010
1	-18.247126	2.145829	0.041209
6	-20.892865	0.000008	-0.000001
1	-20.696003	-2.145632	-0.007076
1	-20.695996	2.145647	0.007074
6	-22.376650	0.000010	-0.000001
6	-23.098345	0.903710	0.794146
6	-23.098348	-0.903687	-0.794148
6	-24.490039	0.903542	0.794776
1	-22.563042	1.594372	1.437662
6	-24.490042	-0.903514	-0.794779
1	-22.563047	-1.594352	-1.437665
6	-25.192623	0.000015	-0.000001
1	-25.026928	1.606069	1.424532
1	-25.026933	-1.606040	-1.424534
1	-26.277843	0.000017	-0.000001

P[12]-cation

6	-14.429284	-1.024302	0.630310
6	-13.698013	0.000000	0.000000
6	-14.429284	1.024302	-0.630310
6	-15.813398	1.028800	-0.622692
6	-16.545124	0.000000	0.000000
6	-15.813398	-1.028800	0.622692
1	-13.903902	-1.843165	1.109068
1	-13.903902	1.843165	-1.109068
1	-16.339841	1.828998	-1.130698
1	-16.339841	-1.828998	1.130698
6	-12.226358	0.000000	0.000000
6	-11.493678	0.526388	-1.081261
6	-11.493679	-0.526388	1.081261
6	-10.109926	0.525814	-1.081524
1	-12.018281	0.900473	-1.953243
6	-10.109926	-0.525813	1.081524
1	-12.018282	-0.900473	1.953243
6	-9.377252	0.000000	0.000000
1	-9.586581	0.898935	-1.954699
1	-9.586581	-0.898935	1.954699
6	-7.905289	0.000000	0.000000
6	-7.172966	-1.009979	0.651927
6	-7.172966	1.009979	-0.651926
6	-5.788897	-1.013801	0.646153
1	-7.697362	-1.818757	1.148143
6	-5.788897	1.013801	-0.646153
1	-7.697362	1.818757	-1.148143
6	-5.056868	0.000000	0.000000
1	-5.264801	-1.802134	1.174638
1	-5.264801	1.802134	-1.174638
6	-3.584340	0.000000	0.000000
6	-2.852143	1.201995	-0.011873
6	-2.852143	-1.201995	0.011873
6	-1.467919	1.202015	-0.005147
1	-3.376064	2.151155	0.000436
6	-1.467919	-1.202015	0.005148
1	-3.376064	-2.151155	-0.000436
6	-0.735813	0.000000	0.000000
1	-0.943900	2.150870	-0.030856
1	-0.943900	-2.150870	0.030857
6	0.736949	0.000000	0.000000
6	1.468793	-1.021726	-0.633370
6	1.468793	1.021726	0.633370
6	2.853065	-1.018029	-0.639068
1	0.944586	-1.816631	-1.151849
6	2.853065	1.018029	0.639069
1	0.944586	1.816631	1.151849
6	3.584976	0.000000	0.000000
1	3.377613	-1.832915	-1.125134
1	3.377613	1.832915	1.125135

6	5.057535	0.000000	0.000000
6	5.789855	0.533674	1.077474
6	5.789855	-0.533674	-1.077474
6	7.173884	0.534625	1.077077
1	5.266209	0.913421	1.947612
6	7.173884	-0.534625	-1.077077
1	5.266209	-0.913422	-1.947612
6	7.905995	0.000000	0.000000
1	7.698517	0.915588	1.946124
1	7.698517	-0.915588	-1.946124
6	9.378084	0.000000	0.000000
6	10.109224	-1.031516	-0.618302
6	10.109224	1.031515	0.618302
6	11.493302	-1.036318	-0.610390
1	9.583581	-1.855473	-1.087879
6	11.493302	1.036318	0.610390
1	9.583581	1.855473	1.087879
6	12.224937	0.000000	0.000000
1	12.019062	-1.842594	-1.109437
1	12.019062	1.842594	1.109437
6	13.696933	0.000000	0.000000
6	14.428292	1.201444	-0.055350
6	14.428292	-1.201444	0.055350
6	15.812465	1.200693	-0.064029
1	13.903179	2.147966	-0.120705
6	15.812465	-1.200693	0.064029
1	13.903179	-2.147966	0.120705
6	16.544347	0.000000	0.000000
1	16.338698	2.148199	-0.094729
1	16.338698	-2.148199	0.094729
6	18.017255	0.000000	0.000000
6	18.747930	-0.968596	0.712512
6	18.747930	0.968596	-0.712512
6	20.133150	-0.966136	0.714578
1	18.223004	-1.705425	1.310520
6	20.133150	0.966136	-0.714579
1	18.223004	1.705425	-1.310520
6	20.863378	0.000000	0.000000
1	20.661373	-1.701189	1.311653
1	20.661373	1.701189	-1.311654
6	22.341536	0.000000	0.000000
6	23.063485	-1.205395	0.003342
6	23.063485	1.205395	-0.003342
6	24.453579	-1.204933	-0.000114
1	22.531050	-2.150136	-0.025369
6	24.453579	1.204933	0.000113
1	22.531050	2.150136	0.025369
6	25.154947	0.000000	0.000000
1	24.991573	-2.147127	-0.010371
1	24.991573	2.147127	0.010371
1	26.239784	0.000000	0.000000
6	-18.018110	0.000000	0.000000
6	-18.748416	-1.201383	-0.051560
6	-18.748416	1.201383	0.051559
6	-20.133724	-1.200281	-0.058935
1	-18.223066	-2.148094	-0.114659
6	-20.133724	1.200281	0.058934
1	-18.223066	2.148094	0.114659
6	-20.863399	0.000000	0.000000
1	-20.662715	-2.146532	-0.087605
1	-20.662715	2.146532	0.087605
6	-22.341586	0.000000	0.000000
6	-23.063292	0.925045	0.773103
6	-23.063292	-0.925045	-0.773104
6	-24.453388	0.922127	0.775698
1	-22.530621	1.629672	1.402841
6	-24.453388	-0.922127	-0.775699
1	-22.530621	-1.629672	-1.402841
6	-25.154722	0.000000	0.000000
1	-24.991369	1.636533	1.390073
1	-24.991369	-1.636533	-1.390074
1	-26.239551	0.000000	0.000000

PP16

6	-14.447854	0.381869	-1.136334
6	-13.719627	0.000000	0.000000
6	-14.447854	-0.381868	1.136334
6	-15.836780	-0.382396	1.136241
6	-16.564917	0.000000	0.000000
6	-15.836780	0.382396	-1.136241
1	-13.919172	0.702046	-2.028219
1	-13.919172	-0.702045	2.028219
1	-16.365524	-0.666047	2.040384
1	-16.365524	0.666048	-2.040384
6	-12.237563	0.000000	0.000000
6	-11.509379	0.401635	1.129752
6	-11.509379	-0.401634	-1.129752
6	-10.120427	0.400755	1.130107
1	-12.037914	0.755256	2.008998
6	-10.120427	-0.400754	-1.130107
1	-12.037914	-0.755255	-2.008998
6	-9.392728	0.000001	0.000000
1	-9.591041	0.752623	2.009631
1	-9.591041	-0.752622	-2.009630
6	-7.910603	0.000001	0.000000
6	-7.183279	0.415097	-1.125033
6	-7.183279	-0.415096	1.125034
6	-5.794196	0.417419	-1.124231
1	-7.713206	0.760104	-2.006954
6	-5.794196	-0.417417	1.124233
1	-7.713206	-0.760102	2.006955
6	-5.067044	0.000001	0.000001
1	-5.264103	0.729738	-2.018148
1	-5.264103	-0.729736	2.018149
6	-3.584637	0.000001	0.000001
6	-2.857840	-1.049454	0.580662
6	-2.857840	1.049455	-0.580661
6	-1.468703	-1.051185	0.577502
1	-3.388386	-1.886146	1.023542
6	-1.468703	1.051186	-0.577501
1	-3.388386	1.886147	-1.023541
6	-0.741864	0.000001	0.000001
1	-0.938276	-1.872362	1.048704
1	-0.938276	1.872363	-1.048703
6	0.740580	0.000001	0.000001
6	1.467522	1.172800	0.250627
6	1.467522	-1.172799	-0.250625
6	2.856665	1.172111	0.253709
1	0.937224	2.094840	0.465797
6	2.856665	-1.172109	-0.253708
1	0.937224	-2.094839	-0.465796

6	3.583725	0.000001	0.000001
1	3.386850	2.101241	0.436399
1	3.386850	-2.101240	-0.436397
6	5.065912	0.000001	0.000001
6	5.793431	-0.727533	-0.953114
6	5.793431	0.727535	0.953115
6	7.182433	-0.726469	-0.953860
1	5.263801	-1.271731	-1.728329
6	7.182433	0.726470	0.953861
1	5.263801	1.271732	1.728330
6	7.910586	0.000000	0.000001
1	7.710962	-1.268946	-1.730909
1	7.710962	1.268947	1.730910
6	9.392655	0.000000	0.000001
6	10.120961	1.160936	0.298734
6	10.120961	-1.160935	-0.298733
6	11.509868	1.161060	0.298384
1	9.592388	2.083427	0.515880
6	11.509868	-1.161059	-0.298384
1	9.592388	-2.083426	-0.515879
6	12.238109	0.000000	0.000000
1	12.038441	2.073850	0.553030
1	12.038441	-2.073849	-0.553029
6	13.720230	0.000000	0.000000
6	14.448388	-1.095609	0.486845
6	14.448388	1.095610	-0.486844
6	15.837255	-1.095262	0.487445
1	13.919614	-1.953571	0.889106
6	15.837255	1.095262	-0.487444
1	13.919614	1.953572	-0.889105
6	16.565475	0.000000	0.000000
1	16.366056	-1.968530	0.855195
1	16.366056	1.968530	-0.855195
6	18.047509	0.000000	0.000000
6	18.775582	0.564365	-1.057944
6	18.775582	-0.564365	1.057944
6	20.164472	0.564831	-1.057718
1	18.246785	0.976322	-1.911245
6	20.164472	-0.564832	1.057718
1	18.246785	-0.976322	1.911245
6	20.892305	0.000000	0.000000
1	20.693748	0.977596	-1.910379
1	20.693748	-0.977596	1.910379
6	22.374377	0.000000	0.000000
6	23.102139	1.103417	-0.469101
6	23.102139	-1.103417	0.469100
6	24.491116	1.104053	-0.467717
1	22.572756	1.982340	-0.822385
6	24.491116	-1.104054	0.467716
1	22.572756	-1.982341	0.822384
6	25.218845	0.000000	0.000000
1	25.020531	1.968820	-0.854336
1	25.020531	-1.968821	0.854335
6	-18.047102	0.000000	0.000000
6	-18.774926	1.012525	-0.642093
6	-18.774926	-1.012525	0.642093
6	-20.163885	1.013099	-0.641158
1	-18.245675	1.822624	-1.133126
6	-20.163885	-1.013099	0.641158
1	-18.245675	-1.822624	1.133126
6	-20.891808	0.000000	0.000000
1	-20.692944	1.803164	-1.163987
1	-20.692944	-1.803164	1.163987
6	-22.374039	0.000000	0.000000
6	-23.102001	-1.191126	-0.136778
6	-23.102001	1.191125	0.136778
6	-24.490985	-1.190917	-0.138214
1	-22.573066	-2.130099	-0.263771
6	-24.490986	1.190917	0.138213
1	-22.573067	2.130098	0.263771
6	-25.218738	0.000000	0.000000
1	-25.020447	-2.133780	-0.229025
1	-25.020448	2.133779	0.229024
6	-26.701004	-0.000001	0.000000
6	-27.428681	0.834527	0.860871
6	-27.428681	-0.834528	-0.860872
6	-28.817872	0.833007	0.862158
1	-26.899641	1.480571	1.554027
6	-28.817872	-0.833008	-0.862159
1	-26.899641	-1.480572	-1.554028
6	-29.545124	-0.000001	-0.000001
1	-29.347753	1.503572	1.530995
1	-29.347753	-1.503574	-1.530996
6	-31.028842	-0.000001	-0.000001
6	-31.750536	-0.072222	-1.200888
6	-31.750536	0.072220	1.200887
6	-33.142204	-0.071796	-1.201232
1	-31.215023	-0.101217	-2.144283
6	-33.142204	0.071794	1.201231
1	-31.215023	0.101216	2.144282
6	-33.844733	-0.000001	-0.000001
1	-33.679202	-0.119471	-2.143437
1	-33.679202	0.119469	2.143435
1	-34.929958	-0.000001	-0.000001
6	26.701183	-0.000001	-0.000001
6	27.428779	1.150525	0.337443
6	27.428778	-1.150526	-0.337444
6	28.817960	1.150013	0.338755
1	26.899528	2.054002	0.622345
6	28.817959	-1.150014	-0.338756
1	26.899528	-2.054003	-0.622346
6	29.545233	-0.000001	-0.000001
1	29.347878	2.063455	0.588666
1	29.347878	-2.063456	-0.588668
6	31.029056	-0.000001	-0.000001
6	31.750643	0.653512	1.010153
6	31.750643	-0.653514	-1.010154
6	33.142320	0.653336	1.010639
1	31.215015	1.142457	1.817378
6	33.142320	-0.653338	-1.010642
1	31.215014	-1.142458	-1.817380
6	33.844757	-0.000001	-0.000001
1	33.679403	1.157959	1.807691
1	33.679402	-1.157961	-1.807693
1	34.929989	-0.000001	-0.000001

PP[16]-cation

6	-14.433015	0.667517	-0.999019
6	-13.702516	-0.000062	0.000015
6	-14.433038	-0.667626	0.999042
6	-15.818374	-0.673323	0.995359

6	-16.548909	-0.000031	0.000003
6	-15.818351	0.673244	-0.995348
1	-13.906931	1.211449	-1.775809
1	-13.906972	-1.211569	1.775837
1	-16.344823	-1.186749	1.792356
1	-16.344783	1.186682	-1.792349
6	-12.227615	-0.000076	0.000021
6	-11.496632	0.001180	1.201499
6	-11.496622	-0.001343	-1.201450
6	-10.111154	0.001036	1.201445
1	-12.022000	0.046408	2.149164
6	-10.111144	-0.001219	-1.201384
1	-12.021983	-0.046565	-2.149120
6	-9.380514	-0.000096	0.000033
1	-9.585152	0.045597	2.148844
1	-9.585135	-0.045787	-2.148779
6	-7.905009	-0.000102	0.000040
6	-7.175309	0.684018	-0.987565
6	-7.175322	-0.684226	0.987651
6	-5.789365	0.689702	-0.983617
1	-7.702002	1.240634	-1.755026
6	-5.789378	-0.689918	0.983715
1	-7.702025	-1.240840	1.755106
6	-5.059944	-0.000109	0.000053
1	-5.262025	1.216934	-1.771160
1	-5.262047	-1.217152	1.771263
6	-3.583835	-0.000110	0.000061
6	-2.854331	-1.136483	0.390033
6	-2.854327	1.136262	-0.389904
6	-1.468269	-1.138707	0.383342
1	-3.381172	-2.039628	0.678475
6	-1.468264	1.138485	-0.383200
1	-3.381164	2.039407	-0.678351
6	-0.738770	-0.000112	0.000074
1	-0.941329	-2.030537	0.704788
1	-0.941320	2.030314	-0.704641
6	0.737467	-0.000112	0.000080
6	1.466982	1.147780	0.354449
6	1.466985	-1.148002	-0.354285
6	2.853037	1.145682	0.361036
1	0.940090	2.047438	0.653340
6	2.853040	-1.145901	-0.360866
1	0.940096	-2.047661	-0.653178
6	3.582691	-0.000109	0.000086
1	3.379769	2.055916	0.626470
1	3.379775	-2.056135	-0.626299
6	5.058566	-0.000106	0.000085
6	5.788762	-0.726593	-0.956680
6	5.788759	0.726387	0.956848
6	7.174507	-0.726431	-0.956841
1	5.262314	-1.264384	-1.737618
6	7.174504	0.726238	0.957004
1	5.262309	1.264173	1.737789
6	7.904975	-0.000092	0.000079
1	7.700394	-1.263804	-1.738387
1	7.700390	1.263616	1.738548
6	9.380459	-0.000082	0.000073
6	10.110809	1.140052	0.378606
6	10.110823	-1.140205	-0.378467
6	11.496440	1.142223	0.372498
1	9.584701	2.046392	0.657922
6	11.496454	-1.142353	-0.372375
1	9.584726	-2.046553	-0.657777
6	12.226831	-0.000059	0.000057
1	12.022379	2.037204	0.686382
1	12.022404	-2.037326	-0.686265
6	13.701912	-0.000046	0.000046
6	14.432462	-1.152563	0.339775
6	14.432435	1.152484	-0.339695
6	15.817798	-1.150620	0.346149
1	13.906540	-2.056174	0.627829
6	15.817771	1.150566	-0.346092
1	13.906492	2.056085	-0.627741
6	16.548742	-0.000020	0.000022
1	16.343558	-2.064728	0.599232
1	16.343511	2.064683	-0.599183
6	18.022999	-0.000006	0.000010
6	18.754406	0.767622	-0.924540
6	18.754437	-0.767621	0.924546
6	20.139370	0.767520	-0.924627
1	18.229327	1.338286	-1.682633
6	20.139401	-0.767490	0.924611
1	18.229383	-1.338295	1.682648
6	20.871137	0.000023	-0.000014
1	20.664807	1.338126	-1.682416
1	20.664862	-1.338085	1.682392
6	22.345172	0.000039	-0.000026
6	23.075868	1.151829	-0.342886
6	23.075899	-1.151734	0.342823
6	24.461150	1.153638	-0.336254
1	22.550136	2.066862	-0.593084
6	24.461181	-1.153512	0.336169
1	22.550191	-2.066779	0.593029
6	25.192110	0.000071	-0.000048
1	24.987969	2.057817	-0.620652
1	24.988025	-2.057679	0.620558
6	-18.023346	-0.000015	-0.000004
6	-18.754018	1.118334	-0.440300
6	-18.754048	-1.118347	0.440286
6	-20.139114	1.121026	-0.433288
1	-18.228219	2.008295	-0.768481
6	-20.139143	-1.121007	0.433263
1	-18.228272	-2.008320	0.768472
6	-20.870222	0.000018	-0.000016
1	-20.665300	1.997851	-0.794237
1	-20.665353	-1.997819	0.794206
6	-22.344389	0.000035	-0.000023
6	-23.075086	-1.171389	-0.268665
6	-23.075060	1.171477	0.268613
6	-24.460299	-1.169573	-0.275323
1	-22.549454	-2.091015	-0.501383
6	-24.460273	1.169696	0.275255
1	-22.549408	2.091091	0.501336
6	-25.191286	0.000071	-0.000039
1	-24.987370	-2.096474	-0.472872
1	-24.987324	2.096610	0.472798
6	-26.666488	0.000090	-0.000048
6	-27.396175	0.805140	0.891953
6	-27.396183	-0.804941	-0.892060
6	-28.782480	0.800220	0.895502
1	-26.870346	1.424400	1.610756
6	-28.782489	-0.799984	-0.895630

1	-26.870361	-1.424216	-1.610855
6	-29.511545	0.000128	-0.000069
1	-29.311620	1.444028	1.589755
1	-29.311636	-1.443777	-1.589891
6	-30.991258	0.000149	-0.000080
6	-31.712795	-0.081304	-1.202225
6	-31.712809	0.081622	1.202055
6	-33.103325	-0.078299	-1.202093
1	-31.179309	-0.114863	-2.146317
6	-33.103340	0.078656	1.201904
1	-31.179336	0.115165	2.146154
6	-33.804911	0.000188	-0.000100
1	-33.641087	-0.129993	-2.143193
1	-33.641113	0.130365	2.142997
1	-34.889832	0.000204	-0.000107
6	26.667482	0.000088	-0.000060
6	27.396982	1.138587	0.384191
6	27.397002	-1.138395	-0.384324
6	28.783324	1.136119	0.389495
1	26.870821	2.030064	0.708154
6	28.783344	-1.135895	-0.389651
1	26.870856	-2.029884	-0.708278
6	29.512377	0.000121	-0.000084
1	29.312440	2.037467	0.679394
1	29.312476	-2.037230	-0.679559
6	30.992221	0.000138	-0.000097
6	31.713613	0.655522	1.011006
6	31.713612	-0.655228	-1.011212
6	33.104165	0.652906	1.012312
1	31.179860	1.143206	1.819874
6	33.104163	-0.652578	-1.012543
1	31.179856	-1.142926	-1.820071
6	33.805654	0.000173	-0.000122
1	33.642014	1.155143	1.809819
1	33.642011	-1.154802	-1.810059
1	34.890584	0.000186	-0.000131

PP24

6	-14.451194	-1.139638	0.373042
6	-13.723470	0.000075	0.000406
6	-14.451188	1.139783	-0.372252
6	-15.840166	1.139890	-0.371880
6	-16.568078	0.000066	0.000358
6	-15.840172	-1.139753	0.372623
1	-13.921822	-2.051154	0.630959
1	-13.921813	2.051303	-0.630153
1	-16.369196	2.051758	-0.629156
1	-16.369205	-2.051624	0.629881
6	-12.241494	0.000078	0.000425
6	-11.513970	0.643188	-1.011660
6	-11.513992	-0.643030	1.012528
6	-10.125022	0.642662	-1.012001
1	-12.043750	1.118898	-1.830583
6	-10.125043	-0.642503	1.012899
1	-12.043790	-1.118742	1.831438
6	-9.397169	0.000080	0.000457
1	-9.595952	1.117397	-1.831854
1	-9.595992	-1.117238	1.832764
6	-7.915099	0.000078	0.000471
6	-7.186824	-1.132171	0.394233
6	-7.186814	1.132326	-0.393279
6	-5.797930	-1.132314	0.393978
1	-7.715443	-2.033505	0.686906
6	-5.797920	1.132463	-0.393007
1	-7.715426	2.033661	-0.685959
6	-5.069609	0.000072	0.000489
1	-5.269492	-2.020908	0.723493
1	-5.269475	2.021054	-0.722516
6	-3.587481	0.000068	0.000493
6	-2.859125	1.133265	0.391529
6	-2.859131	-1.133133	-0.390542
6	-1.470229	1.133134	0.391950
1	-3.387506	2.022598	0.719137
6	-1.470235	-1.133009	-0.390964
1	-3.387517	-2.022463	-0.718149
6	-0.741910	0.000061	0.000491
1	-0.941787	2.035149	0.682789
1	-0.941797	-2.035027	-0.681804
6	0.740230	0.000059	0.000486
6	1.468226	-0.640591	-1.012899
6	1.468237	0.640708	1.013863
6	2.857125	-0.640157	-1.013099
1	0.939187	-1.130293	-1.823912
6	2.857137	0.640273	1.014048
1	0.939208	1.130411	1.824882
6	3.585273	0.000058	0.000470
1	3.385940	-1.162579	-1.803582
1	3.385961	1.162694	1.804526
6	5.067318	0.000059	0.000461
6	5.795648	-0.121257	1.193244
6	5.795630	0.121376	-1.192333
6	7.184568	-0.120620	1.193329
1	5.267270	-0.255467	2.131495
6	7.184550	0.120738	-1.192440
1	5.267238	0.255586	-2.130577
6	7.912570	0.000058	0.000439
1	7.713486	-0.253618	2.131503
1	7.713454	0.253735	-2.130622
6	9.394665	0.000057	0.000427
6	10.122234	-0.659724	-1.000790
6	10.122254	0.659836	1.001631
6	11.511253	-0.661083	-0.999983
1	9.592670	-1.196673	-1.781018
6	11.511272	0.661195	1.000797
1	9.592705	1.196787	1.781869
6	12.238674	0.000056	0.000400
1	12.041044	-1.167371	-1.800314
1	12.041079	1.167483	1.801118
6	13.720950	0.000056	0.000383
6	14.448574	1.148871	0.343878
6	14.448566	-1.148758	-0.343131
6	15.837596	1.149258	0.342267
1	13.919214	2.061725	0.596993
6	15.837588	-1.149143	-0.341560
1	13.919201	-2.061612	-0.596232
6	16.565249	0.000059	0.000342
1	16.367065	2.051604	0.630355
1	16.367051	-2.051487	-0.629663
6	18.047312	0.000060	0.000316
6	18.775192	-1.106383	0.462377

6	18.775173	1.106503	-0.461774
6	20.164094	-1.106061	0.463030
1	18.246036	-1.965459	0.861870
6	20.164075	1.106181	-0.462486
1	18.246001	1.965580	-0.861245
6	20.892332	0.000059	0.000256
1	20.692620	-1.964828	0.863875
1	20.692585	1.964947	-0.863353
6	22.374349	0.000057	0.000219
6	23.102700	-1.156410	-0.315153
6	23.102720	1.156521	0.315552
6	24.491587	-1.156458	-0.315368
1	22.574178	-2.065385	-0.583232
6	24.491607	1.156565	0.315689
1	22.574216	2.065497	0.583660
6	25.219997	0.000053	0.000139
1	25.019918	-2.075853	-0.545695
1	25.019954	2.075960	0.545986
6	-18.050080	0.000060	0.000329
6	-18.777786	-0.654379	1.005097
6	-18.777750	0.654490	-1.004471
6	-20.166756	-0.654671	1.004959
1	-18.248349	-1.138865	1.819042
6	-20.166720	0.654765	-1.004394
1	-18.248283	1.138982	-1.818393
6	-20.894338	0.000042	0.000266
1	-20.696275	-1.139513	1.818634
1	-20.696209	1.139600	-1.818093
6	-22.376461	0.000031	0.000230
6	-23.104247	1.143154	-0.361373
6	-23.104248	-1.143104	0.361795
6	-24.493245	1.143571	-0.360169
1	-22.574982	2.051993	-0.628727
6	-24.493245	-1.143545	0.360515
1	-22.574982	-2.051934	0.629178
6	-25.221023	0.000007	0.000152
1	-25.022429	2.041231	-0.662958
1	-25.022431	-2.041213	0.663273
6	-26.703251	-0.000007	0.000105
6	-27.430969	-1.113649	-0.444330
6	-27.431017	1.113623	0.444492
6	-28.819958	-1.113016	-0.445959
1	-26.901698	-1.986363	-0.812848
6	-28.820007	1.112968	0.446026
1	-26.901785	1.986346	0.813046
6	-29.547695	-0.000029	0.000007
1	-29.349290	-1.999126	-0.780856
1	-29.349376	1.999070	0.780886
6	-31.029956	-0.000039	-0.000048
6	-31.757423	0.575775	1.051772
6	-31.757337	-0.575862	-1.051923
6	-33.146430	0.573757	1.052803
1	-31.227698	1.014401	1.891160
6	-33.146343	-0.573859	-1.053059
1	-31.227543	-1.014482	-1.891270
6	-33.873903	-0.000054	-0.000156
1	-33.676081	1.042973	1.875552
1	-33.675927	-1.043081	-1.875849
6	26.702106	0.000051	0.000094
6	27.430438	-0.710412	-0.965430
6	27.430500	0.710513	0.965572
6	28.819330	-0.710420	-0.965483
1	26.901966	-1.255809	-1.740453
6	28.819392	0.710517	0.965539
1	26.902078	1.255912	1.740628
6	29.547748	0.000047	0.000005
1	29.347663	-1.288038	-1.716853
1	29.347774	1.288133	1.716876
6	31.029852	0.000044	-0.000041
6	31.758302	0.037712	-1.198221
6	31.758378	-0.037630	1.198091
6	33.147178	0.038075	-1.198240
1	31.230026	0.087181	-2.144767
6	33.147255	-0.038007	1.198022
1	31.230162	-0.087094	2.144671
6	33.875583	0.000030	-0.000132
1	33.675671	0.048817	-2.145893
1	33.675807	-0.048755	2.145641
6	35.357637	0.000018	-0.000182
6	36.085957	0.773831	-0.915709
6	36.086007	-0.773810	0.915293
6	37.474856	0.774062	-0.915507
1	35.557514	1.400269	-1.626907
6	37.474906	-0.774074	0.914988
1	35.557602	-1.400235	1.626530
6	38.203412	-0.000016	-0.000288
1	38.002959	1.370904	-1.651960
1	38.003049	-1.370930	1.651400
6	39.685500	-0.000038	-0.000348
6	40.413843	1.173934	-0.242938
6	40.413827	-1.174033	0.242177
6	41.802734	1.173871	-0.242737
1	39.885350	2.105818	-0.415486
6	41.802718	-1.174016	0.241848
1	39.885319	-2.105900	0.414773
6	42.531059	-0.000085	-0.000479
1	42.331427	2.097817	-0.453142
1	42.331400	-2.097979	0.452204
6	44.013199	-0.000110	-0.000554
6	44.741244	1.074205	0.531904
6	44.741151	-1.074451	-0.533087
6	46.130315	1.074348	0.531241
1	44.212573	1.905729	0.986476
6	46.130222	-1.074641	-0.532573
1	44.212404	-1.905956	-0.987603
6	46.857641	-0.000158	-0.000705
1	46.660220	1.906232	0.983852
1	46.660051	-1.906542	-0.985240
6	48.341277	-0.000183	-0.000786
6	49.063077	-1.168627	0.285493
6	49.063084	1.168237	-0.287144
6	50.454735	-1.168963	0.285715
1	48.527717	-2.078354	0.537255
6	50.454743	1.168526	-0.287522
1	48.527727	2.077982	-0.538846
6	51.157263	-0.000230	-0.000943
1	50.991705	-2.083148	0.518774
1	50.991717	2.082693	-0.520640
1	52.242488	-0.000249	-0.001004
6	-35.356175	-0.000059	-0.000215
6	-36.083772	0.227703	-1.177417
6	-36.083865	-0.227826	1.176928

6	-37.472792	0.229559	-1.177115
1	-35.554340	0.425844	-2.103713
6	-37.472885	-0.229691	1.176515
1	-35.554506	-0.425963	2.103267
6	-38.200554	-0.000068	-0.000329
1	-38.002095	0.392695	-2.110297
1	-38.002262	-0.392830	2.109654
6	-39.682792	-0.000072	-0.000390
6	-40.410638	-0.923945	0.763736
6	-40.410580	0.923796	-0.764577
6	-41.799690	-0.924952	0.762474
1	-39.881629	-1.666117	1.352734
6	-41.799632	0.924795	-0.763433
1	-39.881526	1.665972	-1.353530
6	-42.527318	-0.000081	-0.000510
1	-42.329147	-1.643689	1.379451
1	-42.329041	1.643528	-1.380455
6	-44.009660	-0.000085	-0.000574
6	-44.737125	1.198973	0.003986
6	-44.737120	-1.199145	-0.005197
6	-46.126318	1.198813	0.005660
1	-44.207607	2.145930	0.026559
6	-46.126314	-1.198990	-0.006993
1	-44.207598	-2.146101	-0.027723
6	-46.853435	-0.000090	-0.000698
1	-46.656560	2.145560	-0.007296
1	-46.656553	-2.145739	0.005916
6	-48.337208	-0.000091	-0.000765
6	-49.058865	-0.907125	-0.791131
6	-49.058936	0.906944	0.789537
6	-50.450560	-0.906942	-0.791849
1	-48.523478	-1.600465	-1.431690
6	-50.450631	0.906763	0.790126
1	-48.523606	1.600283	1.430144
6	-51.153177	-0.000088	-0.000894
1	-50.987430	-1.612123	-1.418647
1	-50.987557	1.611946	1.416875
1	-52.238395	-0.000087	-0.000944

PP[24]-cation

6	-14.471329	1.776613	-0.256556
6	-13.706930	0.670736	0.150657
6	-14.400709	-0.480824	0.55781
6	-15.786802	-0.524901	0.556422
6	-16.551326	0.58035	0.1477
6	-15.857727	1.732495	-0.258186
1	-13.972829	2.69789	-0.538562
1	-13.845454	-1.36898	0.839915
1	-16.285002	-1.446602	0.837416
1	-16.413041	2.620324	-0.541398
6	-12.229471	0.713175	0.148447
6	-11.480565	0.057405	1.139444
6	-11.520448	1.405492	-0.846933
6	-10.094078	0.088324	1.132794
1	-11.993119	-0.451623	1.948661
6	-10.133685	1.436763	-0.853517
1	-12.062718	1.89043	-1.651606
6	-9.384907	0.776711	0.134661
1	-9.551620	-0.396979	1.93708
1	-9.621152	1.94574	-1.662808
6	-7.906922	0.80018	0.121915
6	-7.197326	1.942893	-0.282099
6	-7.158644	-0.323007	0.510527
6	-5.810246	1.962409	-0.293948
1	-7.740013	2.836929	-0.570334
6	-5.771981	-0.306748	0.489739
1	-7.670920	-1.230966	0.810419
6	-5.062229	0.836756	0.088162
1	-5.297964	2.858326	-0.628191
1	-5.229327	-1.189037	0.811865
6	-3.584160	0.852136	0.066911
6	-2.850397	-0.285724	-0.306652
6	-2.859999	2.00274	0.419527
6	-1.463786	-0.272594	-0.329982
1	-3.374306	-1.187403	-0.605237
6	-1.472851	2.01303	0.405351
1	-3.390980	2.895531	0.732178
6	-0.739337	0.876164	0.028223
1	-0.932510	-1.176634	-0.607805
1	-0.949334	2.925679	0.66966
6	0.738765	0.884771	0.010468
6	1.476495	1.57863	0.983548
6	1.458801	0.19446	-0.978272
6	2.863628	1.57462	0.973669
1	0.955739	2.108181	1.774195
6	2.845617	0.197965	-0.993287
1	0.923853	-0.335155	-1.759291
6	3.583669	0.884422	-0.015178
1	3.398202	2.134062	1.733898
1	3.366096	-0.362423	-1.762494
6	5.061614	0.873962	-0.024216
6	5.784281	0.88764	-1.228876
6	5.798120	0.842419	1.1716
6	7.170858	0.865	-1.237299
1	5.252556	0.955537	-2.171947
6	7.184846	0.819817	1.163191
1	5.276113	0.790941	2.12111
6	7.907330	0.82761	-0.041538
1	7.692961	0.915839	-2.186789
1	7.716353	0.751204	2.106339
6	9.384796	0.78999	-0.050593
6	10.139047	1.454857	0.930069
6	10.088118	0.081588	-1.038724
6	11.525562	1.414735	0.922153
1	9.632387	2.029597	1.697951
6	11.474166	0.033843	-1.04151
1	9.540207	-0.460685	-1.80183
6	12.228379	0.699971	-0.061674
1	12.072739	1.925838	1.707089
1	11.981987	-0.511533	-1.829741
6	13.705503	0.646476	-0.064184
6	14.390353	-0.522132	-0.436248
6	14.477827	1.759586	0.30642
6	15.776077	-0.576602	-0.43235
1	13.828506	-1.40886	-0.709671
6	15.863944	1.707933	0.301035
1	13.985464	2.686358	0.581067
6	16.548712	0.537648	-0.065611
1	16.268503	-1.49249	-0.74113
1	16.425255	2.583425	0.609487
6	18.025321	0.479075	-0.065543

6	18.801035	1.589817	-0.437512
6	18.707818	-0.691548	0.305581
6	20.186687	1.532255	-0.43997
1	18.310824	2.498786	-0.769368
6	20.093165	-0.749286	0.302803
1	18.145291	-1.556476	0.640209
6	20.869005	0.360894	-0.070852
1	20.749165	2.397454	-0.774105
1	20.583197	-1.658149	0.635113
6	22.345153	0.297085	-0.075723
6	23.125943	1.407343	0.286506
6	23.021734	-0.878233	-0.442204
6	24.511327	1.343372	0.289013
1	22.640129	2.327249	0.593831
6	24.406961	-0.939301	-0.449727
1	22.454162	-1.750472	-0.748147
6	25.187727	0.168933	-0.081145
1	25.079381	2.226778	0.560373
1	24.892228	-1.870169	-0.722825
6	-18.028367	0.529389	0.141712
6	-18.776889	1.177831	-0.854458
6	-18.737444	-0.174115	1.129458
6	-20.162700	1.122038	-0.865008
1	-18.263782	1.697644	-1.656419
6	-20.122977	-0.230726	1.118656
1	-18.196422	-0.651073	1.939655
6	-20.871387	0.414428	0.120085
1	-20.703503	1.599081	-1.675335
1	-20.636050	-0.75098	1.920333
6	-22.347534	0.346456	0.104404
6	-23.026089	-0.81966	0.495651
6	-23.125669	1.442208	-0.30417
6	-24.410821	-0.889063	0.472632
1	-22.459377	-1.693339	0.799331
6	-24.511003	1.37646	-0.31746
1	-22.638785	2.367057	-0.594583
6	-25.189224	0.207871	0.067113
1	-24.898452	-1.80221	0.796665
1	-25.076459	2.238198	-0.655534
6	-26.664654	0.133116	0.044937
6	-27.458020	1.242054	0.383756
6	-27.328044	-1.051789	-0.315386
6	-28.842679	1.167653	0.370228
1	-26.982778	2.169246	0.6856
6	-28.712433	-1.123069	-0.339538
1	-26.750343	-1.923427	-0.603499
6	-29.506034	-0.016305	0.006043
1	-29.420313	2.050094	0.623814
1	-29.187421	-2.060694	-0.607374
6	-30.980731	-0.097197	-0.010887
6	-31.658387	-0.857216	-0.97934
6	-31.759801	0.579297	0.942931
6	-33.042442	-0.935296	-0.994139
1	-31.093060	-1.37615	-1.745967
6	-33.143456	0.492246	0.934896
1	-31.272660	1.161467	1.717681
6	-33.821405	-0.266371	-0.034618
1	-33.527790	-1.546148	-1.747622
1	-33.710305	1.04058	1.679463
6	26.663483	0.099303	-0.080801
6	27.425011	0.763378	0.895349
6	27.358800	-0.637005	-1.054654
6	28.809509	0.687167	0.903006
1	26.923406	1.326985	1.67462
6	28.743679	-0.704466	-1.053397
1	26.806862	-1.145522	-1.837835
6	29.505052	-0.047762	-0.071941
1	29.362893	1.225612	1.664787
1	29.243201	-1.297501	-1.811843
6	30.979749	-0.129928	-0.063897
6	31.700718	-0.179479	1.141236
6	31.715745	-0.164484	-1.260449
6	33.084269	-0.267294	1.149331
1	31.167680	-0.174564	2.085901
6	33.100047	-0.240909	-1.25226
1	31.196699	-0.107515	-2.211218
6	33.820720	-0.29833	-0.04716
1	33.605238	-0.288824	2.100425
1	33.631253	-0.281795	-2.197066
6	35.294538	-0.390364	-0.03832
6	35.971759	-1.146306	0.933709
6	36.073592	0.27283	-1.001629
6	37.354979	-1.238663	0.93874
1	35.404634	-1.689698	1.681755
6	37.457425	0.189489	-0.989716
1	35.588787	0.882271	-1.756701
6	38.134638	-0.570466	-0.020673
1	37.841997	-1.819663	1.714361
1	38.023191	0.702959	-1.759636
6	39.608571	-0.663115	-0.010436
6	40.262446	-1.852069	0.354678
6	40.410682	0.434715	-0.364773
6	41.646271	-1.939659	0.360364
1	39.677878	-2.728135	0.614624
6	41.794551	0.349595	-0.348992
1	39.943335	1.376094	-0.633248
6	42.448793	-0.840334	0.011682
1	42.114839	-2.870058	0.662621
1	42.379661	1.214102	-0.64353
6	43.923703	-0.931621	0.024246
6	44.584553	-2.111243	-0.356056
6	44.718001	0.158161	0.417189
6	45.969308	-2.195679	-0.345769
1	44.007297	-2.960793	-0.705227
6	46.102559	0.071499	0.430797
1	44.243577	1.072743	0.756942
6	46.763232	-1.106938	0.048675
1	46.445856	-3.109263	-0.684965
1	46.681878	0.919722	0.779521
6	48.241755	-1.197891	0.060974
6	49.035090	-0.1082	-0.331158
6	48.889017	-2.376178	0.464929
6	50.423402	-0.194264	-0.321408
1	48.559068	0.804066	-0.675374
6	50.277368	-2.461205	0.477604
1	48.299342	-3.222616	0.801157
6	51.050974	-1.370912	0.083689
1	51.016886	0.657168	-0.638725
1	50.756660	-3.378659	0.803767
1	52.133922	-1.437569	0.092388
6	-35.295040	-0.360016	-0.043103
6	-36.031094	-0.386349	1.153784

6	-36.015622	-0.429105	-1.247681
6	-37.413828	-0.484576	1.14654
1	-35.510390	-0.354816	2.104786
6	-37.399197	-0.516174	-1.25497
1	-35.485141	-0.390735	-2.193043
6	-38.135043	-0.550086	-0.057991
1	-37.946716	-0.487223	2.091207
1	-37.917973	-0.583855	-2.205102
6	-39.608152	-0.653021	-0.065183
6	-40.379593	-0.022319	-1.055905
6	-40.292253	-1.38707	0.918683
6	-41.762971	-0.11607	-1.059097
1	-39.889910	0.570331	-1.821136
6	-41.674955	-1.488845	0.90932
1	-39.730922	-1.905949	1.688274
6	-42.446971	-0.853399	-0.077811
1	-42.322978	0.371692	-1.84966
1	-42.168166	-2.051893	1.694249
6	-43.921173	-0.956454	-0.083179
6	-44.570314	-2.142007	0.298736
6	-44.726001	0.127775	-0.469433
6	-45.954276	-2.239099	0.290743
1	-43.982484	-3.008242	0.583487
6	-46.110073	0.032262	-0.469284
1	-44.262113	1.067056	-0.751331
6	-46.758903	-1.153843	-0.091064
1	-46.421302	-3.166076	0.606042
1	-46.699048	0.885629	-0.788033
6	-48.236746	-1.256037	-0.094441
6	-49.035581	-0.176894	0.315657
6	-48.877919	-2.434526	-0.507739
6	-50.423202	-0.273412	0.31427
1	-48.564191	0.734845	0.667493
6	-50.265637	-2.529714	-0.512255
1	-48.284394	-3.272524	-0.857964
6	-51.044708	-1.449956	-0.100434
1	-51.020831	0.56973	0.645598
1	-50.740248	-3.446836	-0.846086
1	-52.127154	-1.524684	-0.10273

α-P[1]

7	0.000000	0.000000	1.121167
6	0.000000	1.123975	0.331046
6	0.000000	0.711908	-0.982058
6	0.000000	-0.711908	-0.982058
6	0.000000	-1.123975	0.331046
1	0.000000	2.111730	0.765259
1	0.000000	-2.111730	0.765259
1	0.000000	1.359500	-1.846640
1	0.000000	-1.359500	-1.846640
1	0.000000	0.000000	2.126747

α-P[1]-cation

7	0.000000	0.000000	1.142521
6	0.000000	1.108684	0.352272
6	0.000000	0.685585	-1.015906
6	0.000000	-0.685585	-1.015906
6	0.000000	-1.108684	0.352272
1	0.000000	2.105232	0.771761
1	0.000000	-2.105232	0.771761
1	0.000000	1.351211	-1.866099
1	0.000000	-1.351211	-1.866099
1	0.000000	0.000000	2.154635

α-P[2]

6	-1.566653	-1.118101	0.309343
6	-2.904466	-0.662089	0.163013
6	-2.850494	0.665819	-0.193928
1	-1.254183	-2.099639	0.636502
1	-3.804437	-1.238772	0.318456
7	-1.526857	1.026383	-0.263758
6	-0.722520	-0.052717	0.034796
6	0.722520	0.052716	0.034819
6	1.566643	1.118110	0.309364
7	1.526865	-1.026390	-0.263688
6	2.904461	0.662094	0.163096
1	1.254161	2.099656	0.636489
6	2.850499	-0.665825	-0.193811
1	3.804427	1.238779	0.318558
1	-3.633965	1.378027	-0.400916
1	3.633977	-1.378038	-0.400750
1	-1.179774	1.913534	-0.588219
1	1.179794	-1.913545	-0.588152

α-P[2]-cation

6	-1.567143	-1.166786	0.000038
6	-2.871975	-0.704945	0.000008
6	-2.817576	0.699167	-0.000020
1	-1.258636	-2.201706	0.000085
1	-3.774795	-1.295838	0.000021
7	-1.520687	1.080964	-0.000029
6	-0.700013	-0.038103	-0.000008
6	0.700013	0.038103	-0.000006
6	1.567143	1.166786	0.000034
7	1.520687	-1.080964	-0.000017
6	2.871975	0.704945	0.000012
1	1.258636	2.201706	0.000073
6	2.817576	-0.699167	-0.000003

1	3.774795	1.295838	0.000025
1	-3.616215	1.425680	-0.000047
1	3.616215	-1.425680	-0.000020
1	-1.206083	2.039141	-0.000081
1	1.206083	-2.039141	-0.000067

α-P[3]

6	0.708880	-1.791536	-0.411609
6	-0.708880	-1.791537	-0.411604
6	-1.134137	-0.498621	-0.145489
1	1.349536	-2.627984	-0.652455
1	-1.349536	-2.627986	-0.652447
7	0.000000	0.271971	0.003402
6	1.134137	-0.498621	-0.145490
6	2.459029	0.070512	-0.029285
6	2.932621	1.351963	-0.270287
7	3.540803	-0.685840	0.370303
6	4.327251	1.357752	-0.000794
1	2.347929	2.176065	-0.653403
6	4.676031	0.086990	0.396270
1	5.001171	2.195733	-0.101905
6	-2.459029	0.070512	-0.029286
6	-2.932621	1.351962	-0.270290
7	-3.540802	-0.685839	0.370305
6	-4.327251	1.357751	-0.000797
1	-2.347930	2.176063	-0.653408
1	-5.001171	2.195732	-0.101910
6	-4.676031	0.086991	0.396272
1	-5.626683	-0.328857	0.691587
1	5.626683	-0.328858	0.691583
1	-3.474304	-1.634844	0.698354
1	0.000000	1.213023	0.361913
1	3.474304	-1.634845	0.698350

α-P[3]-cation

6	0.689652	-1.821577	-0.000022
6	-0.689652	-1.821577	-0.000022
6	-1.132532	-0.471848	-0.000005
1	1.323525	-2.695628	-0.000039
1	-1.323525	-2.695628	-0.000040
7	0.000000	0.309068	0.000005
6	1.132532	-0.471848	-0.000005
6	2.439042	0.062684	0.000001
6	2.886582	1.399551	-0.000012
7	3.577531	-0.729970	0.000026
6	4.281431	1.387853	-0.000004
1	2.260409	2.279857	-0.000032
6	4.684339	0.053023	0.000011
1	4.939490	2.242818	-0.000013
6	-2.439042	0.062684	0.000001
6	-2.886582	1.399551	-0.000014
7	-3.577531	-0.729970	0.000026
6	-4.281431	1.387853	-0.000006
1	-2.260409	2.279857	-0.000035
1	-4.939490	2.242818	-0.000016
6	-4.684339	0.053023	0.000011
1	-5.673697	-0.377872	0.000022
1	5.673697	-0.377872	0.000022
1	-3.591174	-1.737351	0.000046
1	0.000000	1.316236	0.000036
1	3.591174	-1.737351	0.000045

α-P[4]

6	0.960160	0.695800	-0.000460
6	-0.397370	1.113870	-0.001380
6	-1.192220	-0.023180	0.002680
1	1.832280	1.332760	-0.016460
1	-0.754860	2.132320	-0.057480
7	-0.338180	-1.106090	-0.002960
6	0.967610	-0.680400	0.002130
6	-2.629580	-0.188640	-0.000620
6	-3.437290	-1.201850	-0.497970
7	-3.470210	0.758740	0.542190
6	-4.784610	-0.849330	-0.242100
1	-3.093300	-2.080260	-1.025150
1	-5.657760	-1.442830	-0.472310
6	-5.872590	1.190340	0.907490
6	-4.788200	0.378060	0.406650
7	-7.147330	1.098510	0.386940
6	-5.920270	2.138480	1.919240
1	-5.105560	2.398940	2.579980
6	-7.248100	2.627900	1.994740
1	-7.631520	3.327750	2.723500
6	-7.998180	1.974240	1.028620
6	-9.394030	2.078450	0.664270
6	-10.269870	1.154600	0.112850
7	-10.109550	3.241910	0.855030
6	-11.533110	1.787080	-0.033870
1	-10.037970	0.121930	-0.105330
6	-11.404840	3.076930	0.429010
1	-12.437700	1.341420	-0.420770
1	-12.118980	3.883140	0.491500
1	1.783670	-1.386020	0.006210
1	-9.701990	4.110870	1.157520
1	-7.375480	0.619490	-0.468880
1	-3.161460	1.610240	0.981720
1	-0.639410	-2.061320	0.094530

α-P[4]-cation

6	-6.175474	1.156460	0.043382
6	-4.781208	1.266409	-0.049532
6	-4.239304	-0.024911	0.025088
1	-6.893739	1.960951	0.011303
1	-4.225561	2.182665	-0.187551
7	-5.310092	-0.893607	0.157434
6	-6.475116	-0.192950	0.175647
6	-2.891963	-0.472034	-0.030851
6	-2.360191	-1.779490	-0.120688
7	-1.822042	0.386692	-0.014575
6	-0.978520	-1.681557	-0.147237
1	-2.933035	-2.691644	-0.194947
1	-0.287567	-2.505642	-0.246540
6	0.631534	0.313278	-0.075595
6	-0.631534	-0.313278	-0.075597
7	1.822042	-0.386692	-0.014569
6	0.978520	1.681557	-0.147235
1	0.287568	2.505642	-0.246542
6	2.360191	1.779490	-0.120682

1	2.933035	2.691644	-0.194940
6	2.891963	0.472033	-0.030842
6	4.239304	0.024911	0.025102
6	4.781209	-1.266409	-0.049515
7	5.310092	0.893607	0.157450
6	6.175474	-1.156460	0.043403
1	4.225562	-2.182665	-0.187535
6	6.475115	0.192950	0.175667
1	6.893739	-1.960951	0.011327
1	7.425216	0.693092	0.281312
1	-7.425217	-0.693092	0.281289
1	5.241459	1.891079	0.278353
1	1.896419	-1.379534	0.136434
1	-1.896419	1.379534	0.136426
1	-5.241460	-1.891079	0.278338

α-P[5]

6	2.069610	2.998030	0.484050
6	2.085070	4.390260	0.220790
6	0.897890	4.715310	-0.419700
1	2.817260	2.441980	1.031600
1	2.846580	5.092260	0.529220
7	0.172910	3.546680	-0.534100
6	0.874200	2.486370	0.000950
6	0.337180	1.143570	-0.002330
6	-0.969630	0.677400	0.001100
7	1.156330	0.034070	0.002700
6	-0.924670	-0.742140	0.000550
1	-1.856260	1.292800	0.056050
6	0.400800	-1.112900	-0.002010
1	-1.769270	-1.415180	0.016220
6	0.390090	5.974960	-0.909180
6	-0.906240	6.424070	-1.117750
7	1.232890	7.009660	-1.260480
6	-0.833060	7.748720	-1.613760
1	-1.807660	5.881200	-0.871940
1	-1.668310	8.403670	-1.816470
6	1.151840	9.312140	-2.140960
6	0.507300	8.096620	-1.703620
7	0.539520	10.183030	-3.019030
6	2.387280	9.860530	-1.827550
1	3.088050	9.462910	-1.107370
6	2.515970	11.077790	-2.541390
1	3.333190	11.780890	-2.465330
6	1.358900	11.260300	-3.284400
6	0.954390	12.316330	-4.185900
6	-0.300260	12.794230	-4.535930
7	1.876580	13.071890	-4.879260
6	-0.118380	13.853300	-5.464590
1	-1.239640	12.454750	-4.123410
6	1.235750	14.001350	-5.661450
1	-0.892860	14.449570	-5.924170
1	1.792160	14.683390	-6.285220
1	0.865760	-2.086380	-0.005870
1	2.865520	12.885950	-4.887860
1	-0.290220	9.964250	-3.545930
1	2.228200	6.911270	-1.376420
1	-0.650310	3.445670	-1.105100
1	2.157660	0.072200	-0.089780

α-P[5]-cation

6	-4.282691	1.737066	-0.125324
6	-2.893720	1.745701	-0.209526
6	-2.442634	0.414414	-0.146395
1	-4.929115	2.599101	-0.194436
1	-2.273398	2.617829	-0.356474
7	-3.572609	-0.376397	-0.034204
6	-4.704135	0.398307	-0.006582
6	-6.012033	-0.160122	0.110167
6	-6.459198	-1.477881	-0.025181
7	-7.128963	0.611157	0.377910
6	-7.851689	-1.484485	0.170324
1	-5.849292	-2.332358	-0.281106
6	-8.238343	-0.178747	0.424040
1	-8.509071	-2.338844	0.122296
6	-1.133755	-0.120319	-0.202179
6	-0.693740	-1.452955	-0.356085
7	-0.000001	0.660134	-0.124119
6	0.693741	-1.452955	-0.356084
1	-1.328736	-2.313864	-0.504144
1	1.328738	-2.313863	-0.504141
6	2.442634	0.414415	-0.146389
6	1.133755	-0.120318	-0.202177
7	3.572609	-0.376396	-0.034205
6	2.893719	1.745704	-0.209510
1	2.273396	2.617833	-0.356448
6	4.282691	1.737068	-0.125307
1	4.929113	2.599105	-0.194410
6	4.704135	0.398308	-0.006577
6	6.012033	-0.160122	0.110166
6	6.459197	-1.477880	-0.025191
7	7.128964	0.611155	0.377915
6	7.851689	-1.484485	0.170312
1	5.849291	-2.332355	-0.281122
6	8.238343	-0.178749	0.424037
1	8.509071	-2.338844	0.122277
1	9.211007	0.238200	0.633412
1	-9.211006	0.238204	0.633412
1	7.118243	1.595869	0.588129
1	3.563749	-1.364234	0.161535
1	-0.000001	1.637224	0.119218
1	-3.563748	-1.364233	0.161548
1	-7.118241	1.595872	0.588118

α-P[6]

6	0.921900	6.427000	-1.112010
6	1.363940	7.677390	-1.609480
6	2.747690	7.633640	-1.704790
1	-0.095050	6.160540	-0.862170
1	0.744210	8.540190	-1.808240
7	3.138770	6.386140	-1.262330
6	2.039780	5.630920	-0.907350
6	2.174760	4.279440	-0.417750
6	3.223610	3.636670	0.224060
7	1.153110	3.359030	-0.533660
6	2.820620	2.303920	0.486800
1	4.150130	4.098990	0.533280
6	1.530660	2.145450	0.001920
1	3.382900	1.561270	1.034780

6	3.709810	8.617330	-2.142560
6	5.050630	8.792410	-1.826200
7	3.373010	9.628490	-3.016940
6	5.518280	9.928610	-2.528260
1	5.617850	8.188210	-1.132790
1	6.528370	10.312390	-2.526670
6	4.378050	11.566930	-4.165910
6	4.459080	10.439800	-3.266810
7	5.250540	12.632220	-4.074330
6	3.527630	11.835680	-5.228850
1	2.770910	11.168590	-5.616880
6	3.895430	13.091030	-5.773660
1	3.472130	13.556110	-6.652530
6	4.966080	13.576980	-5.038070
6	0.641370	1.004940	-0.002270
6	-0.743400	0.920050	0.001040
7	1.120320	-0.288350	0.002650
6	-1.094380	-0.456200	0.000590
1	-1.424030	1.757620	0.056190
6	0.076100	-1.180430	-0.002010
1	-2.092620	-0.868310	0.016330
1	0.252500	-2.244730	-0.005980
6	5.731620	14.798910	-5.150710
6	7.046490	15.092140	-4.819400
7	5.185260	15.952160	-5.673760
6	7.283780	16.453700	-5.146710
1	7.770530	14.386440	-4.437930
6	6.116250	16.961880	-5.669300
1	8.210810	16.994830	-5.026950
1	5.871870	17.946770	-6.035530
1	2.092790	-0.529550	-0.091150
1	0.334360	3.491780	-1.104620
1	4.064300	6.009370	-1.385900
1	2.459500	9.755150	-3.420510
1	5.865470	12.794320	-3.293580
1	4.213540	16.056700	-5.913660

α-P[6]-cation

6	-2.541267	1.515205	-0.441245
6	-1.151617	1.562201	-0.489256
6	-0.663864	0.247688	-0.365167
1	-3.210635	2.353629	-0.564077
1	-0.551916	2.444954	-0.656165
7	-1.769468	-0.572598	-0.255916
6	-2.928550	0.169898	-0.285752
6	-4.219078	-0.414526	-0.188018
6	-4.630389	-1.751594	-0.288742
7	-5.364689	0.334919	0.013924
6	-6.017887	-1.791288	-0.136148
1	-3.992750	-2.594826	-0.511573
6	-6.469916	-0.476796	0.062431
1	-6.642835	-2.667921	-0.219120
6	0.663864	-0.247687	-0.365166
6	1.151617	-1.562201	-0.489254
7	1.769467	0.572599	-0.255914
6	2.541267	-1.515204	-0.441242
1	0.551917	-2.444953	-0.656162
1	3.210635	-2.353628	-0.564072
6	4.219078	0.414527	-0.188015
6	2.928550	-0.169896	-0.285749
7	5.364689	-0.334918	0.013925
6	4.630388	1.751597	-0.288734
1	3.992749	2.594830	-0.511561
6	6.017888	1.791290	-0.136141
1	6.642835	2.667923	-0.219110
6	6.469916	0.476797	0.062433
6	-7.788337	0.040314	0.268749
6	-8.289037	1.337887	0.155282
7	-8.853952	-0.767244	0.620119
6	-9.666442	1.297409	0.449964
1	-7.729661	2.208274	-0.156411
6	-9.987225	-0.016249	0.740183
1	-10.355470	2.127937	0.440553
1	-10.926405	-0.466125	1.021579
6	7.788337	-0.040315	0.268748
6	8.289034	-1.337889	0.155286
7	8.853955	0.767243	0.620112
6	9.666441	-1.297413	0.449963
1	7.729656	-2.208277	-0.156401
6	9.987227	0.016246	0.740175
1	10.355467	-2.127942	0.440554
1	10.926409	0.466122	1.021566
1	-8.787766	-1.746332	0.845372
1	-5.374463	1.309177	0.268998
1	-1.730749	-1.548227	-0.009796
1	1.730748	1.548228	-0.009796
1	5.374463	-1.309177	0.268994
1	8.787772	1.746332	0.845360

α-P[7]

6	-4.424140	1.844330	-0.413550
6	-3.874000	2.939070	0.213550
7	-3.440230	0.894070	-0.536510
6	-2.509890	2.640380	0.472640
1	-4.396520	3.848300	0.472060
6	-2.256620	1.362990	-0.006090
1	-1.803940	3.264940	1.001230
6	-1.052800	0.561720	-0.003580
6	-0.861890	-0.812280	0.001680
7	0.199650	1.139090	0.004120
6	0.533650	-1.057790	0.000920
1	-1.642540	-1.556360	0.071700
6	1.181390	0.169250	-0.003140
1	1.014280	-2.023190	0.070040
6	2.584300	0.509790	-0.000280
6	3.253970	1.637980	0.452160
7	3.541610	-0.351590	-0.495790
6	4.636600	1.448810	0.211030
1	2.801660	2.475010	0.964480
6	4.799000	0.206780	-0.386630
1	5.434980	2.114800	0.505680
6	5.980440	-0.487030	-0.840330
6	6.245520	-1.839350	-1.005360
7	7.128430	0.191460	-1.195370
6	7.574200	-1.967470	-1.478440
1	5.577680	-2.647860	-0.744520
6	8.108800	-0.692260	-1.598120
1	8.108330	-2.891880	-1.645560
6	9.409400	-0.237780	-2.028140
6	10.118340	0.920230	-1.740730

7	10.202380	-0.993870	-2.867310
6	11.353030	0.857020	-2.431500
1	9.808950	1.693060	-1.051690
6	11.387190	-0.339050	-3.134510
1	12.160210	1.572600	-2.367610
6	12.394440	-0.911990	-3.995480
6	12.681270	-2.229150	-4.324180
7	13.310220	-0.125130	-4.663830
6	13.784690	-2.224620	-5.213140
1	12.195210	-3.101340	-3.910870
6	14.159820	-0.905210	-5.419940
1	14.295910	-3.093280	-5.603070
6	15.209740	-0.321270	-6.224870
6	15.919270	0.863280	-6.088930
7	15.697750	-0.951380	-7.350470
6	16.844930	0.941160	-7.163290
1	15.819760	1.565510	-5.273570
6	16.684370	-0.191140	-7.929100
1	17.558680	1.731180	-7.344930
1	17.184440	-0.517270	-8.827690
1	15.304930	-1.791230	-7.741650
1	13.239620	0.875680	-4.749220
1	9.877850	-1.801070	-3.374140
1	7.172420	1.186710	-1.341360
1	3.333690	-1.170020	-1.044150
1	0.369710	2.116700	-0.166960
1	-3.529280	0.024920	-1.035850
1	-5.423020	1.662750	-0.778450

7	3.573631	0.651049	-0.350330
6	4.292010	-1.410251	-0.813335
1	2.291552	-2.221396	-1.269722
6	4.709227	-0.120992	-0.437884
1	4.939771	-2.242669	-1.044970
6	6.011356	0.396466	-0.185722
6	6.480532	1.714553	-0.138532
7	7.103064	-0.419206	0.051678
6	7.850284	1.677549	0.138110
1	5.905374	2.601987	-0.359962
6	8.230378	0.333984	0.265360
1	8.512114	2.530153	0.169864
6	9.503827	-0.259303	0.549684
6	9.984540	-1.548598	0.323620
7	10.535750	0.451036	1.133248
6	11.315629	-1.602865	0.786400
1	9.456460	-2.346747	-0.178444
6	11.628319	-0.353698	1.287427
1	11.980499	-2.452041	0.746821
1	12.535069	0.018704	1.737562
1	10.465331	1.392414	1.482091
1	7.044160	-1.404357	0.248993
1	3.550496	1.570454	0.058366
1	0.008664	-1.346201	-0.492090
1	-3.544627	1.594695	0.029215
1	-7.072410	-1.422278	0.169490
1	-10.582194	1.459807	1.192100
1	-12.637334	0.062556	1.437089

α-P[7]-cation

6	-11.690519	-0.330374	1.101414
6	-11.318800	-1.613861	0.749210
7	-10.600134	0.480057	0.962711
6	-9.955404	-1.572484	0.390933
1	-11.963547	-2.479296	0.744082
6	-9.514040	-0.257104	0.530566
1	-9.369258	-2.407820	0.035196
6	-8.229289	0.334172	0.298028
6	-7.831268	1.677510	0.238354
7	-7.104887	-0.420634	0.077427
6	-6.455857	1.710309	-0.010313
1	-8.479548	2.536883	0.323012
6	-5.999743	0.390047	-0.106864
1	-5.862449	2.600994	-0.158359
6	-4.698421	-0.131727	-0.353461
6	-4.279033	-1.433132	-0.682783
7	-3.564481	0.645801	-0.305367
6	-2.892155	-1.419731	-0.817369
1	-4.923672	-2.281608	-0.858056
6	-2.441276	-0.112088	-0.573481
1	-2.278802	-2.257182	-1.116461
6	-1.130146	0.434025	-0.584030
6	-0.694619	1.771332	-0.572931
7	0.005028	-0.347835	-0.618775
6	0.697427	1.774049	-0.588706
1	-1.328819	2.644822	-0.609958
6	1.137544	0.438393	-0.610277
1	1.327389	2.649580	-0.644679
6	2.450761	-0.102499	-0.633230
6	2.903733	-1.397568	-0.932744

α-P[8]

6	-12.725080	-2.814535	-0.090885
6	-12.602877	-2.287266	-1.356379
7	-11.689642	-2.326188	0.667889
6	-11.450717	-1.456924	-1.362149
1	-13.275245	-2.464910	-2.182768
6	-10.892049	-1.497218	-0.092838
1	-11.099071	-0.849879	-2.184146
6	-9.725638	-0.844653	0.459820
6	-9.421680	-0.442589	1.752191
7	-8.651088	-0.494588	-0.330719
6	-8.134587	0.149626	1.732209
1	-10.085158	-0.503716	2.603082
6	-7.665463	0.104079	0.427126
1	-7.634455	0.623352	2.564815
6	-6.428846	0.562252	-0.159928
6	-6.113127	0.942791	-1.456724
7	-5.278738	0.703782	0.589215
6	-4.745019	1.307541	-1.482155
1	-6.810669	1.017099	-2.278666
6	-4.237267	1.146894	-0.200541
1	-4.205783	1.712451	-2.326539
6	-2.917971	1.373203	0.339296
6	-2.491217	1.673958	1.625326
7	-1.790526	1.324005	-0.454772
6	-1.080572	1.795672	1.597928
1	-3.133935	1.856510	2.474644
6	-0.658348	1.567964	0.295455
1	-0.446696	2.088452	2.422704
6	0.658348	1.567965	-0.295450
6	1.080573	1.795681	-1.597922

7	1.790526	1.324003	0.454776
6	2.491217	1.673967	-1.625320
1	0.446696	2.088466	-2.422696
6	2.917971	1.373205	-0.339292
1	3.133935	1.856523	-2.474637
6	4.237267	1.146892	0.200545
6	4.745017	1.307532	1.482160
7	5.278738	0.703785	-0.589213
6	6.113126	0.942782	1.456728
1	4.205781	1.712437	2.326546
6	6.428846	0.562250	0.159930
1	6.810668	1.017085	2.278671
6	7.665464	0.104081	-0.427126
6	8.134589	0.149636	-1.732208
7	8.651087	-0.494590	0.330717
6	9.421682	-0.442578	-1.752192
1	7.634458	0.623367	-2.564812
6	9.725638	-0.844651	-0.459823
1	10.085161	-0.503701	-2.603083
6	10.892049	-1.497218	0.092833
6	11.450715	-1.456933	1.362145
7	11.689644	-2.326183	-0.667899
6	12.602875	-2.287274	1.356372
1	11.099066	-0.849893	2.184146
6	12.725081	-2.814534	0.090874
1	13.275242	-2.464923	2.182760
1	13.454727	-3.488634	-0.329938
1	11.471180	-2.611580	-1.607864
1	8.522729	-0.812090	1.277637
1	5.164285	0.339673	-1.520936
1	1.777609	0.959388	1.393244
1	-1.777610	0.959396	-1.393242
1	-5.164284	0.339664	1.520936
1	-8.522731	-0.812082	-1.277641
1	-11.471176	-2.611592	1.607852
1	-13.454725	-3.488638	0.329924

α-P[8]-cation

6	-13.348250	-0.075121	1.630949
6	-13.063902	-1.372279	1.252897
7	-12.248765	0.693894	1.366547
6	-11.743074	-1.385377	0.752156
1	-13.739655	-2.211413	1.317970
6	-11.243030	-0.088214	0.833244
1	-11.229668	-2.235422	0.326109
6	-9.969650	0.454767	0.451301
6	-9.574024	1.766381	0.169568
7	-8.861804	-0.340279	0.284329
6	-8.209261	1.745992	-0.153951
1	-10.223475	2.628648	0.139095
6	-7.766020	0.423210	-0.074420
1	-7.620790	2.591698	-0.479524
6	-6.482114	-0.150382	-0.318225
6	-6.101288	-1.480642	-0.548393
7	-5.334643	0.606953	-0.381242
6	-4.715942	-1.507588	-0.734892
1	-6.772401	-2.322265	-0.634554
6	-4.236211	-0.196108	-0.621900
1	-4.126523	-2.375839	-0.991607
6	-2.916639	0.325842	-0.739992
6	-2.464883	1.641986	-0.924007
7	-1.795823	-0.475563	-0.705744
6	-1.070025	1.616199	-0.985559
1	-3.092249	2.510164	-1.062617
6	-0.652063	0.284901	-0.839990
1	-0.426603	2.461704	-1.180474
6	0.652063	-0.284895	-0.839991
6	1.070024	-1.616193	-0.985563
7	1.795824	0.475568	-0.705743
6	2.464883	-1.641980	-0.924012
1	0.426602	-2.461697	-1.180481
6	2.916639	-0.325837	-0.739993
1	3.092248	-2.510158	-1.062624
6	4.236211	0.196112	-0.621900
6	4.715943	1.507592	-0.734889
7	5.334643	-0.606951	-0.381244
6	6.101289	1.480644	-0.548391
1	4.126525	2.375843	-0.991603
6	6.482114	0.150384	-0.318225
1	6.772403	2.322267	-0.634549
6	7.766020	-0.423210	-0.074422
6	8.209260	-1.745993	-0.153957
7	8.861804	0.340277	0.284330
6	9.574023	-1.766383	0.169562
1	7.620789	-2.591697	-0.479533
6	9.969650	-0.454770	0.451300
1	10.223473	-2.628650	0.139086
6	11.243030	0.088209	0.833244
6	11.743075	1.385372	0.752160
7	12.248764	-0.693901	1.366546
6	13.063903	1.372272	1.252902
1	11.229670	2.235418	0.326116
6	13.348250	0.075112	1.630950
1	13.739656	2.211405	1.317978
1	14.237561	-0.355046	2.064131
1	12.150822	-1.663940	1.617345
1	8.817491	1.304267	0.572576
1	5.282324	-1.572271	-0.099493
1	1.802864	1.443681	-0.428859
1	-1.802864	-1.443676	-0.428862
1	-5.282325	1.572273	-0.099489
1	-8.817491	-1.304270	0.572572
1	-12.150823	1.663932	1.617349
1	-14.237562	0.355036	2.064131

α-P[12]

6	12.881354	-1.889467	-1.033329
6	11.484527	-2.043045	-0.857162
6	11.112425	-1.307354	0.259291
1	13.491916	-2.385205	-1.774423
1	10.831713	-2.678164	-1.438734
7	12.261705	-0.728186	0.757419
6	13.349774	-1.061488	-0.022753
6	14.676064	-0.577315	0.278103
6	15.253042	-0.160652	1.469202
7	15.647826	-0.469092	-0.695736
6	16.592523	0.211950	1.196090
1	14.782122	-0.191225	2.441355
6	16.820081	0.020518	-0.158868
1	17.332308	0.518292	1.921903

6	9.828900	-1.108737	0.888508
6	9.486665	-0.779207	2.192702
7	8.647905	-1.247071	0.188255
6	8.074310	-0.708252	2.267053
1	10.177516	-0.671502	3.016637
1	7.487328	-0.537129	3.158044
6	6.210256	-1.066357	0.519011
6	7.566484	-0.995830	1.007964
7	5.185958	-0.361005	1.116959
6	5.648594	-1.777528	-0.531944
1	6.167241	-2.488228	-1.159291
6	4.264232	-1.480857	-0.566653
1	3.533125	-1.924971	-1.227128
6	3.992681	-0.590349	0.462653
6	17.994188	0.238527	-0.974644
6	18.426209	-0.372427	-2.142960
7	18.942359	1.184184	-0.644775
6	19.656069	0.229899	-2.519132
1	17.937254	-1.199588	-2.637500
6	19.949837	1.190499	-1.578235
1	20.264451	-0.023441	-3.374842
6	2.763717	0.036863	0.887461
6	2.369680	0.540155	2.120558
7	1.702953	0.220869	0.026446
6	1.050348	1.033409	1.987477
1	2.957587	0.518159	3.026915
6	0.647476	0.826104	0.674517
1	0.468422	1.522710	2.755303
6	-0.584586	1.145640	-0.006632
6	-0.863734	1.367381	-1.348080
7	-1.772289	1.300359	0.678827
6	-2.247107	1.647353	-1.464516
1	-0.137866	1.394863	-2.148382
6	-2.800526	1.595107	-0.193022
1	-2.769980	1.928376	-2.367418
6	-4.152213	1.800256	0.269902
6	-4.648663	2.218676	1.496474
7	-5.240929	1.592425	-0.552366
6	-6.061370	2.249898	1.405885
1	-4.053741	2.535981	2.340880
6	-6.415376	1.850156	0.124611
1	-6.744275	2.594446	2.169241
6	-7.704865	1.701896	-0.505987
6	-8.085912	1.742774	-1.839986
7	-8.851905	1.487875	0.230723
6	-9.485998	1.537946	-1.898953
1	-7.435970	1.966916	-2.673734
6	-9.947554	1.374030	-0.600335
1	-10.102561	1.577816	-2.785477
6	-11.273090	1.141481	-0.078693
6	-11.836563	1.431907	1.155945
7	-12.258842	0.543453	-0.837261
6	-13.181122	0.988061	1.135483
1	-11.351891	1.970051	1.957987
6	-13.426862	0.430274	-0.111293
1	-13.912625	1.124616	1.918998
6	-14.614919	-0.168566	-0.671695
6	-15.044607	-0.303647	-1.984066
7	-15.587972	-0.733737	0.127171
6	-16.294556	-0.970791	-1.965518
1	-14.546270	0.099318	-2.854165
6	-16.615264	-1.237922	-0.642545
1	-16.926120	-1.170223	-2.819517
6	-17.758442	-1.891594	-0.044920
6	-18.349491	-1.747337	1.202011
7	-18.491291	-2.840755	-0.726146
6	-19.454461	-2.637335	1.264861
1	-18.051426	-1.037517	1.960404
6	-19.517066	-3.302789	0.061665
1	-20.135901	-2.763628	2.093251
1	-18.235511	-3.212133	-1.625785
1	-15.470544	-0.931036	1.107598
1	-12.090041	0.071335	-1.710432
1	-8.857704	1.240650	1.206769
1	-5.193505	1.122429	-1.441573
1	-1.909349	1.027974	1.638447
1	1.699595	-0.049614	-0.943184
1	5.327211	0.373545	1.790998
1	8.591591	-1.310326	-0.815078
1	12.270846	-0.004754	1.457684
1	15.468454	-0.540209	-1.684031
1	18.843349	1.842115	0.110188
1	20.782933	1.870759	-1.494274
1	-20.198572	-4.058155	-0.297273

α-P[12]-cation

6	20.216998	-1.601849	-0.681645
6	18.819708	-1.533009	-0.464623
6	18.386646	-0.276210	-0.872037
1	20.865374	-2.436008	-0.459749
1	18.206319	-2.297335	-0.008934
7	19.501659	0.403851	-1.318634
6	20.610874	-0.393184	-1.215357
6	17.078555	0.326749	-0.860127
6	16.682081	1.664184	-0.865048
7	15.930311	-0.427100	-0.816828
6	15.276313	1.699401	-0.820185
1	17.342473	2.518845	-0.862900
1	14.660535	2.587015	-0.840614
6	13.481778	-0.144724	-0.756848
6	14.813831	0.384410	-0.789034
7	12.396799	0.627546	-0.405037
6	12.990349	-1.418722	-1.051155
1	13.569841	-2.249746	-1.425781
6	11.599155	-1.402464	-0.855910
1	10.921610	-2.220373	-1.055035
6	11.235886	-0.119717	-0.443479
6	9.958443	0.438035	-0.117678
6	9.539916	1.767702	-0.005164
7	8.855560	-0.345414	0.138312
6	8.175351	1.766410	0.319270
1	10.154036	2.639898	-0.174553
6	7.753066	0.437095	0.409782
1	7.563455	2.638968	0.496209
6	6.475967	-0.121860	0.732659
6	6.104734	-1.424128	1.078303
7	5.326438	0.639371	0.767215
6	4.720052	-1.435084	1.307262
1	6.774614	-2.261715	1.207774
6	4.239119	-0.139881	1.103478
1	4.138085	-2.277717	1.651113

6	2.918000	0.398988	1.218215
6	2.475276	1.714002	1.378675
7	1.794394	-0.400780	1.210351
6	1.073457	1.692974	1.455362
1	3.107169	2.581931	1.498454
6	0.654953	0.365382	1.341278
1	0.433079	2.542381	1.643679
6	-0.654684	-0.211973	1.366658
6	-1.072631	-1.524267	1.598963
7	-1.794301	0.538677	1.166103
6	-2.474300	-1.552981	1.522603
1	-0.431983	-2.352729	1.864041
6	-2.917454	-0.257967	1.244181
1	-3.106100	-2.406869	1.719278
6	-4.239053	0.266570	1.079474
6	-4.723485	1.573355	1.169242
7	-5.323621	-0.541513	0.809266
6	-6.107507	1.539045	0.938931
1	-4.144180	2.444154	1.439531
6	-6.474952	0.210758	0.706130
1	-6.779046	2.383548	0.992227
6	-7.749107	-0.377896	0.428035
6	-8.161625	-1.713453	0.431614
7	-8.857933	0.375365	0.104162
6	-9.526392	-1.747711	0.110432
1	-7.542810	-2.567448	0.665794
6	-9.955198	-0.432350	-0.093998
1	-10.133818	-2.634271	0.002792
6	-11.237627	0.090952	-0.455080
6	-11.612838	1.339485	-0.953142
7	-12.391711	-0.662346	-0.364531
6	-13.004268	1.329900	-1.147224
1	-10.942873	2.148057	-1.208227
6	-13.483866	0.074405	-0.766550
1	-13.591671	2.128219	-1.576633
6	-14.810880	-0.468247	-0.761224
6	-15.260508	-1.786815	-0.704470
7	-15.935240	0.328830	-0.840600
6	-16.666611	-1.768271	-0.748869
1	-14.636095	-2.667836	-0.667582
6	-17.076115	-0.437318	-0.831621
1	-17.318695	-2.627194	-0.688914
6	-18.390108	0.150859	-0.880331
6	-18.835147	1.426892	-0.553616
7	-19.498832	-0.567415	-1.280309
6	-20.233347	1.467851	-0.771937
1	-18.228863	2.224810	-0.148838
6	-20.615816	0.223618	-1.226259
1	-20.889720	2.308092	-0.602770
1	-21.582841	-0.158006	-1.513973
1	21.581085	-0.040446	-1.528120
1	-19.469574	-1.499685	-1.658596
1	-15.928114	1.333832	-0.899186
1	-12.456647	-1.544597	0.116269
1	-8.872689	1.379950	0.044663
1	-5.252690	-1.508880	0.539519
1	-1.794982	1.482262	0.814409
1	1.794848	-1.371950	0.944196
1	5.258883	1.579274	0.412710
1	8.861037	-1.351851	0.144374
1	12.470110	1.539665	0.014967
1	15.913345	-1.433659	-0.809725
1	19.480889	1.310241	-1.755789

α-P[16]

6	-12.467829	-2.914504	0.980023
6	-11.057063	-2.895527	0.859736
6	-10.742649	-2.385248	-0.392304
1	-13.035138	-3.314881	1.807990
1	-10.348181	-3.278381	1.579974
7	-11.938563	-2.111029	-1.023736
6	-13.002648	-2.416220	-0.199729
6	-14.369098	-2.217833	-0.620339
6	-14.947048	-2.194444	-1.881849
7	-15.387084	-2.017566	0.289735
6	-16.335035	-1.964954	-1.719881
1	-14.434759	-2.394339	-2.812053
6	-16.592356	-1.849797	-0.360761
1	-17.078492	-1.955737	-2.504070
6	-9.472233	-2.147645	-1.033993
6	-9.121971	-2.057536	-2.374182
7	-8.313613	-1.970905	-0.305658
6	-7.729327	-1.811065	-2.444213
1	-9.785482	-2.221869	-3.211129
1	-7.133162	-1.753819	-3.343641
6	-5.908390	-1.537150	-0.636124
6	-7.241101	-1.753626	-1.146395
7	-4.959957	-0.838762	-1.355217
6	-5.302990	-1.935587	0.547268
1	-5.750989	-2.565634	1.302219
6	-3.970735	-1.455739	0.536724
1	-3.216079	-1.652901	1.284825
6	-3.774320	-0.767376	-0.652424
6	-17.819494	-1.614763	0.361572
6	-18.196621	-1.928983	1.659683
7	-18.897391	-0.984388	-0.226065
6	-19.521408	-1.466525	1.851766
1	-17.606566	-2.493243	2.367650
6	-19.941508	-0.874048	0.669170
1	-20.129430	-1.612131	2.733122
6	-2.619016	-0.083185	-1.182432
6	-2.248618	0.216518	-2.487147
7	-1.618573	0.398418	-0.365472
6	-1.005206	0.890087	-2.442402
1	-2.798156	-0.056412	-3.376615
6	-0.624323	0.995250	-1.110861
1	-0.462187	1.289755	-3.286800
6	-21.189134	-0.245605	0.304899
6	-21.806539	-0.077474	-0.926259
7	-22.021479	0.319305	1.249670
6	-23.026613	0.609740	-0.710050
1	-21.451220	-0.471759	-1.867596
6	-23.141826	0.855616	0.650333
1	-23.774437	0.836516	-1.456565
6	-24.171153	1.517253	1.421222
6	-24.577851	1.357226	2.738000
7	-24.975061	2.493656	0.871309
6	-25.643492	2.265163	2.977026
1	-24.187831	0.626271	3.431855
6	-25.865930	2.957121	1.808180
1	-26.195071	2.385942	3.897745

1	-26.576400	3.732003	1.566024
6	0.535659	1.593718	-0.494353
6	0.742219	2.096291	0.782916
7	1.715963	1.768902	-1.187572
6	2.075514	2.568056	0.855029
1	-0.006470	2.179696	1.557891
6	2.671212	2.350592	-0.379244
1	2.530693	3.077513	1.692241
6	4.001825	2.636184	-0.860683
6	4.481481	2.893301	-2.137315
7	5.082326	2.708280	-0.005257
6	5.877381	3.111925	-2.041141
1	3.878051	2.984646	-3.029047
6	6.237696	2.985823	-0.706618
1	6.537412	3.400247	-2.846749
6	7.516211	3.103693	-0.047813
6	7.848848	3.414463	1.263504
7	8.702361	2.907268	-0.724973
6	9.260592	3.391323	1.371318
1	7.152174	3.696335	2.040036
6	9.777749	3.067011	0.124899
1	9.840969	3.653927	2.244156
6	11.137267	2.910244	-0.334128
6	11.705691	3.068336	-1.590306
7	12.157660	2.556057	0.524858
6	13.090116	2.792748	-1.478755
1	11.190584	3.415120	-2.474656
6	13.354953	2.467814	-0.155426
1	13.826943	2.889266	-2.263291
6	14.581829	2.101678	0.510189
6	14.967449	2.190054	1.840704
7	15.648864	1.563710	-0.179952
6	16.285830	1.684006	1.946071
1	14.387700	2.635966	2.636226
6	16.694114	1.291782	0.678896
1	16.898918	1.673444	2.835831
6	17.932775	0.719124	0.208304
6	18.551251	0.765083	-1.033172
7	18.754351	-0.017398	1.037355
6	19.760054	0.032812	-0.943979
1	18.203913	1.326950	-1.888391
6	19.868505	-0.454874	0.350895
1	20.505646	-0.068965	-1.719498
6	20.885958	-1.258117	0.985872
6	21.257288	-1.388429	2.316479
7	21.717965	-2.083046	0.256756
6	22.325657	-2.317002	2.380589
1	20.850573	-0.822357	3.142289
6	22.595931	-2.745212	1.089117
1	22.884902	-2.588796	3.264517
6	23.573163	-3.676771	0.570911
6	24.200405	-3.754881	-0.664143
7	24.066641	-4.713323	1.335193
6	25.081643	-4.868204	-0.634330
1	24.078899	-3.051963	-1.475900
6	24.976524	-5.444328	0.611254
1	25.731095	-5.199529	-1.431193
1	25.468124	-6.303746	1.039722
1	23.720988	-4.954660	2.248968
1	21.572318	-2.321096	-0.710742
1	18.479663	-0.359558	1.943604

1	15.596547	1.226292	-1.127162
1	12.012615	2.210684	1.459463
1	8.767020	2.503278	-1.645000
1	5.064351	2.395315	0.951618
1	1.916896	1.341923	-2.077067
1	-1.614585	0.325225	0.638485
1	-5.167399	-0.283740	-2.169305
1	-8.290248	-1.814753	0.688765
1	-12.019508	-1.573443	-1.871253
1	-15.238764	-1.813471	1.264522
1	-18.853632	-0.492697	-1.103642
1	-21.755443	0.495400	2.204751
1	-24.843841	2.879639	-0.048730

α-P[16]-cation

6	-12.819988	2.467843	-0.701867
6	-11.416720	2.484314	-0.599634
6	-11.063039	1.809077	0.567706
1	-13.410028	2.962101	-1.459951
1	-10.734189	2.995112	-1.263211
7	-12.238329	1.402500	1.164808
6	-13.323848	1.781720	0.403120
6	-14.671022	1.482335	0.792438
6	-15.211354	1.127343	2.027948
7	-15.721434	1.533441	-0.101147
6	-16.597688	0.953963	1.862044
1	-14.668873	1.069499	2.960511
6	-16.905094	1.203880	0.524382
1	-17.312181	0.740172	2.643490
6	-9.779938	1.544503	1.152792
6	-9.414453	1.250428	2.465533
7	-8.616729	1.571790	0.411584
6	-8.016543	1.089072	2.500652
1	-10.081163	1.228622	3.315302
1	-7.416140	0.919089	3.382584
6	-6.192372	1.237345	0.688533
6	-7.528953	1.283700	1.209341
7	-5.169342	0.595164	1.354740
6	-5.641675	1.773714	-0.473753
1	-6.158170	2.401866	-1.184924
6	-4.275753	1.432816	-0.503754
1	-3.556999	1.753085	-1.244259
6	-3.993110	0.689014	0.640433
6	-18.155790	1.182262	-0.177070
6	-18.544234	1.782349	-1.373546
7	-19.261082	0.512737	0.309533
6	-19.893724	1.455950	-1.605075
1	-17.936301	2.444033	-1.973576
6	-20.329042	0.655037	-0.549656
1	-20.509050	1.819287	-2.415082
6	-2.769739	0.101584	1.110032
6	-2.379579	-0.303734	2.385959
7	-1.703435	-0.145063	0.272915
6	-1.063960	-0.795251	2.301650
1	-2.972820	-0.217990	3.284681
6	-0.651020	-0.692883	0.973627
1	-0.486099	-1.214535	3.112360
6	-21.605481	0.053071	-0.285151
6	-22.173883	-0.410139	0.897920
7	-22.543844	-0.140996	-1.279980

6	-23.464406	-0.894460	0.598994
1	-21.731979	-0.337487	1.881339
6	-23.678532	-0.727297	-0.766496
1	-24.189599	-1.261143	1.310758
6	-24.811022	-1.042462	-1.600982
6	-25.228562	-0.508258	-2.813941
7	-25.733276	-2.007527	-1.251251
6	-26.419043	-1.175364	-3.194628
1	-24.758293	0.312437	-3.336517
6	-26.705358	-2.099739	-2.213343
1	-27.009400	-0.990010	-4.079408
1	-27.513334	-2.808645	-2.122503
6	0.578746	-1.071915	0.336190
6	0.878018	-1.330590	-1.000006
7	1.741244	-1.274293	1.050745
6	2.239807	-1.679520	-1.080480
1	0.171875	-1.334464	-1.817804
6	2.771512	-1.633081	0.206586
1	2.764492	-1.999702	-1.968871
6	4.096373	-1.900593	0.690094
6	4.560827	-2.221387	1.964475
7	5.194920	-1.890950	-0.143742
6	5.956360	-2.392272	1.887403
1	3.945476	-2.383035	2.837646
6	6.342819	-2.176641	0.565799
1	6.605960	-2.710453	2.689862
6	7.631062	-2.236330	-0.063997
6	7.989456	-2.426749	-1.397588
7	8.804506	-2.124270	0.652302
6	9.394563	-2.415705	-1.474871
1	7.306975	-2.624949	-2.211233
6	9.894364	-2.218159	-0.188251
1	9.986044	-2.602165	-2.359467
6	11.242164	-2.131876	0.294836
6	11.771748	-2.297285	1.574157
7	12.304357	-1.865191	-0.544088
6	13.164617	-2.114248	1.494500
1	11.216773	-2.588528	2.454117
6	13.486491	-1.837608	0.165889
1	13.871756	-2.240511	2.301319
6	14.747774	-1.583956	-0.467632
6	15.139063	-1.691639	-1.801631
7	15.859982	-1.179209	0.242209
6	16.497412	-1.335275	-1.885615
1	14.524734	-2.059046	-2.610897
6	16.936492	-1.008584	-0.602291
1	17.114905	-1.378111	-2.770909
6	18.221198	-0.585942	-0.125324
6	18.779288	-0.608827	1.151544
7	19.181382	-0.064695	-0.969695
6	20.082721	-0.083790	1.065506
1	18.317465	-1.026795	2.034418
6	20.320076	0.260031	-0.265075
1	20.801926	-0.023999	1.869237
6	21.473909	0.826267	-0.905329
6	21.877295	0.819211	-2.237392
7	22.446573	1.506006	-0.198468
6	23.102039	1.513332	-2.323677
1	21.377444	0.304393	-3.045344
6	23.441036	1.943628	-1.043779
1	23.710243	1.628523	-3.209010
6	24.574187	2.691013	-0.558100
6	25.162087	2.746705	0.699753
7	25.307550	3.523410	-1.378677
6	26.262139	3.636510	0.625121
1	24.865471	2.164377	1.560389
6	26.325858	4.105468	-0.669248
1	26.941268	3.893298	1.424222
1	27.005720	4.799285	-1.138323
1	25.060726	3.748422	-2.328139
1	22.347641	1.812947	0.755562
1	19.005031	0.226345	-1.917379
1	15.835925	-0.857887	1.196226
1	12.208209	-1.537076	-1.491164
1	8.853662	-1.814553	1.609215
1	5.188104	-1.528044	-1.083035
1	1.868934	-0.999314	2.010963
1	-1.695003	0.047829	-0.715038
1	-5.307845	-0.027561	2.133848
1	-8.590292	1.588036	-0.594935
1	-12.285614	0.750370	1.930642
1	-15.612270	1.600286	-1.099894
1	-19.235083	-0.147112	1.069696
1	-22.354698	-0.055969	-2.265436
1	-25.642105	-2.621885	-0.459250

α-P[24]

6	-24.687605	-4.327622	-0.594693
6	-23.330501	-3.972405	-0.788125
6	-23.298406	-2.800044	-1.530350
1	-25.053291	-5.223142	-0.112998
1	-22.467943	-4.546541	-0.481378
7	-24.609035	-2.457087	-1.792947
6	-25.472195	-3.369282	-1.221094
6	-26.904703	-3.236132	-1.338078
6	-27.694833	-2.616005	-2.295836
7	-27.762230	-3.783924	-0.405869
6	-29.049310	-2.788945	-1.920218
1	-27.335748	-2.152408	-3.203516
6	-29.074203	-3.512558	-0.736016
1	-29.915832	-2.481624	-2.488028
6	-22.194065	-2.001571	-2.005713
6	-22.083821	-1.132733	-3.082476
7	-20.966621	-2.014408	-1.375347
6	-20.767945	-0.609392	-3.086029
1	-22.847422	-0.950548	-3.825070
1	-20.341221	0.045963	-3.831754
6	-18.732572	-0.984624	-1.543596
6	-20.086187	-1.163437	-2.011544
7	-18.016730	0.163764	-1.813693
6	-17.900215	-1.812441	-0.803396
1	-18.130877	-2.821175	-0.492062
6	-16.668562	-1.137956	-0.619312
1	-15.786161	-1.539066	-0.141320
6	-16.759683	0.095753	-1.248240
6	-30.172183	-3.965353	0.083991
6	-30.278144	-5.025854	0.972943
7	-31.396294	-3.328037	0.074705
6	-31.587796	-5.012728	1.511554
1	-29.516709	-5.769661	1.159383
6	-32.270136	-3.944310	0.946684

1	-32.010772	-5.744418	2.184877
6	-15.811616	1.177277	-1.376832
6	-15.670309	2.163927	-2.344029
7	-14.805639	1.377221	-0.455859
6	-14.559735	2.965447	-1.988377
1	-16.279416	2.268445	-3.230410
6	-14.030383	2.461432	-0.807305
1	-14.205810	3.840751	-2.513902
6	-33.620134	-3.467829	1.132155
6	-34.459987	-2.740024	0.301312
7	-34.325531	-3.719497	2.291295
6	-35.686388	-2.547187	0.984307
1	-34.238624	-2.443544	-0.714016
6	-35.583393	-3.157866	2.225587
1	-36.573611	-2.076287	0.585514
6	-36.521649	-3.272866	3.319970
6	-36.664628	-4.236751	4.307665
7	-37.510007	-2.334780	3.532265
6	-37.759216	-3.857856	5.129530
1	-36.080597	-5.142165	4.391523
6	-38.260875	-2.677501	4.629952
1	-38.144789	-4.398198	5.981538
1	-39.081255	-2.059041	4.959126
6	-12.918038	2.898581	0.002767
6	-12.648589	2.743023	1.355330
7	-11.873196	3.624945	-0.531359
6	-11.413378	3.379103	1.629175
1	-13.304456	2.283863	2.081316
6	-10.939371	3.918068	0.441427
1	-10.954131	3.494431	2.600487
6	-9.741160	4.665616	0.144028
6	-9.454819	5.582342	-0.857935
7	-8.605928	4.554809	0.920698
6	-8.119038	6.017532	-0.680412
1	-10.155891	5.950449	-1.593209
6	-7.601379	5.362948	0.428614
1	-7.612110	6.779249	-1.255339
6	-6.304821	5.429411	1.059158
6	-5.907108	5.182550	2.365751
7	-5.174513	5.801940	0.360675
6	-4.510378	5.401834	2.443856
1	-6.564653	4.941197	3.188594
6	-4.067327	5.780460	1.184132
1	-3.904407	5.358628	3.337529
6	-2.752153	6.122611	0.698414
6	-2.342502	6.911944	-0.367268
7	-1.608222	5.660376	1.316319
6	-0.926622	6.910504	-0.390323
1	-2.992936	7.483830	-1.013521
6	-0.484070	6.120326	0.661514
1	-0.296535	7.481109	-1.057539
6	0.845497	5.775806	1.104387
6	1.327915	5.393677	2.348509
7	1.926026	5.798154	0.246295
6	2.721216	5.173229	2.225640
1	0.750410	5.348570	3.260742
6	3.077570	5.423032	0.907709
1	3.404190	4.929282	3.026711
6	4.353568	5.358410	0.236409
6	4.835536	6.016192	-0.886723
7	5.373809	4.550082	0.694781
6	6.165479	5.582862	-1.107074
1	4.310052	6.778823	-1.443477
6	6.484038	4.664060	-0.116809
1	6.842804	5.953484	-1.863058
6	7.692234	3.918006	0.141081
6	8.202751	3.374043	1.311323
7	8.597989	3.633494	-0.860346
6	9.431585	2.743986	0.997730
1	7.771823	3.482146	2.296363
6	9.660690	2.908119	-0.361247
1	10.110033	2.283217	1.701593
6	10.751161	2.481416	-1.205818
6	11.243232	2.995178	-2.398765
7	11.543070	1.400414	-0.882701
6	12.348325	2.202928	-2.790380
1	10.869147	3.871108	-2.909067
6	12.523611	1.212100	-1.833065
1	12.931403	2.316224	-3.693031
1	11.424211	0.828450	-0.062758
1	8.407668	3.751522	-1.842028
1	5.254105	3.830747	1.389066
1	1.849685	5.871528	-0.755021
1	-1.597773	4.929559	2.008865
1	-5.129497	5.871922	-0.642780
1	-8.463827	3.837221	1.612580
1	-11.712006	3.737715	-1.518868
1	-14.660000	0.810724	0.363557
1	-18.424198	1.008607	-2.179898
1	-20.803302	-2.419398	-0.468068
1	-24.895683	-1.564618	-2.160627
1	-27.468143	-4.141157	0.488402
1	-31.560416	-2.428048	-0.345857
1	-33.914545	-4.080920	3.136507
1	-37.590185	-1.473543	3.017925
6	27.114319	-4.854664	0.069997
6	28.438317	-4.823437	0.571432
6	29.087003	-3.740255	-0.005213
1	26.370732	-5.612151	0.272671
1	28.892087	-5.552840	1.226950
7	28.178718	-3.132986	-0.847902
6	26.965958	-3.790339	-0.808350
6	25.838437	-3.349720	-1.594229
6	25.770160	-2.621990	-2.774146
7	24.540098	-3.639194	-1.227355
6	24.403345	-2.464804	-3.109626
1	26.616020	-2.301499	-3.365335
6	23.649157	-3.098505	-2.131947
1	24.012269	-2.002172	-4.004482
6	30.433084	-3.241746	0.145235
6	31.234805	-2.491823	-0.703918
7	31.175806	-3.487868	1.282140
6	32.475132	-2.277909	-0.054716
1	30.978752	-2.192806	-1.710286
1	33.340907	-1.785176	-0.473450
6	33.392065	-2.999666	2.247598
6	32.419896	-2.899162	1.185053
7	34.387596	-2.058314	2.411879
6	33.568661	-3.948814	3.244216
1	32.998407	-4.860246	3.353410
6	34.686898	-3.558867	4.022224
1	35.127373	-4.118702	4.834977

6	35.181132	-2.374919	3.494454
6	22.222264	-3.248183	-1.973676
6	21.466379	-4.215746	-1.326478
7	21.333207	-2.344448	-2.518647
6	20.100504	-3.874734	-1.479887
1	21.855316	-5.107990	-0.857065
6	20.034495	-2.701744	-2.218844
1	19.253287	-4.458299	-1.149126
6	36.293852	-1.539507	3.888412
6	37.100125	-0.679616	3.156682
7	36.747398	-1.500444	5.190276
6	38.049374	-0.110926	4.046965
1	37.046175	-0.523754	2.088680
6	37.806496	-0.632600	5.297255
1	38.832162	0.589452	3.795453
6	18.908739	-1.913858	-2.660534
6	18.758560	-1.045625	-3.732921
7	17.700756	-1.938237	-1.993926
6	17.438480	-0.534291	-3.696914
1	19.497943	-0.856033	-4.497845
6	16.794097	-1.094948	-2.602965
1	16.983840	0.117255	-4.429331
6	15.453523	-0.928099	-2.094628
6	14.649392	-1.764716	-1.333434
7	14.721762	0.215987	-2.339053
6	13.418820	-1.099987	-1.110632
1	14.896470	-2.772822	-1.032847
6	13.482455	0.136696	-1.737179
1	12.553823	-1.509198	-0.608289
1	36.289685	-1.958240	5.960736
1	34.409109	-1.169510	1.939074
1	30.793592	-3.859154	2.136444
1	28.315711	-2.227465	-1.266332
1	24.276650	-4.002956	-0.326195
1	21.599489	-1.448346	-2.892737
1	17.568354	-2.344989	-1.082409
1	15.112185	1.065024	-2.714009
1	38.293654	-0.462116	6.244607

α-P[24]-cation

6	-25.742317	-3.682801	0.297202
6	-24.356614	-3.448972	0.184745
6	-24.162163	-2.495558	-0.811124
1	-26.216703	-4.414862	0.934597
1	-23.575357	-3.970319	0.718735
7	-25.410465	-2.168694	-1.299692
6	-26.390869	-2.871176	-0.630432
6	-27.785112	-2.715089	-0.939914
6	-28.423148	-2.230600	-2.078588
7	-28.776821	-3.085293	-0.054386
6	-29.814247	-2.303342	-1.861200
1	-27.935022	-1.925764	-2.993051
6	-30.022288	-2.832464	-0.589701
1	-30.586567	-2.064645	-2.577880
6	-22.961128	-1.904425	-1.333863
6	-22.697020	-1.291412	-2.555770
7	-21.783610	-1.885508	-0.615175
6	-21.344721	-0.892320	-2.557698
1	-23.388705	-1.208789	-3.381595
1	-20.811521	-0.446943	-3.385150
6	-19.456283	-1.100933	-0.817654
6	-20.786875	-1.261968	-1.336861
7	-18.586470	-0.156186	-1.321685
6	-18.774819	-1.778864	0.188930
1	-19.146875	-2.631373	0.738534
6	-17.484313	-1.218826	0.292448
1	-16.690029	-1.566483	0.937349
6	-17.381534	-0.200791	-0.651337
6	-31.232129	-3.123026	0.129473
6	-31.484955	-3.996289	1.183036
7	-32.433018	-2.518201	-0.184028
6	-32.854395	-3.900447	1.507651
1	-30.771676	-4.680674	1.619393
6	-33.433189	-2.967676	0.651391
1	-33.381445	-4.495585	2.239112
6	-16.296920	0.683624	-0.982760
6	-16.027888	1.406103	-2.142617
7	-15.264321	0.941040	-0.106965
6	-14.817519	2.101678	-1.949760
1	-16.624434	1.398691	-3.043301
6	-14.350186	1.803658	-0.671969
1	-14.350217	2.777334	-2.651384
6	-34.785577	-2.488958	0.544513
6	-35.467969	-1.895333	-0.511224
7	-35.680047	-2.587756	1.591845
6	-36.786792	-1.628264	-0.080301
1	-35.077364	-1.739913	-1.506720
6	-36.901305	-2.059010	1.236547
1	-37.588855	-1.230741	-0.685216
6	-38.011543	-2.033223	2.158622
6	-38.312894	-2.837210	3.250020
7	-39.033306	-1.113058	2.046363
6	-39.536528	-2.379253	3.801522
1	-37.743334	-3.695742	3.576125
6	-39.957043	-1.310500	3.041072
1	-40.058741	-2.795116	4.650253
1	-40.828703	-0.680509	3.124764
6	-13.183335	2.256306	0.036804
6	-12.888995	2.292382	1.396440
7	-12.095584	2.793549	-0.620361
6	-11.601338	2.848951	1.548041
1	-13.558706	2.012346	2.196898
6	-11.113815	3.150785	0.280278
1	-11.108724	3.073884	2.482886
6	-9.870187	3.736027	-0.143478
6	-9.527125	4.414562	-1.308895
7	-8.742228	3.710543	0.650480
6	-8.170033	4.787896	-1.210282
1	-10.204500	4.673821	-2.109721
6	-7.689705	4.336161	0.015058
1	-7.618474	5.385483	-1.921583
6	-6.392208	4.451855	0.624974
6	-5.996515	4.393345	1.957652
7	-5.254044	4.682941	-0.119568
6	-4.598871	4.582085	2.004262
1	-6.656992	4.297483	2.807329
6	-4.146592	4.755105	0.699738
1	-3.993689	4.657236	2.896128
6	-2.827531	4.991782	0.177197
6	-2.404250	5.564140	-1.018271
7	-1.690898	4.662162	0.886420

6	-0.993258	5.564172	-1.024078
1	-3.045817	6.000000	-1.770385
6	-0.560203	4.991967	0.167924
1	-0.357760	6.000199	-1.781222
6	0.763164	4.756340	0.680184
6	1.226974	4.592349	1.981725
7	1.863010	4.676496	-0.148643
6	2.623973	4.401500	1.923794
1	0.629877	4.675229	2.878345
6	3.007590	4.449364	0.587179
1	3.291934	4.310830	2.768183
6	4.299095	4.325642	-0.033870
6	4.767174	4.760095	-1.270077
7	5.357786	3.708171	0.599367
6	6.123015	4.384209	-1.377525
1	4.208782	5.347973	-1.984149
6	6.477493	3.721777	-0.206428
1	6.792543	4.631822	-2.188562
6	7.725337	3.141981	0.213147
6	8.229920	2.867656	1.480316
7	8.693308	2.761600	-0.692961
6	9.514126	2.304261	1.323172
1	7.751104	3.115418	2.416556
6	9.788942	2.236363	-0.039229
1	10.194344	2.040491	2.120296
6	10.943886	1.762965	-0.754213
6	11.391319	2.025637	-2.046643
7	11.864899	0.913018	-0.181190
6	12.596561	1.321149	-2.240450
1	10.914752	2.683980	-2.758423
6	12.882438	0.629063	-1.066326
1	13.178582	1.288654	-3.150062
1	11.805632	0.553521	0.757135
1	8.536473	2.684425	-1.684579
1	5.269166	3.150028	1.432811
1	1.809773	4.591663	-1.150588
1	-1.687290	4.080306	1.708216
1	-5.210329	4.605531	-1.122573
1	-8.645126	3.141074	1.475266
1	-11.953224	2.738363	-1.615619
1	-15.192251	0.557888	0.821073
1	-18.862212	0.592411	-1.936084
1	-21.718811	-2.102865	0.365878
1	-25.592044	-1.384820	-1.905102
1	-28.615379	-3.309362	0.913909
1	-32.522833	-1.718267	-0.788989
1	-35.424453	-2.821397	2.537459
1	-39.036704	-0.345649	1.395232
6	28.123124	-3.929975	0.897365
6	29.504649	-3.824357	1.157939
6	30.060618	-2.990236	0.190975
1	27.419923	-4.555845	1.427707
1	30.053060	-4.354498	1.922937
7	29.032637	-2.608829	-0.645299
6	27.838447	-3.160234	-0.227365
6	26.604608	-2.920653	-0.923098
6	26.353432	-2.488983	-2.223264
7	25.377514	-3.125300	-0.327137
6	24.956041	-2.424915	-2.397171
1	27.100192	-2.309043	-2.982960
6	24.356950	-2.818140	-1.203410
1	24.436816	-2.188464	-3.314678
6	31.413131	-2.551861	-0.018767
6	32.057566	-2.082755	-1.159397
7	32.351445	-2.561225	0.993994
6	33.395935	-1.798412	-0.816260
1	31.625239	-2.023125	-2.147868
1	34.175446	-1.479151	-1.492616
6	34.714746	-1.993079	1.391259
6	33.564041	-2.094224	0.533803
7	35.778713	-1.165800	1.091041
6	35.028984	-2.633883	2.584285
1	34.440091	-3.404912	3.060160
6	36.296524	-2.172306	3.004229
1	36.853594	-2.524805	3.860226
6	36.747967	-1.250913	2.066009
6	22.973501	-2.944511	-0.836129
6	22.353236	-3.695985	0.158538
7	21.974047	-2.276386	-1.512802
6	20.965281	-3.461194	0.078006
1	22.845759	-4.392889	0.821099
6	20.741565	-2.566758	-0.965213
1	20.200510	-3.945553	0.667746
6	37.964503	-0.477584	1.993375
6	38.640376	0.064775	0.908239
7	38.696338	-0.159676	3.118826
6	39.794334	0.725069	1.401642
1	38.362942	-0.053238	-0.129474
6	39.801768	0.574192	2.770790
1	40.543527	1.239491	0.818493
6	19.526512	-1.999283	-1.482391
6	19.229292	-1.446595	-2.724975
7	18.369520	-1.941559	-0.732918
6	17.877938	-1.043947	-2.708933
1	19.897613	-1.405952	-3.572908
6	17.353946	-1.351813	-1.456596
1	17.322283	-0.638681	-3.542189
6	16.037360	-1.164197	-0.910179
6	15.377372	-1.801959	0.135785
7	15.159761	-0.234067	-1.427669
6	14.091392	-1.232657	0.248613
1	15.758941	-2.636294	0.706358
6	13.970574	-0.248859	-0.728592
1	13.311335	-1.552944	0.924368
1	38.399254	-0.349452	4.061488
1	35.763340	-0.456684	0.376179
1	32.131243	-2.690006	1.968066
1	29.108004	-1.875030	-1.330677
1	25.247591	-3.274246	0.660172
1	22.138525	-1.530902	-2.169430
1	18.330781	-2.110890	0.258922
1	15.424341	0.490298	-2.075115
1	40.495564	0.924839	3.518708

α-F[1]			
8	0.000000	0.000000	1.159331
6	0.000000	1.093380	0.346499
6	0.000000	0.717367	-0.958284
6	0.000000	-0.717367	-0.958284
6	0.000000	-1.093380	0.346499
1	0.000000	2.046705	0.849036
1	0.000000	-2.046705	0.849036
1	0.000000	1.373423	-1.815649
1	0.000000	-1.373423	-1.815649

α-F[1]-cation			
8	0.000000	0.000000	1.173789
6	0.000000	1.080407	0.369321
6	0.000000	0.690349	-0.989428
6	0.000000	-0.690349	-0.989428
6	0.000000	-1.080407	0.369321
1	0.000000	2.043944	0.860740
1	0.000000	-2.043944	0.860740
1	0.000000	1.362698	-1.835254
1	0.000000	-1.362698	-1.835254

α-F[2]			
6	1.544962	1.160724	0.000238
6	2.878714	0.645722	0.000009
6	2.765419	-0.707988	-0.000113
1	1.235735	2.194136	0.000332
1	3.797611	1.212343	0.000264
8	1.452542	-1.077343	-0.000150
6	0.714633	0.073856	0.000006
6	-0.714633	-0.073856	0.000003
6	-1.544962	-1.160724	0.000221
8	-1.452542	1.077343	-0.000155
6	-2.878714	-0.645722	0.000010
1	-1.235735	-2.194136	0.000304
6	-2.765419	0.707988	-0.000087
1	-3.797611	-1.212343	0.000268
1	3.474575	-1.519156	-0.000253
1	-3.474575	1.519156	-0.000200

α-F[2]-cation			
6	1.556700	1.167601	0.000005
6	2.853522	0.654920	-0.000002
6	2.725738	-0.725427	-0.000012
1	1.249699	2.202538	0.000013
1	3.781511	1.205971	-0.000001
8	1.432491	-1.094238	-0.000011
6	0.694199	0.058846	0.000000
6	-0.694199	-0.058846	0.000002
6	-1.556700	-1.167601	-0.000005
8	-1.432491	1.094238	0.000012
6	-2.853522	-0.654920	0.000002
1	-1.249699	-2.202538	-0.000014
6	-2.725738	0.725427	0.000012
1	-3.781511	-1.205971	-0.000001
1	3.444469	-1.530793	-0.000020
1	-3.444469	1.530793	0.000020

α-F[3]			
6	0.711135	1.864026	0.000086
6	-0.711135	1.864026	0.000085
6	-1.101438	0.551063	-0.000001
1	1.370062	2.718146	0.000089
1	-1.370061	2.718146	0.000088
8	0.000000	-0.262000	0.000013
6	1.101438	0.551063	0.000000
6	2.382502	-0.092784	-0.000004
6	2.776075	-1.403968	0.000299
8	3.480470	0.723242	-0.000031
6	4.205068	-1.393087	-0.000202
1	2.122639	-2.262151	0.000319
6	4.577638	-0.086512	-0.000123
1	4.864679	-2.247698	-0.000223
6	-2.382502	-0.092784	-0.000007
6	-2.776075	-1.403968	0.000285
8	-3.480471	0.723242	-0.000033
6	-4.205068	-1.393087	-0.000206
1	-2.122639	-2.262151	0.000298
1	-4.864679	-2.247698	-0.000225
6	-4.577638	-0.086512	-0.000112
1	-5.527891	0.421334	-0.000262
1	5.527891	0.421334	-0.000288

α-F[3]-cation			
6	0.692851	-1.846135	0.000005
6	-0.692851	-1.846135	0.000004
6	-1.096498	-0.502642	0.000000
1	1.356267	-2.697148	0.000008
1	-1.356267	-2.697148	0.000007
8	0.000000	0.308938	-0.000002
6	1.096498	-0.502642	0.000000
6	2.364387	0.094350	0.000000
6	2.799234	1.416051	-0.000001
8	3.448151	-0.745278	0.000007
6	4.203842	1.369951	-0.000004
1	2.167321	2.290733	-0.000003
6	4.545450	0.037078	0.000000
1	4.889084	2.203359	-0.000008
6	-2.364387	0.094350	-0.000002
6	-2.799234	1.416051	-0.000003
8	-3.448151	-0.745278	0.000004
6	-4.203842	1.369951	-0.000006
1	-2.167321	2.290733	-0.000004
1	-4.889084	2.203359	-0.000011
6	-4.545450	0.037078	-0.000002
1	-5.490757	-0.482394	-0.000002
1	5.490757	-0.482394	0.000000

α-F[4]			
6	-2.504803	-1.551418	0.000037
6	-1.085749	-1.600023	0.000037
6	-0.648870	-0.299286	0.000007
1	-3.191564	-2.383245	0.000050
1	-0.457486	-2.476884	0.000059
8	-1.722726	0.551192	-0.000001
6	-2.851797	-0.224034	0.000012
6	0.648870	0.299271	-0.000011

6	1.085745	1.600009	-0.000044
8	1.722731	-0.551205	0.000006
6	2.504799	1.551407	-0.000023
1	0.457479	2.476869	-0.000108
1	3.191560	2.383234	0.000002
6	4.106047	-0.461886	0.000013
6	2.851798	0.224023	0.000005
8	5.235276	0.313831	0.000008
6	4.453473	-1.788630	0.000006
1	3.767514	-2.621128	-0.000007
6	5.873604	-1.835808	0.000010
1	6.503647	-2.711431	0.000013
6	6.308271	-0.535990	0.000009
6	7.610313	0.062870	0.000009
6	8.049227	1.359858	0.000053
8	8.679455	-0.790830	-0.000059
6	9.476705	1.299269	0.000035
1	7.426168	2.240347	0.000126
6	9.803708	-0.019566	-0.000052
1	10.165550	2.130457	0.000049
1	10.735909	-0.559841	-0.000097
1	-3.863811	0.153098	0.000004

α-F[4]-cation

6	-2.500485	-1.553717	0.000011
6	-1.090932	-1.633329	0.000011
6	-0.627968	-0.329106	0.000008
1	-3.203837	-2.371795	0.000013
1	-0.481358	-2.523557	0.000012
8	-1.689465	0.537423	0.000008
6	-2.809036	-0.218208	0.000009
6	0.660263	0.243580	0.000007
6	1.091354	1.572196	0.000004
8	1.734107	-0.592770	0.000008
6	2.481846	1.540593	0.000004
1	0.448097	2.438143	0.000003
1	3.160160	2.379663	0.000002
6	4.099433	-0.444942	0.000006
6	2.855966	0.193917	0.000006
8	5.221293	0.341744	0.000003
6	4.473553	-1.791617	0.000008
1	3.795239	-2.630687	0.000010
6	5.864045	-1.823221	0.000007
1	6.507301	-2.689170	0.000009
6	6.295138	-0.494606	0.000004
6	7.583368	0.078078	0.000001
6	8.046342	1.382297	-0.000001
8	8.644863	-0.788459	0.000003
6	9.455893	1.302677	-0.000006
1	7.436773	2.272529	-0.000003
6	9.764441	-0.032833	0.000001
1	10.159248	2.120752	-0.000012
1	10.695062	-0.577373	0.000002
1	-3.739659	0.326329	0.000009

α-F[5]

6	-2.504803	-1.551418	0.000037
6	-1.085749	-1.600023	0.000037
6	-0.648870	-0.299286	0.000007
1	-3.191564	-2.383245	0.000050
1	-0.457486	-2.476884	0.000059
8	-1.722726	0.551192	-0.000001
6	-2.851797	-0.224034	0.000012
6	-4.106044	0.461879	0.000001
6	-4.453464	1.788625	-0.000008
8	-5.235281	-0.313834	-0.000001
6	-5.873595	1.835808	-0.000018
1	-3.767500	2.621119	-0.000006
6	-6.308269	0.535991	-0.000008
1	-6.503635	2.711432	-0.000026
6	0.648870	0.299271	-0.000011
6	1.085745	1.600009	-0.000044
8	1.722731	-0.551205	0.000006
6	2.504799	1.551407	-0.000023
1	0.457479	2.476869	-0.000108
1	3.191560	2.383234	0.000002
6	4.106047	-0.461886	0.000013
6	2.851798	0.224023	0.000005
8	5.235276	0.313831	0.000008
6	4.453473	-1.788630	0.000006
1	3.767514	-2.621128	-0.000007
6	5.873604	-1.835808	0.000010
1	6.503647	-2.711431	0.000013
6	6.308271	-0.535990	0.000009
6	7.610313	0.062870	0.000009
6	8.049227	1.359858	0.000053
8	8.679455	-0.790830	-0.000059
6	9.476705	1.299269	0.000035
1	7.426168	2.240347	0.000126
6	9.803708	-0.019566	-0.000052
1	10.165550	2.130457	0.000049
1	10.735909	-0.559841	-0.000097
1	-7.343447	0.228083	-0.000006

α-F[5]-cation

6	4.171768	1.763723	0.000004
6	2.775631	1.774022	0.000005
6	2.363068	0.444589	0.000001
1	4.840183	2.610174	0.000006
1	2.124241	2.634169	0.000008
8	3.462272	-0.376312	-0.000003
6	4.560046	0.427477	0.000000
6	5.834408	-0.188802	-0.000003
6	6.255351	-1.502673	-0.000007
8	6.920481	0.645583	-0.000002
6	7.670749	-1.466179	-0.000007
1	5.619298	-2.374107	-0.000009
6	8.019410	-0.143735	-0.000005
1	8.347946	-2.306063	-0.000008
6	1.099662	-0.163560	-0.000001
6	0.695753	-1.500382	-0.000005
8	0.000001	0.648697	0.000003
6	-0.695749	-1.500382	-0.000004
1	1.355418	-2.353937	-0.000009
1	-1.355415	-2.353937	-0.000006
6	-2.363066	0.444587	0.000003
6	-1.099659	-0.163560	0.000001
8	-3.462270	-0.376314	0.000000
6	-2.775631	1.774019	0.000008

1	-2.124242	2.634168	0.000011
6	-4.171768	1.763720	0.000009
1	-4.840183	2.610170	0.000013
6	-4.560046	0.427474	0.000003
6	-5.834407	-0.188805	0.000001
6	-6.255357	-1.502675	-0.000005
8	-6.920480	0.645584	0.000006
6	-7.670753	-1.466175	-0.000006
1	-5.619306	-2.374111	-0.000009
6	-8.019414	-0.143730	0.000002
1	-8.347951	-2.306059	-0.000011
1	-8.964954	0.373957	0.000005
1	8.964950	0.373954	-0.000004

α-F[6]

6	-2.504803	-1.551418	0.000037
6	-1.085749	-1.600023	0.000037
6	-0.648870	-0.299286	0.000007
1	-3.191564	-2.383245	0.000050
1	-0.457486	-2.476884	0.000059
8	-1.722726	0.551192	-0.000001
6	-2.851797	-0.224034	0.000012
6	-4.106044	0.461879	0.000001
6	-4.453464	1.788625	-0.000008
8	-5.235281	-0.313834	-0.000001
6	-5.873595	1.835808	-0.000018
1	-3.767500	2.621119	-0.000006
6	-6.308269	0.535991	-0.000008
1	-6.503635	2.711432	-0.000026
6	0.648870	0.299271	-0.000011
6	1.085745	1.600009	-0.000044
8	1.722731	-0.551205	0.000006
6	2.504799	1.551407	-0.000023
1	0.457479	2.476869	-0.000108
1	3.191560	2.383234	0.000002
6	4.106047	-0.461886	0.000013
6	2.851798	0.224023	0.000005
8	5.235276	0.313831	0.000008
6	4.453473	-1.788630	0.000006
1	3.767514	-2.621128	-0.000007
6	5.873604	-1.835808	0.000010
1	6.503647	-2.711431	0.000013
6	6.308271	-0.535990	0.000009
6	-7.610315	-0.062861	-0.000011
6	-8.049238	-1.359847	-0.000032
8	-8.679449	0.790845	0.000031
6	-9.476715	-1.299249	-0.000033
1	-7.426184	-2.240340	-0.000085
6	-9.803708	0.019588	0.000029
1	-10.165566	-2.130432	-0.000043
1	-10.735905	0.559870	0.000052
6	7.610313	0.062870	0.000009
6	8.049227	1.359858	0.000053
8	8.679455	-0.790830	-0.000059
6	9.476705	1.299269	0.000035
1	7.426168	2.240347	0.000126
6	9.803708	-0.019566	-0.000052
1	10.165550	2.130457	0.000049
1	10.735909	-0.559841	-0.000097

α-F[6]-cation

6	-2.487831	1.549774	0.000002
6	-1.094080	1.600825	0.000002
6	-0.642010	0.283175	0.000001
1	-3.178400	2.378331	0.000003
1	-0.467378	2.478957	0.000002
8	-1.713689	-0.569663	0.000000
6	-2.840510	0.201647	0.000002
6	-4.084883	-0.454426	0.000002
6	-4.451635	-1.792536	0.000001
8	-5.210610	0.330161	0.000003
6	-5.851824	-1.828448	0.000001
1	-3.772964	-2.631303	0.000000
6	-6.281871	-0.509240	0.000003
1	-6.491417	-2.696782	0.000001
6	0.642010	-0.283175	0.000000
6	1.094080	-1.600824	-0.000002
8	1.713689	0.569663	-0.000001
6	2.487831	-1.549774	-0.000001
1	0.467377	-2.478957	-0.000003
1	3.178400	-2.378331	-0.000001
6	4.084883	0.454426	-0.000003
6	2.840510	-0.201647	-0.000002
8	5.210610	-0.330161	-0.000003
6	4.451635	1.792535	-0.000003
1	3.772964	2.631303	-0.000003
6	5.851824	1.828448	-0.000003
1	6.491417	2.696782	-0.000002
6	6.281871	0.509239	-0.000004
6	-7.577507	0.070670	0.000004
6	-8.036086	1.369063	0.000005
8	-8.637306	-0.796038	0.000004
6	-9.452467	1.290390	0.000009
1	-7.426310	2.259025	0.000006
6	-9.761433	-0.039838	0.000005
1	-10.153804	2.110270	0.000012
1	-10.690219	-0.586723	0.000004
6	7.577507	-0.070671	-0.000004
6	8.036086	-1.369063	-0.000004
8	8.637306	0.796039	-0.000003
6	9.452467	-1.290390	-0.000007
1	7.426310	-2.259025	-0.000004
6	9.761432	0.039838	-0.000004
1	10.153804	-2.110270	-0.000009
1	10.690219	0.586723	-0.000003

α-F7

6	0.709771	-1.729249	0.000017
6	-0.709771	-1.729249	0.000017
6	-1.102078	-0.414220	0.000020
1	1.367686	-2.584074	0.000016
1	-1.367686	-2.584074	0.000015
8	0.000000	0.399235	0.000022
6	1.102078	-0.414220	0.000020
6	2.379019	0.227184	0.000020
6	2.772868	1.541611	0.000021
8	3.480342	-0.587467	0.000013
6	4.192695	1.539826	0.000017
1	2.116085	2.397325	0.000026

6	4.583229	0.224478	0.000012
1	4.851703	2.393806	0.000018
6	-2.379019	0.227184	0.000019
6	-2.772868	1.541611	0.000021
8	-3.480342	-0.587467	0.000013
6	-4.192695	1.539826	0.000017
1	-2.116085	2.397325	0.000026
1	-4.851703	2.393806	0.000018
6	-5.859285	-0.419913	0.000006
6	-4.583229	0.224478	0.000012
8	-6.962618	0.392243	-0.000002
6	-6.249796	-1.734678	0.000004
1	-5.591354	-2.589111	0.000010
6	-7.670658	-1.735462	-0.000004
1	-8.328954	-2.590041	-0.000006
6	-8.062692	-0.422160	-0.000007
6	5.859285	-0.419913	0.000006
6	6.249796	-1.734678	0.000005
8	6.962618	0.392243	-0.000001
6	7.670658	-1.735462	-0.000003
1	5.591354	-2.589111	0.000010
6	8.062692	-0.422160	-0.000006
1	8.328954	-2.590041	-0.000006
6	-9.344615	0.218598	-0.000016
6	-9.741286	1.529100	-0.000020
8	-10.440810	-0.600025	-0.000024
6	-11.169963	1.514820	-0.000032
1	-9.090022	2.388935	-0.000013
6	-11.539497	0.207224	-0.000034
1	-11.831542	2.367868	-0.000039
1	-12.488693	-0.302603	-0.000041
6	9.344615	0.218598	-0.000015
6	9.741286	1.529100	-0.000020
8	10.440810	-0.600025	-0.000024
6	11.169963	1.514820	-0.000032
1	9.090022	2.388935	-0.000013
6	11.539497	0.207224	-0.000034
1	11.831542	2.367868	-0.000039
1	12.488693	-0.302603	-0.000041

α-F[7]-cation

6	0.698125	-1.725071	0.000003
6	-0.698125	-1.725071	0.000003
6	-1.100299	-0.392810	0.000000
1	1.356931	-2.579223	0.000006
1	-1.356932	-2.579222	0.000006
8	0.000000	0.420049	-0.000003
6	1.100299	-0.392810	0.000000
6	2.366391	0.219388	-0.000002
6	2.775992	1.547132	-0.000006
8	3.465013	-0.600061	0.000000
6	4.174103	1.539641	-0.000003
1	2.122983	2.405923	-0.000009
6	4.566690	0.205681	-0.000002
1	4.838403	2.389295	-0.000004
6	-2.366391	0.219389	-0.000002
6	-2.775992	1.547133	-0.000006
8	-3.465013	-0.600061	0.000000
6	-4.174103	1.539641	-0.000004
1	-2.122984	2.405924	-0.000009
1	-4.838404	2.389295	-0.000004
6	-5.833202	-0.415390	0.000000
6	-4.566690	0.205681	-0.000002
8	-6.933679	0.404010	-0.000001
6	-6.239658	-1.738627	0.000002
1	-5.587682	-2.598279	0.000004
6	-7.643699	-1.730941	0.000004
1	-8.309543	-2.579264	0.000007
6	-8.031276	-0.401800	0.000001
6	5.833203	-0.415390	0.000000
6	6.239658	-1.738626	0.000003
8	6.933679	0.404010	-0.000001
6	7.643699	-1.730941	0.000004
1	5.587683	-2.598279	0.000004
6	8.031276	-0.401800	0.000001
1	8.309543	-2.579264	0.000007
6	-9.309202	0.222387	0.000000
6	-9.723404	1.533771	0.000000
8	-10.396713	-0.608693	0.000004
6	-11.143502	1.502471	-0.000002
1	-9.084209	2.402808	-0.000001
6	-11.496613	0.184628	0.000001
1	-11.816724	2.345651	-0.000005
1	-12.442493	-0.331923	0.000002
6	9.309202	0.222388	0.000001
6	9.723404	1.533771	0.000000
8	10.396713	-0.608693	0.000005
6	11.143503	1.502471	-0.000002
1	9.084210	2.402808	-0.000001
6	11.496613	0.184627	0.000002
1	11.816725	2.345650	-0.000004
1	12.442493	-0.331924	0.000003

α-F[8]

6	-0.997359	1.656635	0.000000
6	-0.358462	2.924306	0.000000
6	0.992466	2.682809	0.000000
1	-2.056886	1.454138	0.000000
1	-0.825890	3.896449	0.000000
8	1.222722	1.332656	0.000000
6	0.000408	0.714395	0.000000
6	-0.000408	-0.714395	0.000000
6	0.997359	-1.656635	0.000000
8	-1.222722	-1.332656	0.000000
6	0.358462	-2.924306	0.000000
1	2.056886	-1.454138	0.000000
6	-0.992466	-2.682809	0.000000
1	0.825890	-3.896449	0.000000
6	2.140622	3.533490	0.000000
6	3.491483	3.292707	0.000000
8	1.909820	4.883741	0.000000
6	4.129800	4.560960	0.000000
1	3.959526	2.320842	0.000000
1	5.189181	4.764151	0.000000
6	3.131592	6.931874	0.000000
6	3.131592	5.502410	0.000000
8	4.354195	7.550009	0.000000
6	2.134648	7.873793	0.000000
1	1.074946	7.672168	0.000000
6	2.775317	9.142109	0.000000

1	2.309641	10.115135	0.000000
6	4.124181	8.899186	0.000000
6	-2.140622	-3.533490	0.000000
6	-3.491483	-3.292707	0.000000
8	-1.909820	-4.883741	0.000000
6	-4.129800	-4.560960	0.000000
1	-3.959526	-2.320842	0.000000
6	-3.131592	-5.502410	0.000000
1	-5.189181	-4.764151	0.000000
6	5.275357	9.752834	0.000000
6	6.623574	9.514096	0.000000
8	5.040910	11.100686	0.000000
6	7.256876	10.794820	0.000000
1	7.096151	8.544505	0.000000
6	6.257695	11.715712	0.000000
1	8.316909	10.999022	0.000000
1	6.232066	12.792858	0.000000
6	-3.131592	-6.931874	0.000000
6	-2.134648	-7.873793	0.000000
8	-4.354195	-7.550009	0.000000
6	-2.775317	-9.142109	0.000000
1	-1.074946	-7.672168	0.000000
6	-4.124181	-8.899186	0.000000
1	-2.309641	-10.115135	0.000000
6	-5.275357	-9.752834	0.000000
6	-6.623574	-9.514096	0.000000
8	-5.040910	-11.100686	0.000000
6	-7.256876	-10.794820	0.000000
1	-7.096151	-8.544505	0.000000
6	-6.257695	-11.715712	0.000000
1	-8.316909	-10.999022	0.000000
1	-6.232066	-12.792858	0.000000

1	2.205899	10.114136	0.000000
6	4.034225	8.902269	0.000000
6	-2.090368	-3.542275	0.000000
6	-3.459478	-3.323127	0.000000
8	-1.840535	-4.890112	0.000000
6	-4.071846	-4.583420	0.000000
1	-3.941980	-2.358182	0.000000
6	-3.049945	-5.522596	0.000000
1	-5.127611	-4.803580	0.000000
6	5.163360	9.770197	0.000000
6	6.520810	9.557383	0.000000
8	4.903009	11.113609	0.000000
6	7.125641	10.844129	0.000000
1	7.014435	8.598184	0.000000
6	6.103615	11.746544	0.000000
1	8.180512	11.071106	0.000000
1	6.061178	12.823379	0.000000
6	-3.049945	-6.936178	0.000000
6	-2.044060	-7.883732	0.000000
8	-4.271249	-7.560748	0.000000
6	-2.672965	-9.142123	0.000000
1	-0.984684	-7.679382	0.000000
6	-4.034225	-8.902269	0.000000
1	-2.205899	-10.114136	0.000000
6	-5.163360	-9.770197	0.000000
6	-6.520810	-9.557383	0.000000
8	-4.903009	-11.113609	0.000000
6	-7.125641	-10.844129	0.000000
1	-7.014435	-8.598184	0.000000
6	-6.103615	-11.746544	0.000000
1	-8.180512	-11.071106	0.000000
1	-6.061178	-12.823379	0.000000

α-F[8]-cation

6	-1.011930	1.652422	0.000000
6	-0.393152	2.906982	0.000000
6	0.977345	2.677610	0.000000
1	-2.069685	1.440571	0.000000
1	-0.867646	3.875615	0.000000
8	1.219469	1.332226	0.000000
6	0.002946	0.704072	0.000000
6	-0.002946	-0.704072	0.000000
6	1.011930	-1.652422	0.000000
8	-1.219469	-1.332226	0.000000
6	0.393152	-2.906982	0.000000
1	2.069685	-1.440571	0.000000
6	-0.977345	-2.677610	0.000000
1	0.867646	-3.875615	0.000000
6	2.090368	3.542275	0.000000
6	3.459478	3.323127	0.000000
8	1.840535	4.890112	0.000000
6	4.071846	4.583420	0.000000
1	3.941980	2.358182	0.000000
1	5.127611	4.803580	0.000000
6	3.049945	6.936178	0.000000
6	3.049945	5.522596	0.000000
8	4.271249	7.560748	0.000000
6	2.044060	7.883732	0.000000
1	0.984684	7.679382	0.000000
6	2.672965	9.142123	0.000000

α-F[12]

6	19.884073	-1.448187	-0.000096
6	18.455584	-1.474427	-0.000116
6	18.047981	-0.167279	0.000019
1	20.552765	-2.295666	-0.000179
1	17.811560	-2.339701	-0.000216
8	19.137283	0.660485	0.000120
6	20.242643	-0.137538	0.000049
6	16.760789	0.462821	0.000071
6	16.357986	1.772902	0.000206
8	15.667496	-0.360584	-0.000027
6	14.937211	1.760402	0.000190
1	17.009232	2.632859	0.000303
1	14.271787	2.609410	0.000273
6	13.286854	-0.212406	-0.000033
6	14.557532	0.442487	0.000047
8	12.177318	0.590291	0.000042
6	12.907327	-1.531017	-0.000174
1	13.573434	-2.379461	-0.000258
6	11.487621	-1.544650	-0.000187
1	10.838056	-2.405862	-0.000282
6	11.082819	-0.233547	-0.000053
6	9.800627	0.397207	0.000003
6	9.397538	1.709103	0.000133
8	8.705397	-0.425222	-0.000087
6	7.978162	1.697412	0.000124
1	10.048410	2.569288	0.000224

6	7.596621	0.379183	-0.000010
1	7.313324	2.546874	0.000207
6	6.325295	-0.272893	-0.000080
6	5.943259	-1.591096	-0.000212
8	5.216929	0.531815	-0.000004
6	4.523895	-1.602221	-0.000216
1	6.607794	-2.440780	-0.000294
6	4.121231	-0.290198	-0.000088
1	3.872802	-2.462261	-0.000303
6	2.839881	0.341918	-0.000029
6	2.437777	1.654161	0.000096
8	1.743915	-0.479641	-0.000105
6	1.018460	1.643616	0.000096
1	3.089266	2.513890	0.000176
6	0.635859	0.325596	-0.000028
1	0.354294	2.493594	0.000176
6	-0.635859	-0.325636	-0.000085
6	-1.018462	-1.643655	-0.000204
8	-1.743914	0.479603	-0.000008
6	-2.437779	-1.654199	-0.000200
1	-0.354297	-2.493634	-0.000284
6	-2.839881	-0.341955	-0.000079
1	-3.089269	-2.513926	-0.000276
6	-4.121230	0.290163	-0.000016
6	-4.523890	1.602188	0.000101
8	-5.216931	-0.531845	-0.000080
6	-5.943254	1.591068	0.000109
1	-3.872794	2.462226	0.000171
6	-6.325294	0.272866	-0.000002
1	-6.607786	2.440753	0.000188
6	-7.596622	-0.379205	-0.000047
6	-7.978170	-1.697432	-0.000155
8	-8.705395	0.425206	0.000030
6	-9.397547	-1.709116	-0.000142
1	-7.313337	-2.546898	-0.000232
6	-9.800629	-0.397218	-0.000029
1	-10.048422	-2.569298	-0.000209
6	-11.082817	0.233543	0.000035
6	-11.487611	1.544649	0.000144
8	-12.177321	-0.590288	-0.000019
6	-12.907317	1.531025	0.000158
1	-10.838040	2.405857	0.000206
6	-13.286852	0.212417	0.000058
1	-13.573418	2.379474	0.000234
6	-14.557535	-0.442467	0.000021
6	-14.937223	-1.760379	-0.000077
8	-15.667493	0.360611	0.000095
6	-16.357998	-1.772869	-0.000061
1	-14.271806	-2.609393	-0.000150
6	-16.760791	-0.462785	0.000044
1	-17.009251	-2.632821	-0.000120
6	-18.047979	0.167324	0.000107
6	-18.455573	1.474475	0.000210
8	-19.137287	-0.660433	0.000057
6	-19.884063	1.448244	0.000224
1	-17.811544	2.339745	0.000268
6	-20.242641	0.137597	0.000130
1	-20.552750	2.295727	0.000296
1	-21.187557	-0.380120	0.000103
1	21.187555	0.380185	0.000115

α-F[12]-cation

6	19.846231	-1.442152	-0.000158
6	18.422079	-1.477274	-0.000162
6	18.005704	-0.170103	-0.000044
1	20.520965	-2.284356	-0.000233
1	17.784660	-2.347519	-0.000241
8	19.089937	0.664267	0.000032
6	20.195907	-0.126337	-0.000040
6	16.720415	0.452087	0.000012
6	16.321023	1.770427	0.000133
8	15.628368	-0.366065	-0.000062
6	14.908683	1.763038	0.000131
1	16.976628	2.626731	0.000211
1	14.247445	2.615459	0.000209
6	13.254510	-0.201955	-0.000044
6	14.520518	0.441536	0.000013
8	12.145718	0.595857	0.000030
6	12.876085	-1.530732	-0.000165
1	13.545899	-2.375961	-0.000243
6	11.467703	-1.548605	-0.000165
1	10.821694	-2.412614	-0.000244
6	11.053443	-0.231976	-0.000044
6	9.777013	0.384145	0.000014
6	9.372116	1.706511	0.000136
8	8.682669	-0.434986	-0.000059
6	7.965449	1.697533	0.000138
1	10.025421	2.564643	0.000214
6	7.575750	0.371920	0.000017
1	7.302789	2.548772	0.000218
6	6.310282	-0.264107	-0.000039
6	5.924497	-1.592395	-0.000161
8	5.203213	0.538878	0.000038
6	4.518420	-1.604449	-0.000159
1	6.590126	-2.441086	-0.000240
6	4.109038	-0.284038	-0.000036
1	3.868321	-2.465263	-0.000238
6	2.834090	0.332199	0.000024
6	2.427417	1.654101	0.000148
8	1.739280	-0.488236	-0.000050
6	1.021526	1.644348	0.000150
1	3.079480	2.513317	0.000226
6	0.632907	0.317326	0.000028
1	0.357901	2.494721	0.000231
6	-0.632906	-0.317350	-0.000028
6	-1.021527	-1.644371	-0.000150
8	-1.739278	0.488214	0.000050
6	-2.427419	-1.654122	-0.000147
1	-0.357903	-2.494745	-0.000231
6	-2.834090	-0.332219	-0.000024
1	-3.079482	-2.513337	-0.000225
6	-4.109037	0.284019	0.000036
6	-4.518417	1.604431	0.000159
8	-5.203213	-0.538895	-0.000038
6	-5.924494	1.592379	0.000161
1	-3.868316	2.465244	0.000237
6	-6.310280	0.264091	0.000039
1	-6.590122	2.441071	0.000241
6	-7.575750	-0.371933	-0.000017
6	-7.965453	-1.697544	-0.000138
8	-8.682666	0.434977	0.000060

6	-9.372121	-1.706518	-0.000137
1	-7.302797	-2.548786	-0.000218
6	-9.777013	-0.384150	-0.000014
1	-10.025428	-2.564648	-0.000216
6	-11.053440	0.231975	0.000045
6	-11.467695	1.548607	0.000166
8	-12.145719	-0.595853	-0.000031
6	-12.876076	1.530739	0.000167
1	-10.821682	2.412612	0.000245
6	-13.254508	0.201964	0.000044
1	-13.545887	2.375971	0.000247
6	-14.520518	-0.441522	-0.000014
6	-14.908689	-1.763022	-0.000135
8	-15.628367	0.366082	0.000062
6	-16.321029	-1.770407	-0.000136
1	-14.247455	-2.615446	-0.000214
6	-16.720419	-0.452067	-0.000013
1	-16.976636	-2.626709	-0.000215
6	-18.005703	0.170128	0.000044
6	-18.422080	1.477298	0.000163
8	-19.089944	-0.664242	-0.000035
6	-19.846228	1.442180	0.000164
1	-17.784657	2.347542	0.000244
6	-20.195914	0.126366	0.000038
1	-20.520955	2.284389	0.000244
1	-21.138978	-0.394922	-0.000012
1	21.138967	0.394958	0.000007

α-F[16]

6	-12.899599	1.586335	-0.000155
6	-11.480202	1.593272	-0.000160
6	-11.081401	0.280083	-0.000044
1	-13.561622	2.437976	-0.000229
1	-10.826600	2.451411	-0.000239
8	-12.179524	-0.538695	0.000033
6	-13.285506	0.269243	-0.000036
6	-14.558665	-0.379252	0.000026
6	-14.943763	-1.696446	0.000144
8	-15.665259	0.428160	-0.000041
6	-16.363150	-1.704303	0.000150
1	-14.281226	-2.547704	0.000216
6	-16.762687	-0.391316	0.000036
1	-17.016349	-2.562719	0.000229
6	-9.802055	-0.356074	0.000010
6	-9.404433	-1.669695	0.000127
8	-8.703342	0.461766	-0.000066
6	-7.985122	-1.663978	0.000123
1	-10.058859	-2.527184	0.000205
1	-7.323859	-2.516218	0.000199
6	-6.323978	0.299356	-0.000055
6	-7.598044	-0.347271	0.000005
8	-5.219045	-0.510075	0.000018
6	-5.936342	1.615938	-0.000174
1	-6.597230	2.468464	-0.000251
6	-4.516991	1.621024	-0.000176
1	-3.862251	2.478285	-0.000254
6	-4.119920	0.307268	-0.000057
6	-18.043235	0.242761	-0.000014
6	-18.444739	1.554871	-0.000127
8	-19.139804	-0.578323	0.000065
6	-19.864475	1.544814	-0.000119
1	-17.793017	2.414453	-0.000207
6	-20.247313	0.227151	0.000000
1	-20.528445	2.394931	-0.000191
6	-2.841226	-0.330178	0.000000
6	-2.444564	-1.644076	0.000120
8	-1.741888	0.486843	-0.000074
6	-1.025239	-1.639415	0.000120
1	-3.099588	-2.501114	0.000198
6	-0.637202	-0.322966	0.000000
1	-0.364610	-2.492142	0.000198
6	-21.519618	-0.424581	0.000064
6	-21.902544	-1.741558	0.000182
8	-22.627596	0.381228	0.000001
6	-23.323341	-1.750550	0.000192
1	-21.239222	-2.592210	0.000252
6	-23.722907	-0.439478	0.000080
1	-23.976708	-2.608895	0.000272
6	-25.008552	0.193771	0.000034
6	-25.412961	1.501907	-0.000078
8	-26.099868	-0.631333	0.000115
6	-26.841508	1.479159	-0.000065
1	-24.766828	2.365608	-0.000159
6	-27.203274	0.169383	0.000053
1	-27.508131	2.328265	-0.000135
1	-28.149447	-0.346033	0.000106
6	0.637202	0.322991	-0.000058
6	1.025240	1.639440	-0.000178
8	1.741888	-0.486819	0.000018
6	2.444565	1.644100	-0.000177
1	0.364611	2.492167	-0.000258
6	2.841226	0.330203	-0.000056
1	3.099589	2.501138	-0.000255
6	4.119920	-0.307245	0.000005
6	4.516989	-1.621001	0.000127
8	5.219046	0.510097	-0.000069
6	5.936341	-1.615917	0.000129
1	3.862248	-2.478261	0.000205
6	6.323978	-0.299335	0.000008
1	6.597227	-2.468443	0.000209
6	7.598045	0.347290	-0.000049
6	7.985125	1.663996	-0.000171
8	8.703342	-0.461749	0.000029
6	9.404437	1.669711	-0.000168
1	7.323864	2.516237	-0.000252
6	9.802056	0.356088	-0.000045
1	10.058863	2.527199	-0.000246
6	11.081400	-0.280071	0.000017
6	11.480198	-1.593261	0.000141
8	12.179525	0.538704	-0.000056
6	12.899595	-1.586328	0.000144
1	10.826593	-2.451398	0.000220
6	13.285505	-0.269237	0.000022
1	13.561616	-2.437970	0.000226
6	14.558666	0.379255	-0.000035
6	14.943768	1.696448	-0.000157
8	15.665258	-0.428160	0.000044
6	16.363155	1.704301	-0.000154
1	14.281233	2.547708	-0.000239
6	16.762688	0.391313	-0.000030
1	17.016357	2.562715	-0.000233

6	18.043234	-0.242768	0.000032
6	18.444734	-1.554879	0.000156
8	19.139806	0.578312	-0.000042
6	19.864470	-1.544828	0.000159
1	17.793009	-2.414459	0.000235
6	20.247312	-0.227166	0.000036
1	20.528436	-2.394947	0.000240
6	21.519619	0.424561	-0.000022
6	21.902550	1.741537	-0.000144
8	22.627594	-0.381252	0.000056
6	23.323347	1.750524	-0.000142
1	21.239231	2.592191	-0.000225
6	23.722909	0.439450	-0.000019
1	23.976717	2.608866	-0.000221
6	25.008552	-0.193803	0.000042
6	25.412955	-1.501941	0.000164
8	26.099870	0.631297	-0.000034
6	26.841502	-1.479198	0.000164
1	24.766819	-2.365639	0.000244
6	27.203273	-0.169424	0.000042
1	27.508122	-2.328307	0.000244
1	28.149448	0.345989	-0.000005

α-F[16]-cation

6	-12.873176	1.587954	-0.000150
6	-11.463212	1.595678	-0.000151
6	-11.059706	0.276703	-0.000030
1	-13.536056	2.438792	-0.000228
1	-10.810486	2.454478	-0.000230
8	-12.156445	-0.542847	0.000045
6	-13.261492	0.263678	-0.000029
6	-14.530370	-0.373529	0.000030
6	-14.921141	-1.695988	0.000151
8	-15.635507	0.435605	-0.000044
6	-16.331320	-1.702040	0.000153
1	-14.260156	-2.548490	0.000228
6	-16.732156	-0.381523	0.000032
1	-16.986221	-2.558971	0.000232
6	-9.784731	-0.348423	0.000027
6	-9.384285	-1.668777	0.000148
8	-8.686963	0.468448	-0.000049
6	-7.974248	-1.663602	0.000149
1	-10.039134	-2.525842	0.000226
1	-7.313585	-2.516271	0.000229
6	-6.313037	0.294728	-0.000032
6	-7.583114	-0.340946	0.000026
8	-5.209362	-0.514359	0.000044
6	-5.922102	1.617561	-0.000155
1	-6.582867	2.470100	-0.000235
6	-4.511789	1.622507	-0.000153
1	-3.857241	2.479861	-0.000231
6	-4.111434	0.302724	-0.000031
6	-18.008615	0.241817	-0.000023
6	-18.417143	1.557823	-0.000144
8	-19.103305	-0.582393	0.000053
6	-19.828637	1.544396	-0.000138
1	-17.768203	2.419588	-0.000224
6	-20.210362	0.219276	-0.000018
1	-20.495486	2.392008	-0.000213
6	-2.836845	-0.324475	0.000027
6	-2.437199	-1.644480	0.000149
8	-1.738597	0.492027	-0.000048
6	-1.026757	-1.640080	0.000149
1	-3.092198	-2.501467	0.000227
6	-0.635305	-0.317708	0.000028
1	-0.366488	-2.493023	0.000229
6	-21.479160	-0.424417	0.000042
6	-21.868041	-1.743953	0.000161
8	-22.585587	0.384595	-0.000028
6	-23.282719	-1.749387	0.000165
1	-21.207725	-2.597044	0.000236
6	-23.679840	-0.432383	0.000048
1	-23.939169	-2.605102	0.000244
6	-24.964254	0.195004	-0.000004
6	-25.375172	1.503046	-0.000119
8	-26.051655	-0.635122	0.000075
6	-26.800603	1.473591	-0.000112
1	-24.734016	2.370516	-0.000199
6	-27.155642	0.160000	0.000008
1	-27.471767	2.318742	-0.000185
1	-28.100376	-0.358171	0.000057
6	0.635305	0.317711	-0.000029
6	1.026757	1.640083	-0.000151
8	1.738597	-0.492024	0.000046
6	2.437199	1.644483	-0.000149
1	0.366488	2.493026	-0.000230
6	2.836845	0.324478	-0.000028
1	3.092198	2.501470	-0.000227
6	4.111434	-0.302721	0.000030
6	4.511789	-1.622504	0.000151
8	5.209362	0.514362	-0.000044
6	5.922102	-1.617558	0.000152
1	3.857241	-2.479859	0.000229
6	6.313037	-0.294726	0.000031
1	6.582867	-2.470098	0.000230
6	7.583114	0.340948	-0.000026
6	7.974248	1.663604	-0.000147
8	8.686963	-0.468446	0.000049
6	9.384286	1.668779	-0.000148
1	7.313585	2.516273	-0.000225
6	9.784731	0.348425	-0.000026
1	10.039135	2.525844	-0.000227
6	11.059706	-0.276701	0.000031
6	11.463212	-1.595677	0.000152
8	12.156445	0.542848	-0.000045
6	12.873176	-1.587953	0.000152
1	10.810485	-2.454477	0.000231
6	13.261492	-0.263677	0.000030
1	13.536055	-2.438791	0.000230
6	14.530370	0.373530	-0.000029
6	14.921141	1.695988	-0.000151
8	15.635507	-0.435605	0.000044
6	16.331320	1.702039	-0.000152
1	14.260157	2.548490	-0.000230
6	16.732156	0.381523	-0.000032
1	16.986222	2.558971	-0.000231
6	18.008615	-0.241817	0.000023
6	18.417142	-1.557824	0.000143
8	19.103305	0.582392	-0.000053
6	19.828636	-1.544397	0.000139
1	17.768202	-2.419589	0.000223

6	20.210362	-0.219277	0.000018
1	20.495485	-2.392010	0.000215
6	21.479160	0.424415	-0.000042
6	21.868042	1.743950	-0.000162
8	22.585586	-0.384598	0.000028
6	23.282720	1.749384	-0.000166
1	21.207726	2.597042	-0.000238
6	23.679841	0.432380	-0.000048
1	23.939170	2.605099	-0.000244
6	24.964254	-0.195008	0.000004
6	25.375171	-1.503050	0.000121
8	26.051655	0.635118	-0.000073
6	26.800602	-1.473595	0.000109
1	24.734015	-2.370519	0.000201
6	27.155642	-0.160004	-0.000005
1	27.471766	-2.318747	0.000179
1	28.100377	0.358166	-0.000053

α-F[24]

6	41.101117	-0.756060	0.000180
6	40.809459	0.571048	0.000161
8	39.956736	-1.497021	0.000168
6	39.384144	0.669708	0.000135
1	41.520252	1.383527	0.000165
6	38.910776	-0.615095	0.000140
1	38.784849	1.566537	0.000114
6	37.593293	-1.179138	0.000122
6	37.124439	-2.467086	0.000128
8	36.543191	-0.301280	0.000093
6	35.706139	-2.382349	0.000102
1	37.731092	-3.359062	0.000149
6	35.393907	-1.046893	0.000082
1	34.998490	-3.196490	0.000099
6	34.157977	-0.328548	0.000053
6	33.844879	1.007358	0.000031
8	33.009695	-1.074621	0.000044
6	32.427562	1.092058	0.000008
1	34.552508	1.821490	0.000032
6	31.957665	-0.197158	0.000016
1	31.821981	1.984750	-0.000013
6	30.646073	-0.764264	0.000004
6	30.180264	-2.055255	0.000013
8	29.591749	0.110044	-0.000021
6	28.763198	-1.975129	-0.000007
1	30.788960	-2.945773	0.000032
6	28.445607	-0.640097	-0.000026
1	28.058199	-2.791554	-0.000006
6	27.206255	0.070904	-0.000049
6	26.884331	1.405031	-0.000068
8	26.062542	-0.682520	-0.000050
6	25.466767	1.480538	-0.000083
1	27.586556	2.223845	-0.000071
6	25.005040	0.188116	-0.000070
1	24.855473	2.369322	-0.000099
6	23.697574	-0.388052	-0.000074
6	23.241873	-1.682707	-0.000063
8	22.636434	0.478079	-0.000090
6	21.824409	-1.613719	-0.000072
1	23.857542	-2.568417	-0.000049
6	21.496354	-0.281124	-0.000089
1	21.125768	-2.435574	-0.000066
6	20.250753	0.418798	-0.000102
6	19.915759	1.749707	-0.000118
8	19.114415	-0.345736	-0.000097
6	18.497486	1.811330	-0.000121
1	20.609868	2.575424	-0.000125
6	18.048446	0.514409	-0.000108
1	17.877556	2.694113	-0.000131
6	16.747154	-0.075546	-0.000103
6	16.306293	-1.375322	-0.000092
8	15.676243	0.778505	-0.000108
6	14.888231	-1.322560	-0.000090
1	16.932083	-2.253909	-0.000085
6	14.544984	0.006235	-0.000100
1	14.198970	-2.152288	-0.000083
6	-1.034831	2.239885	-0.000004
6	-2.454539	2.236367	0.000009
6	-2.843675	0.920242	0.000014
1	-0.379369	3.096622	-0.000011
1	-3.114233	3.089848	0.000014
8	-1.739428	0.109986	0.000004
6	-0.639192	0.925698	-0.000007
6	0.636172	0.281609	-0.000018
6	1.020494	-1.035946	-0.000020
8	1.742860	1.088742	-0.000030
6	2.439407	-1.044572	-0.000033
1	0.357278	-1.886628	-0.000012
6	2.839685	0.268241	-0.000039
1	3.092245	-1.903244	-0.000038
6	-4.115876	0.269925	0.000026
6	-4.493871	-1.049452	0.000029
8	-5.226430	1.071719	0.000035
6	-5.912739	-1.064908	0.000042
1	-3.826582	-1.896943	0.000023
1	-6.561437	-1.926714	0.000048
6	-7.605264	0.868656	0.000055
6	-6.319316	0.245973	0.000045
8	-8.691921	0.034891	0.000061
6	-8.022497	2.176159	0.000061
1	-7.381232	3.043572	0.000059
6	-9.441926	2.149214	0.000070
1	-10.115615	2.991687	0.000076
6	-9.809326	0.826870	0.000069
6	4.122742	0.896865	-0.000051
6	4.534184	2.206201	-0.000058
8	5.213084	0.067948	-0.000057
6	5.953739	2.185553	-0.000068
1	3.889093	3.070774	-0.000055
6	6.326992	0.864848	-0.000068
1	6.623675	3.031016	-0.000076
6	-11.070936	0.156235	0.000074
6	-11.428401	-1.168826	0.000070
8	-12.193832	0.940620	0.000082
6	-12.846914	-1.206363	0.000075
1	-10.748054	-2.005874	0.000063
6	-13.273810	0.098058	0.000083
1	-13.482108	-2.078173	0.000074
6	7.591360	0.199430	-0.000074
6	7.953845	-1.124274	-0.000072
8	8.711253	0.988109	-0.000083
6	9.372455	-1.156415	-0.000081

1	7.276661	-1.963880	-0.000066
6	9.794393	0.149614	-0.000087
1	10.010971	-2.025792	-0.000083
6	11.087424	0.757460	-0.000096
6	11.519413	2.060167	-0.000104
8	12.164590	-0.088558	-0.000096
6	12.938429	2.017157	-0.000108
1	10.887990	2.934769	-0.000107
6	13.290855	0.690755	-0.000103
1	13.621609	2.851948	-0.000114
6	-14.568895	0.701506	0.000090
6	-15.004781	2.002911	0.000103
8	-15.643511	-0.147781	0.000082
6	-16.423624	1.955652	0.000103
1	-14.375957	2.879383	0.000111
6	-16.772074	0.628197	0.000091
1	-17.109327	2.788366	0.000111
6	-18.024484	-0.059464	0.000083
6	-18.365101	-1.388926	0.000066
8	-19.157310	0.710505	0.000090
6	-19.783111	-1.444512	0.000063
1	-17.674223	-2.217313	0.000056
6	-20.226558	-0.145613	0.000078
1	-20.407134	-2.324358	0.000051
6	-21.528699	0.442462	0.000083
6	-21.978909	1.738965	0.000102
8	-22.593877	-0.418713	0.000063
6	-23.397084	1.676066	0.000095
1	-21.359747	2.622285	0.000120
6	-23.730869	0.344849	0.000071
1	-24.091979	2.501115	0.000105
6	-24.976280	-0.355426	0.000052
6	-25.304848	-1.687868	0.000025
8	-26.116138	0.404145	0.000059
6	-26.722423	-1.756330	0.000014
1	-24.606548	-2.510021	0.000014
6	-27.177635	-0.461509	0.000035
1	-27.338413	-2.641819	-0.000007
6	-28.484548	0.115981	0.000037
6	-28.944211	1.409074	0.000060
8	-29.543442	-0.753066	0.000011
6	-30.361905	1.335806	0.000046
1	-28.331488	2.296875	0.000083
6	-30.685887	0.002228	0.000017
1	-31.062907	2.155659	0.000057
6	-31.926975	-0.705992	-0.000009
6	-32.248789	-2.039824	-0.000040
8	-33.070852	0.047718	-0.000004
6	-33.666447	-2.115325	-0.000055
1	-31.546479	-2.858577	-0.000050
6	-34.127878	-0.823040	-0.000032
1	-34.278077	-3.003832	-0.000079
6	-35.437696	-0.250397	-0.000034
6	-35.902003	1.040172	-0.000013
8	-36.493410	-1.123603	-0.000061
6	-37.320682	0.960455	-0.000029
1	-35.293110	1.930602	0.000010
6	-37.637755	-0.372911	-0.000058
1	-38.026190	1.776482	-0.000020
6	-38.880873	-1.086056	-0.000084
6	-39.201220	-2.417207	-0.000111
8	-40.022407	-0.332064	-0.000083
6	-40.628284	-2.485524	-0.000128
1	-38.501453	-3.238047	-0.000118
6	-41.072695	-1.201393	-0.000110
1	-41.239472	-3.375364	-0.000151
1	-42.049709	-0.747141	-0.000113
1	42.018560	-1.321041	0.000201

α-F[24]-cation

6	41.060290	-0.624101	-0.001833
6	40.763569	0.703100	-0.001660
8	39.921054	-1.369646	-0.001895
6	39.339718	0.795702	-0.001424
1	41.471293	1.517988	-0.001628
6	38.871524	-0.492138	-0.001660
1	38.737320	1.690493	-0.001177
6	37.559043	-1.062103	-0.001627
6	37.101201	-2.357325	-0.001781
8	36.503170	-0.194451	-0.001396
6	35.686079	-2.285483	-0.001601
1	37.716488	-3.243170	-0.002010
6	35.360346	-0.950656	-0.001336
1	34.986338	-3.106504	-0.001640
6	34.121193	-0.246569	-0.001091
6	33.799567	1.091886	-0.001007
8	32.978827	-0.998356	-0.000911
6	32.387156	1.168381	-0.000720
1	34.503189	1.909283	-0.001112
6	31.921853	-0.126424	-0.000667
1	31.777119	2.058086	-0.000560
6	30.617461	-0.696161	-0.000337
6	30.160269	-1.995602	-0.000021
8	29.557246	0.168630	-0.000244
6	28.748760	-1.927486	0.000195
1	30.776816	-2.880551	0.000005
6	28.417615	-0.591221	0.000001
1	28.050863	-2.750014	0.000420
6	27.175730	0.103012	-0.000050
6	26.842991	1.439790	-0.000377
8	26.038128	-0.657536	0.000298
6	25.431406	1.505542	-0.000272
1	27.540039	2.262893	-0.000688
6	24.975481	0.206126	0.000233
1	24.814448	2.390392	-0.000446
6	23.675403	-0.371770	0.000767
6	23.226568	-1.674057	0.001819
8	22.608977	0.486308	0.000265
6	21.814970	-1.615430	0.002076
1	23.848668	-2.555176	0.002409
6	21.475169	-0.280977	0.001095
1	21.122377	-2.442349	0.002871
6	20.227407	0.403067	0.000834
6	19.881714	1.736040	-0.000134
8	19.096887	-0.368656	0.001594
6	18.469201	1.788154	0.000053
1	20.570415	2.566202	-0.000854
6	18.026298	0.484373	0.001048
1	17.843640	2.666898	-0.000530
6	16.731584	-0.106799	0.001643
6	16.296046	-1.412937	0.003012

8	15.656506	0.740784	0.000969
6	14.883456	-1.368516	0.002858
1	16.926751	-2.287946	0.003857
6	14.530687	-0.037766	0.001615
1	14.199132	-2.202253	0.003648
6	-1.035139	2.143148	-0.001011
6	-2.449663	2.139790	-0.001105
6	-2.840624	0.820303	-0.000162
1	-0.379721	2.999849	-0.001617
1	-3.109120	2.993389	-0.001790
8	-1.737348	0.010026	0.000535
6	-0.637951	0.825509	-0.000049
6	0.635621	0.188037	0.000445
6	1.023390	-1.132410	0.001499
8	1.740372	0.996403	-0.000169
6	2.437287	-1.139087	0.001572
1	0.361550	-1.984105	0.002161
6	2.837502	0.177644	0.000571
1	3.091048	-1.997003	0.002314
6	-4.111155	0.176867	0.000096
6	-4.492765	-1.145435	0.000640
8	-5.219632	0.980024	-0.000343
6	-5.906557	-1.158743	0.000615
1	-3.826942	-1.994017	0.001064
1	-6.556280	-2.019728	0.001006
6	-7.595125	0.775837	-0.000179
6	-6.312978	0.156143	0.000029
8	-8.683389	-0.054338	0.000167
6	-8.010036	2.088209	-0.000678
1	-7.366138	2.953594	-0.001034
6	-9.424142	2.065833	-0.000626
1	-10.095024	2.910485	-0.000962
6	-9.797482	0.741089	-0.000178
6	4.116968	0.803122	0.000175
6	4.526413	2.117082	-0.000981
8	5.208693	-0.022539	0.001027
6	5.940771	2.100545	-0.000887
1	3.878985	2.979834	-0.001816
6	6.319494	0.777452	0.000315
1	6.608138	2.947978	-0.001639
6	-11.059305	0.081390	-0.000176
6	-11.424155	-1.245908	-0.000540
8	-12.177899	0.870267	0.000116
6	-12.837347	-1.277306	-0.000602
1	-10.747540	-2.085910	-0.000820
6	-13.260719	0.032550	-0.000180
1	-13.476022	-2.146523	-0.000894
6	7.583900	0.122313	0.000899
6	7.953164	-1.203600	0.002049
8	8.699805	0.915038	0.000257
6	9.366629	-1.230170	0.002120
1	7.279400	-2.045887	0.002755
6	9.785422	0.080962	0.001020
1	10.008264	-2.097200	0.002906
6	11.073180	0.688484	0.000585
6	11.500364	1.997083	-0.000677
8	12.153691	-0.151752	0.001417
6	12.913997	1.961579	-0.000442
1	10.864526	2.868407	-0.001592
6	13.275142	0.633281	0.000878
1	13.592703	2.799954	-0.001220
6	-14.550092	0.636008	-0.000040
6	-14.980589	1.943734	0.000302
8	-15.628533	-0.206925	-0.000253
6	-16.393811	1.904813	0.000352
1	-14.346822	2.816568	0.000520
6	-16.751834	0.575400	0.000053
1	-17.074644	2.741452	0.000613
6	-18.006017	-0.097489	-0.000053
6	-18.357593	-1.428752	-0.000655
8	-19.132735	0.679883	0.000412
6	-19.769899	-1.474658	-0.000526
1	-17.672441	-2.261828	-0.001128
6	-20.206930	-0.168696	0.000097
1	-20.399750	-2.350276	-0.000885
6	-21.501739	0.421470	0.000486
6	-21.944837	1.725336	0.001311
8	-22.572440	-0.431712	0.000028
6	-23.357047	1.673270	0.001385
1	-21.319246	2.604073	0.001796
6	-23.702802	0.339988	0.000592
1	-24.045920	2.503258	0.001968
6	-24.951154	-0.342482	0.000297
6	-25.294100	-1.676113	-0.000376
8	-26.083595	0.427331	0.000742
6	-26.705831	-1.731658	-0.000390
1	-24.603426	-2.504675	-0.000850
6	-27.151776	-0.428177	0.000285
1	-27.330005	-2.611285	-0.000872
6	-28.450329	0.153201	0.000570
6	-28.902444	1.453604	0.001564
8	-29.515851	-0.707580	-0.000166
6	-30.314468	1.392010	0.001374
1	-28.282944	2.336707	0.002295
6	-30.650822	0.056267	0.000358
1	-31.009342	2.216899	0.001970
6	-31.896054	-0.633236	-0.000107
6	-32.235070	-1.966620	-0.000385
8	-33.031559	0.133526	-0.000159
6	-33.648141	-2.026062	-0.000542
1	-31.542429	-2.793628	-0.000410
6	-34.096576	-0.724504	-0.000470
1	-34.270250	-2.907079	-0.000732
6	-35.398356	-0.144324	-0.000592
6	-35.854034	1.151990	-0.000297
8	-36.461265	-1.009390	-0.001152
6	-37.269415	1.083864	-0.000587
1	-35.238644	2.038007	0.000112
6	-37.597432	-0.250078	-0.001034
1	-37.968969	1.904787	-0.000525
6	-38.846990	-0.947274	-0.001402
6	-39.184652	-2.275260	-0.001637
8	-39.978563	-0.178591	-0.001401
6	-40.610617	-2.324990	-0.002014
1	-38.496163	-3.105630	-0.001632
6	-41.037999	-1.033844	-0.001824
1	-41.233681	-3.206310	-0.002361
1	-42.009621	-0.568106	-0.001894
1	41.980763	-1.184187	-0.001932

α-T[1]			
16	0.000000	0.000000	1.159331
6	0.000000	1.093380	0.346499
6	0.000000	0.717367	-0.958284
6	0.000000	-0.717367	-0.958284
6	0.000000	-1.093380	0.346499
1	0.000000	2.046705	0.849036
1	0.000000	-2.046705	0.849036
1	0.000000	1.373423	-1.815649
1	0.000000	-1.373423	-1.815649

α-T[1]-cation			
16	-1.227805	-0.001274	0.000000
6	-0.002526	1.217458	0.000000
6	1.317173	0.689350	0.000000
6	1.318600	-0.686617	0.000000
6	0.000000	-1.217459	0.000000
1	-0.278460	2.265255	0.000000
1	-0.273757	-2.265827	0.000000
1	2.197444	1.319321	0.000000
1	2.200176	-1.314760	0.000000

α-T[2]			
6	1.405761	-1.274326	-0.366571
6	2.817527	-1.131318	-0.270842
6	3.200353	0.133157	0.071039
1	0.912811	-2.195213	-0.653989
1	3.518643	-1.934639	-0.461310
16	1.834151	1.173558	0.304779
6	0.716277	-0.116751	-0.094251
6	-0.716277	0.116752	-0.094254
6	-1.405759	1.274332	-0.366564
16	-1.834153	-1.173562	0.304749
6	-2.817525	1.131322	-0.270848
1	-0.912806	2.195222	-0.653966
6	-3.200354	-0.133158	0.071013
1	-3.518640	1.934645	-0.461310
1	4.199485	0.521419	0.202917
1	-4.199487	-0.521422	0.202877

α-T[2]-cation			
6	-1.378125	-1.348520	0.000003
6	-2.759088	-1.210493	-0.000001
6	-3.159899	0.123956	-0.000011
1	-0.868279	-2.303925	0.000011
1	-3.458962	-2.035483	0.000001
16	-1.850374	1.224523	-0.000016
6	-0.693011	-0.112224	-0.000004
6	0.693011	0.112224	0.000000
6	1.378125	1.348520	-0.000005
16	1.850374	-1.224523	0.000015
6	2.759088	1.210493	0.000004
1	0.868279	2.303925	-0.000013
6	3.159899	-0.123956	0.000015
1	3.458962	2.035483	0.000001
1	-4.173522	0.501763	-0.000012
1	4.173522	-0.501763	0.000028

α-T[3]			
6	-0.707815	1.453639	-0.507050
6	0.707813	1.453617	-0.507028
6	1.262328	0.243075	-0.161408
1	-1.305261	2.311296	-0.791963
1	1.305247	2.311279	-0.791956
16	-0.000037	-0.915693	0.210035
6	-1.262341	0.243108	-0.161463
6	-2.658368	-0.131639	-0.071269
6	-3.233166	-1.374156	-0.207796
16	-3.890375	1.070520	0.265893
6	-4.646806	-1.366095	-0.058395
1	-2.658415	-2.263534	-0.436327
6	-5.146969	-0.120663	0.189575
1	-5.266542	-2.250226	-0.144019
6	2.658351	-0.131655	-0.071165
6	3.233121	-1.374239	-0.207275
16	3.890450	1.070577	0.265483
6	4.646768	-1.366181	-0.057981
1	2.658373	-2.263707	-0.435466
1	5.266459	-2.250369	-0.143332
6	5.146996	-0.120681	0.189483
1	6.175388	0.175010	0.335428
1	-6.175345	0.174994	0.335704

α-T[3]-cation			
6	-0.689423	-1.507857	0.000026
6	0.689423	-1.507857	0.000026
6	1.259342	-0.216939	0.000012
1	-1.287258	-2.410527	0.000032
1	1.287258	-2.410527	0.000032
16	0.000000	1.005208	0.000007
6	-1.259342	-0.216939	0.000012
6	-2.629018	0.128138	0.000003
6	-3.206096	1.404007	0.000001
16	-3.888543	-1.106458	-0.000015
6	-4.604100	1.380693	-0.000002
1	-2.622942	2.316773	0.000011
6	-5.111645	0.094680	-0.000015
1	-5.229560	2.263403	0.000002
6	2.629018	0.128138	0.000003
6	3.206096	1.404007	0.000001
16	3.888543	-1.106458	-0.000014
6	4.604100	1.380693	-0.000002
1	2.622942	2.316773	0.000011
1	5.229559	2.263403	0.000002
6	5.111645	0.094680	-0.000015
1	6.150460	-0.204326	-0.000022
1	-6.150460	-0.204326	-0.000022

α-T[4]			
6	-2.640085	-1.375757	0.667951
6	-1.226164	-1.339981	0.691348
6	-0.692289	-0.158969	0.226311
1	-3.222214	-2.213042	1.033615
1	-0.615869	-2.148019	1.076485
16	-1.975674	0.920880	-0.289175
6	-3.216782	-0.223848	0.184014

6	-4.618746	0.103042	0.030798
6	-5.223644	1.338824	0.008558
16	-5.817960	-1.160656	-0.174660
6	-6.633936	1.278422	-0.157776
1	-4.672990	2.263013	0.135788
6	-7.101811	0.000290	-0.260164
1	-7.274763	2.151051	-0.188215
1	-8.120757	-0.335690	-0.383364
6	0.692758	0.238721	0.122618
6	1.230103	1.504648	0.053580
16	1.970481	-0.962638	0.061247
6	2.640615	1.521480	-0.052644
1	0.624096	2.401883	0.090692
1	3.222271	2.431726	-0.134920
6	4.610493	-0.095441	-0.149896
6	3.212310	0.269975	-0.061287
16	5.863237	1.010624	0.384415
6	5.174618	-1.261155	-0.614793
1	4.586264	-2.079487	-1.012041
6	6.594758	-1.267906	-0.557698
1	7.206965	-2.097080	-0.890440
6	7.110926	-0.109666	-0.052632
1	8.146902	0.158228	0.093426

α-T[4]-cation

6	-2.613694	-1.498219	0.000001
6	-1.230245	-1.478165	0.000001
6	-0.679214	-0.184801	0.000002
1	-3.197876	-2.409637	0.000000
1	-0.621941	-2.374174	0.000000
16	-1.964344	1.018074	0.000005
6	-3.200561	-0.221848	0.000001
6	-4.583247	0.106962	-0.000001
6	-5.176965	1.367075	-0.000004
16	-5.820627	-1.145346	0.000004
6	-6.580530	1.323144	-0.000009
1	-4.608784	2.289359	-0.000007
6	-7.068348	0.035330	-0.000001
1	-7.216866	2.198152	-0.000015
1	-8.101119	-0.282649	-0.000001
6	0.679214	0.184799	0.000000
6	1.230244	1.478164	-0.000003
16	1.964345	-1.018075	-0.000002
6	2.613694	1.498218	-0.000004
1	0.621940	2.374172	-0.000002
1	3.197874	2.409637	-0.000006
6	4.583247	-0.106962	-0.000001
6	3.200562	0.221848	-0.000001
16	5.820627	1.145347	0.000006
6	5.176966	-1.367074	-0.000007
1	4.608785	-2.289359	-0.000013
6	6.580531	-1.323142	-0.000003
1	7.216868	-2.198150	-0.000006
6	7.068348	-0.035328	0.000001
1	8.101119	0.282651	0.000004

α-T[5]

6	-0.706688	-1.406202	0.502952
6	0.706704	-1.406199	0.502960
6	1.263152	-0.158493	0.325894
1	-1.303083	-2.295678	0.666421
1	1.303106	-2.295670	0.666428
16	0.000005	1.041601	0.117277
6	-1.263142	-0.158498	0.325875
6	-2.655438	0.221347	0.286011
6	-3.228714	1.452298	0.516789
16	-3.894187	-0.955265	-0.114004
6	-4.638854	1.454384	0.408226
1	-2.650739	2.325074	0.795802
6	-5.173456	0.226553	0.090939
1	-5.250840	2.328429	0.595680
6	2.655445	0.221364	0.286050
6	3.228708	1.452324	0.516811
16	3.894204	-0.955250	-0.113920
6	4.638852	1.454413	0.408276
1	2.650717	2.325100	0.795788
1	5.250833	2.328461	0.595735
6	6.559991	-0.149605	-0.085389
6	5.173462	0.226579	0.091018
16	7.759223	1.038311	-0.563204
6	7.148740	-1.384641	0.062363
1	6.596377	-2.264083	0.370612
6	8.547370	-1.381425	-0.190095
1	9.175507	-2.260275	-0.111982
6	9.022731	-0.147270	-0.527651
1	10.036367	0.142900	-0.761486
6	-6.559981	-0.149634	-0.085477
6	-7.148664	-1.384748	0.061888
16	-7.759310	1.038400	-0.562759
6	-8.547315	-1.381506	-0.190449
1	-6.596234	-2.264280	0.369759
6	-9.022760	-0.147253	-0.527531
1	-9.175404	-2.260413	-0.112598
1	-10.036427	0.142953	-0.761182

α-T[5]-cation

6	-0.691990	1.417911	0.000006
6	0.691990	1.417911	0.000006
6	1.262611	0.134305	0.000000
1	-1.287732	2.322146	0.000008
1	1.287732	2.322146	0.000009
16	0.000000	-1.088228	-0.000001
6	-1.262611	0.134305	-0.000001
6	-2.630711	-0.214748	-0.000006
6	-3.203909	-1.491975	-0.000021
16	-3.894478	1.011196	0.000007
6	-4.592613	-1.486206	-0.000022
1	-2.613844	-2.400291	-0.000032
6	-5.153126	-0.204062	-0.000007
1	-5.192940	-2.387064	-0.000034
6	2.630711	-0.214748	-0.000004
6	3.203909	-1.491975	-0.000015
16	3.894478	1.011196	0.000004
6	4.592614	-1.486206	-0.000014
1	2.613844	-2.400291	-0.000021
1	5.192940	-2.387064	-0.000020
6	6.534248	0.155759	-0.000002
6	5.153126	-0.204062	-0.000004
16	7.794516	-1.070807	0.000014

6	7.101154	1.423433	-0.000004
1	6.515130	2.334577	-0.000012
6	8.509146	1.408134	-0.000001
1	9.126181	2.296992	-0.000004
6	9.022860	0.133863	0.000006
1	10.061027	-0.165261	0.000008
6	-6.534248	0.155759	-0.000005
6	-7.101154	1.423433	-0.000027
16	-7.794516	-1.070807	0.000025
6	-8.509146	1.408134	-0.000013
1	-6.515130	2.334577	-0.000054
6	-9.022860	0.133863	0.000022
1	-9.126181	2.296992	-0.000025
1	-10.061027	-0.165261	0.000040

α-T[6]

6	-2.664642	-1.345082	-0.622759
6	-1.251710	-1.350877	-0.603731
6	-0.694072	-0.136848	-0.266415
1	-3.260769	-2.205251	-0.902587
1	-0.656307	-2.216870	-0.866914
16	-1.957833	1.033884	0.070990
6	-3.220617	-0.126337	-0.300668
6	-4.612046	0.252293	-0.234031
6	-5.177083	1.506016	-0.313862
16	-5.861577	-0.958943	-0.009297
6	-6.588728	1.502116	-0.229003
1	-4.591546	2.404218	-0.468766
6	-7.132938	0.246677	-0.081348
1	-7.194423	2.396405	-0.312502
6	0.697621	0.230691	-0.164599
6	1.269582	1.484000	-0.188824
16	1.940015	-0.995300	0.022963
6	2.676339	1.472981	-0.056182
1	0.689951	2.390944	-0.311539
1	3.280217	2.372219	-0.039117
6	4.596569	-0.179752	0.214080
6	3.214481	0.210816	0.067898
16	5.890381	0.899499	-0.277187
6	5.121865	-1.353712	0.707191
1	4.504403	-2.160330	1.083797
6	6.535599	-1.384234	0.723523
1	7.110234	-2.215376	1.114143
6	7.121632	-0.235569	0.242633
6	-8.523629	-0.140877	0.022234
6	-9.115068	-1.341831	-0.296758
16	-9.725305	0.980897	0.634575
6	-10.517479	-1.363317	-0.067328
1	-8.561518	-2.175935	-0.710772
6	-10.992948	-0.181675	0.423393
1	-11.148002	-2.220178	-0.270446
1	-12.008976	0.081327	0.678060
6	8.525938	0.094509	0.123755
6	9.126822	1.332363	0.101443
16	9.734940	-1.167124	-0.031168
6	10.541234	1.275289	-0.025141
1	8.569673	2.256057	0.200965
6	11.016298	-0.002289	-0.097270
1	11.179550	2.149919	-0.049806
1	12.039442	-0.335871	-0.187899

α-T[6]-cation

6	-2.654909	-1.430623	-0.000028
6	-1.268110	-1.443842	-0.000029
6	-0.685737	-0.169267	-0.000024
1	-3.259207	-2.329078	-0.000033
1	-0.682249	-2.354724	-0.000036
16	-1.939235	1.065254	-0.000017
6	-3.211709	-0.144284	-0.000022
6	-4.580625	0.220314	-0.000018
6	-5.142004	1.497772	-0.000037
16	-5.853749	-0.995117	0.000016
6	-6.534953	1.502857	-0.000030
1	-4.545759	2.402168	-0.000061
6	-7.103548	0.228914	-0.000007
1	-7.127714	2.408744	-0.000051
6	0.685737	0.169267	-0.000025
6	1.268111	1.443841	-0.000033
16	1.939236	-1.065254	-0.000013
6	2.654910	1.430622	-0.000030
1	0.682249	2.354724	-0.000042
1	3.259207	2.329078	-0.000037
6	4.580625	-0.220314	-0.000015
6	3.211709	0.144284	-0.000021
16	5.853748	0.995117	0.000007
6	5.142004	-1.497772	-0.000023
1	4.545760	-2.402168	-0.000038
6	6.534954	-1.502857	-0.000017
1	7.127714	-2.408744	-0.000028
6	7.103547	-0.228915	-0.000002
6	-8.490462	-0.125019	0.000001
6	-9.063817	-1.386757	-0.000067
16	-9.742488	1.108385	0.000108
6	-10.474262	-1.363687	-0.000037
1	-8.483149	-2.301365	-0.000146
6	-10.980972	-0.088828	0.000057
1	-11.095280	-2.249893	-0.000083
1	-12.016904	0.217475	0.000100
6	8.490462	0.125019	0.000005
6	9.063816	1.386757	-0.000051
16	9.742488	-1.108384	0.000092
6	10.474261	1.363688	-0.000024
1	8.483148	2.301365	-0.000114
6	10.980972	0.088829	0.000051
1	11.095280	2.249894	-0.000061
1	12.016904	-0.217474	0.000086

T7

6	0.706416	-1.452188	-0.848565
6	-0.706415	-1.452188	-0.848568
6	-1.263283	-0.213170	-0.616439
1	1.302585	-2.333803	-1.050836
1	-1.302582	-2.333803	-1.050841
16	-0.000001	0.976837	-0.355422
6	1.263282	-0.213169	-0.616434
6	2.654565	0.164454	-0.559323
6	3.226123	1.407972	-0.720070
16	3.895841	-1.032226	-0.231315
6	4.635143	1.406663	-0.613977

1	2.646236	2.294684	-0.946055
6	5.173848	0.162330	-0.369308
1	5.244342	2.291914	-0.750903
6	-2.654566	0.164453	-0.559331
6	-3.226122	1.407973	-0.720069
16	-3.895845	-1.032230	-0.231347
6	-4.635142	1.406665	-0.613982
1	-2.646233	2.294688	-0.946041
1	-5.244340	2.291917	-0.750901
6	-6.558133	-0.217635	-0.217606
6	-5.173850	0.162330	-0.369328
16	-7.768268	0.968189	0.239094
6	-7.143094	-1.454960	-0.373371
1	-6.584393	-2.334529	-0.669753
6	-8.541650	-1.455406	-0.163605
1	-9.162979	-2.334746	-0.283199
6	-9.055551	-0.219891	0.158328
6	6.558130	-0.217635	-0.217576
6	7.143088	-1.454964	-0.373318
16	7.768268	0.968195	0.239102
6	8.541643	-1.455410	-0.163552
1	6.584384	-2.334537	-0.669683
6	9.055548	-0.219890	0.158357
1	9.162969	-2.334755	-0.283128
6	-10.426844	0.160196	0.422953
6	-11.026665	1.391235	0.286518
16	-11.587366	-1.015550	1.013042
6	-12.403921	1.394325	0.636997
1	-10.498891	2.262724	-0.081558
6	-12.852144	0.168878	1.037641
1	-13.037482	2.271006	0.581793
1	-13.846263	-0.115357	1.349522
6	10.426842	0.160198	0.422973
6	11.026650	1.391248	0.286579
16	11.587386	-1.015561	1.012994
6	12.403914	1.394335	0.637027
1	10.498861	2.262750	-0.081447
6	12.852156	0.168875	1.037608
1	13.037465	2.271025	0.581845
1	13.846285	-0.115364	1.349454

α-T[7]-cation

6	0.694065	-1.473323	0.000056
6	-0.694063	-1.473323	0.000056
6	-1.263556	-0.194355	0.000033
1	1.288820	-2.378320	0.000073
1	-1.288819	-2.378320	0.000073
16	0.000001	1.027686	0.000009
6	1.263558	-0.194356	0.000033
6	2.634651	0.157562	0.000026
6	3.207230	1.432662	0.000014
16	3.897107	-1.068204	0.000032
6	4.597337	1.428702	0.000010
1	2.616183	2.340338	0.000009
6	5.160943	0.148791	0.000020
1	5.195505	2.331218	0.000003
6	-2.634650	0.157564	0.000026
6	-3.207229	1.432665	0.000014
16	-3.897106	-1.068203	0.000031
6	-4.597336	1.428704	0.000011
1	-2.616182	2.340341	0.000010
1	-5.195506	2.331220	0.000003
6	-6.535449	-0.210642	0.000018
6	-5.160942	0.148793	0.000020
16	-7.800649	1.012121	-0.000020
6	-7.103151	-1.481574	0.000043
1	-6.512920	-2.389973	0.000071
6	-8.499379	-1.478140	0.000033
1	-9.097131	-2.380806	0.000055
6	-9.058861	-0.203639	0.000001
6	6.535449	-0.210641	0.000018
6	7.103151	-1.481572	0.000043
16	7.800648	1.012122	-0.000019
6	8.499378	-1.478139	0.000033
1	6.512921	-2.389971	0.000070
6	9.058860	-0.203638	0.000001
1	9.097130	-2.380804	0.000054
6	-10.445608	0.162338	-0.000015
6	-11.008964	1.426552	0.000031
16	-11.706221	-1.061324	-0.000103
6	-12.421359	1.414368	-0.000003
1	-10.421487	2.336836	0.000092
6	-12.938021	0.145033	-0.000074
1	-13.034844	2.305917	0.000026
1	-13.975911	-0.154251	-0.000113
6	10.445607	0.162339	-0.000015
6	11.008964	1.426552	0.000030
16	11.706219	-1.061324	-0.000103
6	12.421358	1.414367	-0.000003
1	10.421487	2.336836	0.000091
6	12.938019	0.145032	-0.000073
1	13.034843	2.305916	0.000026
1	13.975909	-0.154252	-0.000111

α-T[8]

6	1.252979	1.582977	0.493884
6	2.665522	1.582171	0.477020
6	3.222235	0.321917	0.510827
1	0.657853	2.488076	0.508726
1	3.262034	2.486465	0.477691
16	1.958373	-0.895795	0.527322
6	0.695703	0.323343	0.540848
6	-0.695338	-0.056123	0.584540
6	-1.262390	-1.238634	1.008191
16	-1.943550	1.049455	0.037218
6	-2.672628	-1.256815	0.926941
1	-0.677561	-2.060486	1.403281
6	-3.217872	-0.088816	0.439411
1	-3.276960	-2.094823	1.252807
6	4.613632	-0.059222	0.521532
6	5.189963	-1.239125	0.939352
16	5.848561	1.040587	-0.065841
6	6.597975	-1.259300	0.822620
1	4.614548	-2.057190	1.355595
1	7.209825	-2.095341	1.139385
6	8.513310	0.246273	0.073012
6	7.131460	-0.095734	0.312793
16	9.735238	-1.003883	-0.084190
6	9.088221	1.489845	-0.069621
1	8.521963	2.410264	0.006704

6	10.481605	1.451124	-0.307790
1	11.085468	2.337305	-0.461509
6	11.003868	0.178448	-0.346709
6	-4.604360	0.255608	0.237562
6	-5.181213	1.500493	0.110164
16	-5.832288	-0.993080	0.115793
6	-6.580029	1.464816	-0.086092
1	-4.611197	2.419836	0.169300
6	-7.107217	0.192076	-0.108923
1	-7.185582	2.352922	-0.220704
6	12.372471	-0.241272	-0.561340
6	12.846334	-1.439518	-1.044362
16	13.710191	0.831023	-0.188366
6	14.263775	-1.497994	-1.128705
1	12.193212	-2.245800	-1.355803
6	14.867829	-0.346753	-0.712879
1	14.810333	-2.358121	-1.495367
1	15.921903	-0.114138	-0.678611
6	-8.479112	-0.222699	-0.281645
6	-8.974866	-1.444840	-0.679044
16	-9.799717	0.889202	0.034383
6	-10.385873	-1.489219	-0.761372
1	-8.336343	-2.279637	-0.942023
6	-10.999324	-0.303161	-0.427945
1	-10.937346	-2.360278	-1.094099
6	-12.409041	0.024618	-0.411580
6	-13.015169	1.252956	-0.544554
16	-13.619160	-1.225549	-0.188233
6	-14.433855	1.196329	-0.482048
1	-12.457461	2.166808	-0.710023
6	-14.906790	-0.071596	-0.303669
1	-15.076064	2.063181	-0.577659
1	-15.931826	-0.403439	-0.229550

6	10.450230	1.497783	-0.029495
1	11.044793	2.402196	-0.056600
6	11.013062	0.228024	0.005749
6	-4.587565	0.161219	-0.037016
6	-5.163653	1.431384	-0.042124
16	-5.845428	-1.068908	-0.022085
6	-6.556599	1.422153	-0.036293
1	-4.576638	2.341704	-0.052166
6	-7.113819	0.142527	-0.026514
1	-7.157990	2.322510	-0.042305
6	12.402512	-0.136093	0.023845
6	12.970847	-1.392494	-0.076928
16	13.655634	1.082897	0.190821
6	14.383708	-1.378754	-0.024330
1	12.387998	-2.297923	-0.196070
6	14.894357	-0.115889	0.116068
1	15.000500	-2.265615	-0.090979
1	15.929933	0.183730	0.182845
6	-8.489577	-0.225193	-0.018344
6	-9.051364	-1.495773	-0.042396
16	-9.758627	0.991640	0.032459
6	-10.450229	-1.497782	-0.029404
1	-8.458163	-2.401618	-0.077211
6	-11.013062	-0.228022	0.005805
1	-11.044791	-2.402197	-0.056474
6	-12.402512	0.136094	0.023897
6	-12.970845	1.392501	-0.076811
16	-13.655637	-1.082905	0.190775
6	-14.383706	1.378759	-0.024238
1	-12.387994	2.297938	-0.195883
6	-14.894359	0.115885	0.116076
1	-15.000497	2.265625	-0.090843
1	-15.929936	-0.183737	0.182817

α-T[8]-cation

6	1.249462	1.458597	-0.045329
6	2.639821	1.463691	-0.043575
6	3.212612	0.188459	-0.040457
1	0.652170	2.362067	-0.048369
1	3.231380	2.370721	-0.045298
16	1.954323	-1.037335	-0.039283
6	0.685302	0.180016	-0.043618
6	-0.685303	-0.180015	-0.043612
6	-1.249462	-1.458597	-0.045309
16	-1.954324	1.037335	-0.039277
6	-2.639821	-1.463691	-0.043546
1	-0.652170	-2.362067	-0.048346
6	-3.212612	-0.188459	-0.040434
1	-3.231380	-2.370721	-0.045257
6	4.587565	-0.161220	-0.037045
6	5.163653	-1.431384	-0.042156
16	5.845428	1.068908	-0.022119
6	6.556600	-1.422153	-0.036332
1	4.576638	-2.341704	-0.052196
1	7.157991	-2.322510	-0.042350
6	8.489578	0.225194	-0.018396
6	7.113819	-0.142527	-0.026557
16	9.758628	-0.991637	0.032448
6	9.051365	1.495774	-0.042484
1	8.458163	2.401617	-0.077330

α-T[12]

6	6.592155	-1.464260	1.423638
6	5.187557	-1.613898	1.426244
6	4.609397	-1.466990	0.183737
1	7.206154	-1.585297	2.307884
1	4.616305	-1.860447	2.313066
16	5.838207	-1.096865	-1.013586
6	7.121757	-1.199055	0.179095
6	8.499397	-1.006015	-0.202181
6	9.083393	-1.125097	-1.444840
16	9.702968	-0.542089	0.988177
6	10.474737	-0.880864	-1.447560
1	8.528243	-1.418561	-2.327594
6	10.987915	-0.568805	-0.207072
1	11.093514	-0.968529	-2.332416
6	3.220635	-1.567866	-0.192537
6	2.670421	-1.802980	-1.434228
16	1.950587	-1.369666	1.002465
6	1.258842	-1.854259	-1.432719
1	3.271989	-1.971241	-2.319300
1	0.669186	-2.065632	-2.316565
6	-0.695766	-1.659823	0.189805
6	0.695770	-1.659829	-0.189802
16	-1.950582	-1.369673	-1.002467
6	-1.258839	-1.854230	1.432726
1	-0.669183	-2.065590	2.316575

6	-2.670417	-1.802943	1.434234
1	-3.271985	-1.971186	2.319309
6	-3.220631	-1.567847	0.192539
6	12.350402	-0.280031	0.168915
6	12.942937	-0.346139	1.411306
16	13.518500	0.249893	-1.029111
6	14.315167	-0.009387	1.408065
1	12.410032	-0.666495	2.298423
6	14.803984	0.322040	0.163173
1	14.940162	-0.045663	2.292153
6	-4.609392	-1.466970	-0.183735
6	-5.187553	-1.613884	-1.426241
16	-5.838201	-1.096834	1.013586
6	-6.592151	-1.464243	-1.423636
1	-4.616302	-1.860440	-2.313062
6	-7.121752	-1.199029	-0.179094
1	-7.206150	-1.585284	-2.307880
6	16.143885	0.697880	-0.220408
6	16.743330	0.635955	-1.459051
16	17.265587	1.350613	0.960495
6	18.088321	1.072566	-1.464404
1	16.238544	0.248417	-2.335756
6	18.545532	1.478522	-0.231282
1	18.718419	1.054016	-2.345449
6	19.855537	1.967067	0.143095
6	20.474029	1.936158	1.372091
16	20.897869	2.737628	-1.038943
6	21.773982	2.510489	1.368660
1	20.017604	1.488376	2.246579
6	22.145077	2.975787	0.140270
1	22.411035	2.564366	2.242886
1	23.072556	3.447558	-0.148771
6	-8.499391	-1.005984	0.202182
6	-9.083385	-1.125047	1.444843
16	-9.702964	-0.542076	-0.988181
6	-10.474729	-0.880815	1.447562
1	-8.528233	-1.418497	2.327601
6	-10.987910	-0.568774	0.207071
1	-11.093504	-0.968466	2.332421
6	-12.350398	-0.280005	-0.168917
6	-12.942928	-0.346105	-1.411312
16	-13.518503	0.249898	1.029109
6	-14.315161	-0.009362	-1.408072
1	-12.410019	-0.666448	-2.298430
6	-14.803984	0.322049	-0.163178
1	-14.940153	-0.045633	-2.292162
6	-16.143889	0.697876	0.220403
6	-16.743339	0.635927	1.459043
16	-17.265589	1.350620	-0.960494
6	-18.088331	1.072531	1.464397
1	-16.238554	0.248378	2.335744
6	-18.545540	1.478504	0.231280
1	-18.718433	1.053963	2.345439
6	-19.855545	1.967048	-0.143095
6	-20.474032	1.936156	-1.372094
16	-20.897887	2.737584	1.038951
6	-21.773988	2.510480	-1.368659
1	-20.017600	1.488391	-2.246587
6	-22.145090	2.975755	-0.140263
1	-22.411037	2.564368	-2.242888
1	-23.072573	3.447517	0.148781

α-T[12]-cation

6	6.560646	-1.439459	-0.202208
6	5.163650	-1.442606	-0.215070
6	4.595107	-0.173311	-0.211005
1	7.156865	-2.343522	-0.206826
1	4.572760	-2.350296	-0.229880
16	5.856436	1.050433	-0.187840
6	7.122505	-0.166444	-0.187908
6	8.500536	0.199210	-0.171796
6	9.064678	1.469014	-0.193913
16	9.765944	-1.019700	-0.112031
6	10.462648	1.470729	-0.169011
1	8.471529	2.374577	-0.233524
6	11.027445	0.200558	-0.126737
1	11.056503	2.376063	-0.188588
6	3.216220	0.186220	-0.219758
6	2.648711	1.456880	-0.231668
16	1.954689	-1.036174	-0.212313
6	1.252092	1.454441	-0.235872
1	3.240910	2.363641	-0.238956
1	0.657162	2.359459	-0.246831
6	-0.688709	-0.182207	-0.227448
6	0.688706	0.182203	-0.227442
16	-1.954692	1.036170	-0.212335
6	-1.252095	-1.454445	-0.235882
1	-0.657165	-2.359463	-0.246832
6	-2.648714	-1.456883	-0.231691
1	-3.240913	-2.363645	-0.238983
6	-3.216223	-0.186224	-0.219790
6	12.408166	-0.161611	-0.092889
6	12.977642	-1.426634	-0.120916
16	13.666872	1.061996	0.004667
6	14.377634	-1.421655	-0.077434
1	12.390174	-2.334604	-0.184844
6	14.933273	-0.150774	-0.014631
1	14.977405	-2.322701	-0.108057
6	-4.595110	0.173308	-0.211049
6	-5.163652	1.442602	-0.215115
16	-5.856440	-1.050436	-0.187901
6	-6.560648	1.439456	-0.202266
1	-4.572763	2.350293	-0.229916
6	-7.122508	0.166441	-0.187977
1	-7.156867	2.343519	-0.206889
6	16.315105	0.221921	0.037676
6	16.881904	1.479623	-0.075252
16	17.569967	-0.983639	0.281347
6	18.284833	1.480891	0.008485
1	16.297171	2.376544	-0.240641
6	18.834065	0.224135	0.189914
1	18.887689	2.375040	-0.089402
6	20.221459	-0.148372	0.309193
6	20.800565	-1.391226	0.156915
16	21.445574	1.046681	0.699744
6	22.205642	-1.386806	0.341802
1	20.234669	-2.277513	-0.103635
6	22.696543	-0.144420	0.633533
1	22.829259	-2.267315	0.253815
1	23.720130	0.146057	0.818843
6	-8.500539	-0.199213	-0.171878

6	-9.064682	-1.469015	-0.194036
16	-9.765946	1.019696	-0.112074
6	-10.462652	-1.470729	-0.169138
1	-8.471534	-2.374578	-0.233679
6	-11.027448	-0.200560	-0.126826
1	-11.056509	-2.376062	-0.188753
6	-12.408169	0.161610	-0.092974
6	-12.977646	1.426631	-0.121042
16	-13.666873	-1.061994	0.004649
6	-14.377637	1.421654	-0.077543
1	-12.390179	2.334599	-0.185019
6	-14.933274	0.150775	-0.014684
1	-14.977410	2.322697	-0.108197
6	-16.315105	-0.221919	0.037653
6	-16.881907	-1.479621	-0.075259
16	-17.569962	0.983642	0.281349
6	-18.284835	-1.480888	0.008507
1	-16.297178	-2.376543	-0.240662
6	-18.834062	-0.224132	0.189945
1	-18.887693	-2.375037	-0.089366
6	-20.221454	0.148377	0.309253
6	-20.800562	1.391229	0.156980
16	-21.445560	-1.046673	0.699843
6	-22.205635	1.386812	0.341900
1	-20.234672	2.277514	-0.103591
6	-22.696530	0.144429	0.633652
1	-22.829253	2.267321	0.253920
1	-23.720113	-0.146046	0.818989

α-T[16]

6	-10.777040	-3.048240	-0.589230
6	-12.040240	-3.607500	-0.883640
6	-11.976550	-4.874070	-1.423390
1	-10.648430	-2.076840	-0.127280
1	-12.977530	-3.108100	-0.670010
16	-10.302540	-5.369500	-1.604260
6	-9.717010	-3.873750	-0.896890
6	-8.303710	-3.645700	-0.719950
6	-7.275770	-4.561370	-0.653640
16	-7.670830	-2.015940	-0.566360
6	-6.004390	-3.978960	-0.453610
1	-7.439180	-5.630800	-0.710320
6	-6.030020	-2.604030	-0.361940
1	-5.094940	-4.556780	-0.341470
6	-13.051860	-5.747550	-1.824890
6	-13.045920	-7.115510	-1.993380
16	-14.642510	-5.101510	-2.189560
6	-14.296080	-7.648650	-2.378260
1	-12.169930	-7.724980	-1.807030
1	-14.474610	-8.708070	-2.517250
6	-16.674380	-6.878040	-2.869680
6	-15.288030	-6.701240	-2.513160
16	-17.205700	-8.318250	-3.720560
6	-17.743930	-6.037660	-2.646830
1	-17.648860	-5.095040	-2.121490
6	-18.975290	-6.543160	-3.119380
1	-19.919220	-6.026800	-2.993200
6	-18.877030	-7.782450	-3.714530
6	-4.940030	-1.684190	-0.144670
6	-4.973930	-0.393600	0.337100
16	-3.288470	-2.145550	-0.518750
6	-3.701380	0.212170	0.436410
1	-5.891320	0.091950	0.647310
6	-2.664680	-0.600940	0.032860
1	-3.544810	1.209260	0.829920
6	-19.915700	-8.601760	-4.289240
6	-19.920970	-9.959100	-4.528800
16	-21.432960	-7.890890	-4.811550
6	-21.125450	-10.434430	-5.093080
1	-19.089370	-10.603060	-4.269370
6	-22.070140	-9.452000	-5.298500
1	-21.310080	-11.479560	-5.310250
6	-1.247700	-0.326800	0.010770
6	-0.190170	-1.209430	-0.003610
16	-0.655000	1.324660	-0.014540
6	1.077020	-0.581670	-0.003120
1	-0.323120	-2.284250	0.023720
6	1.015860	0.793230	0.010500
1	2.013110	-1.126230	0.024770
6	2.095590	1.756870	0.031170
6	2.094650	3.049630	0.503110
16	3.675650	1.349820	-0.613340
6	3.347390	3.706130	0.364320
1	1.225580	3.505120	0.962220
6	4.300000	2.915190	-0.210220
1	3.534400	4.722080	0.689720
1	5.331210	3.152530	-0.426180
6	-23.403580	-9.568800	-5.835800
6	-24.474050	-8.710880	-5.702020
16	-23.852870	-10.943890	-6.829500
6	-25.645420	-9.153430	-6.355610
1	-24.426350	-7.801310	-5.115530
6	-25.498760	-10.360360	-7.004900
1	-26.586290	-8.617650	-6.320330
6	-26.472630	-11.115530	-7.754370
6	-26.477350	-12.456770	-8.071770
16	-27.893870	-10.332140	-8.422830
6	-27.609870	-12.864420	-8.810910
1	-25.700500	-13.138530	-7.747350
6	-28.498180	-11.844600	-9.076870
1	-27.788920	-13.890170	-9.109740
6	-29.754870	-11.893050	-9.783050
6	-30.813780	-11.011930	-9.737370
16	-30.107210	-13.202540	-10.897340
6	-31.904010	-11.386760	-10.553560
1	-30.819500	-10.134920	-9.101460
6	-31.704870	-12.563450	-11.243110
1	-32.829710	-10.826490	-10.605870
6	-32.594920	-13.253520	-12.144280
6	-32.588590	-14.576890	-12.529280
16	-33.907700	-12.400470	-12.937610
6	-33.630730	-14.917300	-13.419900
1	-31.871550	-15.294320	-12.148920
6	-34.458960	-13.862300	-13.737400
1	-33.792960	-15.921990	-13.791160
6	-35.621150	-13.841760	-14.591590
6	-36.661500	-12.938370	-14.624430
16	-35.858050	-15.079510	-15.813100
6	-37.650070	-13.240820	-15.587170
1	-36.729200	-12.097740	-13.944480
6	-37.389230	-14.382880	-16.313210

1	-38.551970	-12.655520	-15.719700
6	-38.173470	-15.000040	-17.355080
6	-38.151550	-16.302510	-17.804480
16	-39.348760	-14.067170	-18.265510
6	-39.077350	-16.564990	-18.838990
1	-37.509360	-17.060500	-17.372480
6	-39.828750	-15.469430	-19.204910
1	-39.216090	-17.544450	-19.280540
6	-40.867940	-15.369580	-20.201680
6	-41.877400	-14.439340	-20.317000
16	-40.964430	-16.529780	-21.514650
6	-42.736680	-14.663280	-21.417610
1	-42.019100	-13.636420	-19.603620
6	-42.402490	-15.767870	-22.167570
1	-43.603230	-14.049880	-21.633040
6	-43.054710	-16.308290	-23.341200
6	-43.052450	-17.599750	-23.816690
16	-44.004680	-15.277460	-24.396000
6	-43.813060	-17.769050	-25.005140
1	-42.541360	-18.409640	-23.310320
6	-44.394120	-16.610280	-25.432660
1	-43.931950	-18.717550	-25.514270
1	-45.025800	-16.452080	-26.294240

α-T[16]-cation

6	-14.380412	-1.432951	0.432408
6	-12.978949	-1.434810	0.427541
6	-12.414089	-0.169462	0.370013
1	-14.975561	-2.336014	0.489049
1	-12.387063	-2.340587	0.478832
16	-13.676769	1.050641	0.307185
6	-14.941496	-0.164994	0.378776
6	-16.323542	0.204509	0.371273
6	-16.887306	1.468352	0.450639
16	-17.586474	-1.010372	0.241571
6	-18.289418	1.469296	0.423261
1	-16.295549	2.370825	0.544742
6	-18.850156	0.204826	0.321897
1	-18.885068	2.370851	0.495547
6	-11.031671	0.196310	0.354154
6	-10.466398	1.462937	0.396071
16	-9.770879	-1.022853	0.266469
6	-9.065505	1.461416	0.367264
1	-11.057996	2.368049	0.457777
1	-8.470719	2.365979	0.403477
6	-7.123637	-0.174544	0.263007
6	-8.504688	0.194310	0.302423
16	-5.860196	1.042896	0.186959
6	-6.561516	-1.443098	0.272990
1	-7.154782	-2.347986	0.321110
6	-5.161155	-1.444853	0.226553
1	-4.568775	-2.351657	0.233555
6	-4.597466	-0.178128	0.179665
6	-20.233385	-0.163217	0.273620
6	-20.801997	-1.423397	0.350487
16	-21.488072	1.052459	0.084877
6	-22.204562	-1.420819	0.279970
1	-20.216357	-2.325661	0.479136
6	-22.756284	-0.157298	0.146709
1	-22.806256	-2.318399	0.351015
6	-3.215831	0.187385	0.129051
6	-2.650918	1.454571	0.123003
16	-1.955240	-1.033639	0.060908
6	-1.250889	1.452871	0.067105
1	-3.241909	2.361419	0.161887
6	-0.690238	0.184447	0.028820
1	-0.656745	2.358460	0.056395
6	-24.139103	0.217035	0.053491
6	-24.711869	1.468509	0.179025
16	-25.379655	-0.983416	-0.269452
6	-26.113793	1.468764	0.046448
1	-24.135644	2.360424	0.393888
6	-26.651475	0.217946	-0.185903
1	-26.723191	2.357875	0.150771
6	-28.033915	-0.158228	-0.361137
6	-28.619797	-1.396939	-0.211184
16	-29.237435	1.028197	-0.832219
6	-30.016241	-1.396510	-0.460022
1	-28.066408	-2.276714	0.094341
6	-30.493138	-0.161178	-0.797732
1	-30.643452	-2.275573	-0.382119
1	-31.507239	0.125832	-1.033575
6	0.690241	-0.184441	-0.029088
6	1.250891	-1.452864	-0.067407
16	1.955245	1.033645	-0.061128
6	2.650920	-1.454563	-0.123297
1	0.656745	-2.358453	-0.056734
6	3.215834	-0.187379	-0.129307
1	3.241910	-2.361412	-0.162212
6	4.597470	0.178135	-0.179908
6	5.161159	1.444858	-0.226816
16	5.860201	-1.042888	-0.187152
6	6.561521	1.443104	-0.273236
1	4.568779	2.351662	-0.233851
6	7.123642	0.174550	-0.263219
1	7.154787	2.347990	-0.321374
6	8.504694	-0.194305	-0.302615
6	9.065510	-1.461410	-0.367471
16	9.770885	1.022856	-0.266610
6	10.466404	-1.462932	-0.396253
1	8.470724	-2.365971	-0.403719
6	11.031677	-0.196306	-0.354301
1	11.058002	-2.368043	-0.457972
6	12.414096	0.169465	-0.370131
6	12.978957	1.434812	-0.427666
16	13.676774	-1.050637	-0.307251
6	14.380421	1.432952	-0.432498
1	12.387074	2.340588	-0.478990
6	14.941503	0.164996	-0.378830
1	14.975572	2.336013	-0.489141
6	16.323548	-0.204509	-0.371287
6	16.887313	-1.468353	-0.450632
16	17.586478	1.010371	-0.241554
6	18.289424	-1.469298	-0.423216
1	16.295557	-2.370825	-0.544748
6	18.850161	-0.204829	-0.321844
1	18.885076	-2.370854	-0.495483
6	20.233389	0.163214	-0.273533
6	20.802005	1.423391	-0.350402
16	21.488069	-1.052461	-0.084738
6	22.204568	1.420813	-0.279846

1	20.216370	2.325655	-0.479081
6	22.756285	0.157293	-0.146551
1	22.806266	2.318391	-0.350888
6	24.139100	-0.217041	-0.053289
6	24.711868	-1.468517	-0.178796
16	25.379645	0.983411	0.269680
6	26.113789	-1.468773	-0.046178
1	24.135649	-2.360433	-0.393669
6	26.651465	-0.217954	0.186179
1	26.723188	-2.357885	-0.150476
6	28.033901	0.158220	0.361450
6	28.619789	1.396929	0.211503
16	29.237406	-1.028203	0.832574
6	30.016225	1.396500	0.460382
1	28.066409	2.276702	-0.094044
6	30.493112	0.161170	0.798115
1	30.643439	2.275562	0.382491
1	31.507206	-0.125840	1.033988

α-T[24]

6	-46.140626	0.522690	-0.522671
6	-45.695930	-0.723504	-0.187464
16	-44.842929	1.668982	-0.592569
6	-44.292995	-0.767939	0.035244
1	-46.348692	-1.582272	-0.090429
6	-43.670388	0.447790	-0.132838
1	-43.761145	-1.662020	0.337392
6	-42.269840	0.782946	0.012253
6	-41.692309	1.996265	0.310117
16	-41.031166	-0.438050	-0.210750
6	-40.281130	1.952539	0.389542
1	-42.273873	2.889399	0.504213
6	-39.749756	0.703454	0.155264
1	-39.671675	2.809245	0.650816
6	-38.368929	0.283207	0.169867
6	-37.845314	-0.980115	0.338141
16	-37.076099	1.446699	-0.061102
6	-36.433216	-1.020611	0.313474
1	-38.463934	-1.852203	0.512140
6	-35.843581	0.210669	0.125511
1	-35.861187	-1.927958	0.465849
6	-34.442996	0.551055	0.064928
6	-33.838989	1.778872	0.229422
16	-33.232202	-0.677809	-0.259981
6	-32.433163	1.746556	0.096566
1	-34.395500	2.681054	0.452750
6	-31.926702	0.492493	-0.168334
1	-31.806575	2.626182	0.181528
6	-30.555540	0.087039	-0.358172
6	-30.058308	-1.052618	-0.952905
16	-29.235547	1.095111	0.210235
6	-28.647431	-1.112210	-0.983205
1	-30.695394	-1.812382	-1.389400
6	-28.031349	-0.019371	-0.412485
1	-28.095064	-1.921277	-1.445683
6	-26.623923	0.267122	-0.280244
6	-25.998061	1.477029	-0.069905
16	-25.434372	-1.020198	-0.368134
6	-24.589775	1.388139	-0.008266
1	-26.539800	2.412401	0.001628
6	-24.104481	0.108330	-0.169889
1	-23.943913	2.249046	0.115692
6	-22.737943	-0.353286	-0.182414
6	-22.220419	-1.524205	-0.692871
16	-21.455509	0.616069	0.522814
6	-20.823975	-1.652855	-0.524446
1	-22.831649	-2.268006	-1.189558
6	-20.238313	-0.581527	0.115020
1	-20.261501	-2.517854	-0.854561
6	-18.851448	-0.368928	0.449565
6	-18.300669	0.497491	1.369195
16	-17.583780	-1.273065	-0.361107
6	-16.892508	0.424685	1.450721
1	-18.900338	1.145942	1.996532
6	-16.332108	-0.499225	0.595174
1	-16.304807	1.010192	2.147362
6	1.277654	-1.451884	-0.939180
6	2.689286	-1.426054	-0.900199
6	3.210031	-0.292638	-0.313826
1	0.708813	-2.252160	-1.396936
1	3.310690	-2.205253	-1.324876
16	1.911400	0.752910	0.235527
6	0.684606	-0.338697	-0.383440
6	-0.716483	-0.018370	-0.261658
6	-1.315545	1.207327	-0.065240
16	-1.934665	-1.278993	-0.343607
6	-2.725802	1.151039	-0.009331
1	-0.753097	2.130836	0.000607
6	-3.239304	-0.118865	-0.161654
1	-3.352403	2.027510	0.103911
6	4.589562	0.080188	-0.117550
6	5.127587	1.325612	0.125336
16	5.862636	-1.127569	-0.166421
6	6.532108	1.322078	0.274367
1	4.524804	2.223920	0.182356
1	7.110847	2.213542	0.483888
6	8.492841	-0.303318	0.231318
6	7.103519	0.074509	0.144873
16	9.762389	0.893957	0.040834
6	9.044537	-1.547356	0.449869
1	8.444714	-2.435157	0.610079
6	10.456233	-1.546521	0.494061
1	11.046663	-2.432908	0.692136
6	11.018493	-0.301535	0.310662
6	-4.615818	-0.549956	-0.175564
6	-5.157974	-1.711053	-0.682791
16	-5.877741	0.449703	0.524211
6	-6.557146	-1.808617	-0.516030
1	-4.562326	-2.469664	-1.176007
6	-7.120146	-0.722529	0.118905
1	-7.137887	-2.662344	-0.843830
6	12.409988	0.077901	0.309178
6	12.973646	1.320195	0.505994
16	13.664177	-1.114141	0.016174
6	14.385100	1.321308	0.453798
1	12.384623	2.203983	0.719318
6	14.935143	0.080165	0.215505
1	14.986143	2.206697	0.622550
6	-8.502450	-0.479010	0.451385
6	-9.035139	0.400847	1.368871
16	-9.788613	-1.357203	-0.358601

6	-10.444599	0.358489	1.449424
1	-8.422083	1.037308	1.995550
6	-11.024097	-0.554872	0.595239
1	-11.020020	0.957910	2.144485
6	-12.418473	-0.878183	0.417455
6	-12.987375	-2.011430	-0.122798
16	-13.669985	0.251497	0.905259
6	-14.399763	-1.996688	-0.122771
1	-12.400211	-2.850016	-0.477137
6	-14.944823	-0.851808	0.417530
1	-15.004363	-2.822843	-0.476986
6	16.323746	-0.297133	0.116000
6	16.895111	-1.546493	0.226956
16	17.563456	0.907855	-0.188729
6	18.298634	-1.549118	0.068917
1	16.317096	-2.440037	0.429500
6	18.835983	-0.301206	-0.162504
1	18.901124	-2.448433	0.111218
6	20.214487	0.072732	-0.363703
6	20.732483	1.212535	-0.940003
16	21.515713	-0.981151	0.163231
6	22.143826	1.236916	-0.989279
1	20.109056	1.997695	-1.350506
6	22.739451	0.116207	-0.451647
1	22.710351	2.041932	-1.441557
6	24.140855	-0.208038	-0.345259
6	24.738914	-1.436755	-0.165462
16	25.361263	1.050482	-0.427870
6	26.149767	-1.384242	-0.122824
1	24.174997	-2.359559	-0.102264
6	26.664880	-0.114251	-0.268976
1	26.775276	-2.263165	-0.023431
6	28.042288	0.313429	-0.293834
6	28.581601	1.478996	-0.793714
16	29.310022	-0.698418	0.377561
6	29.983104	1.570468	-0.643533
1	27.982156	2.245388	-1.270031
6	30.550734	0.475100	-0.029092
1	30.562368	2.426418	-0.968109
6	31.936707	0.222849	0.281353
6	32.479066	-0.665370	1.184820
16	33.214657	1.099318	-0.543403
6	33.890017	-0.630798	1.243384
1	31.872572	-1.302507	1.817201
6	34.460686	0.284865	0.385914
1	34.473330	-1.237586	1.925339
6	35.853972	0.601881	0.186890
6	36.419840	1.737132	-0.351546
16	37.107156	-0.540229	0.639797
6	37.832293	1.713730	-0.377293
1	35.831620	2.582951	-0.686478
6	38.379894	0.560215	0.140357
1	38.435114	2.539755	-0.734960
6	39.769051	0.196611	0.288558
6	40.336857	-0.746826	1.116056
16	41.011914	0.986836	-0.666203
6	41.741737	-0.846565	0.989166
1	39.756655	-1.346255	1.807207
6	42.279774	0.021825	0.067002
1	42.343501	-1.550000	1.551851
6	43.662953	0.203190	-0.319364
6	44.176663	0.701670	-1.494638
16	44.965378	-0.225712	0.775234
6	45.597134	0.729649	-1.527652
1	43.551238	1.014095	-2.322226
6	46.163843	0.251928	-0.381447
1	46.173103	1.080313	-2.375165
1	47.211624	0.151481	-0.139775
1	-47.149738	0.842206	-0.736973

α-T[24]-cation

6	45.505701	-3.552930	0.077781
6	45.002783	-3.719070	1.336897
16	44.249019	-3.387788	-1.100971
6	43.583668	-3.728431	1.365759
1	45.624722	-3.841189	2.214809
6	43.007265	-3.567611	0.124885
1	43.003479	-3.875965	2.268640
6	41.606688	-3.531830	-0.228308
6	41.010142	-3.789708	-1.445051
16	40.395122	-3.101925	0.962228
6	39.604964	-3.672284	-1.425733
1	41.572105	-4.090518	-2.320671
6	39.091525	-3.322718	-0.192928
1	38.979468	-3.874010	-2.286996
6	37.719731	-3.134103	0.196044
6	37.172878	-3.089362	1.465198
16	36.466773	-2.906680	-1.010169
6	35.778227	-2.901338	1.477264
1	37.763938	-3.221372	2.363079
6	35.216379	-2.796832	0.218517
1	35.190414	-2.873643	2.386856
6	33.839020	-2.619010	-0.144956
6	33.239873	-2.770306	-1.383381
16	32.645669	-2.135514	1.047581
6	31.855243	-2.528119	-1.378816
1	33.787439	-3.077510	-2.265870
6	31.350176	-2.183494	-0.137688
1	31.231400	-2.630767	-2.258472
6	29.997450	-1.885069	0.234300
6	29.446969	-1.772355	1.499745
16	28.769359	-1.592950	-0.985499
6	28.072670	-1.479878	1.498388
1	30.021545	-1.925665	2.404984
6	27.525822	-1.359171	0.232587
1	27.484788	-1.384887	2.403265
6	26.169648	-1.082287	-0.141611
6	25.575572	-1.173520	-1.388885
16	24.996526	-0.538949	1.046282
6	24.213324	-0.831196	-1.396742
1	26.111468	-1.500657	-2.271447
6	23.718226	-0.466810	-0.156211
1	23.598894	-0.863682	-2.288287
6	22.387737	-0.070358	0.202195
6	21.874015	0.220137	1.454636
16	21.136426	0.108196	-1.017298
6	20.516970	0.583235	1.443873
1	22.468387	0.172847	2.358949
6	19.945816	0.581904	0.183130
1	19.967667	0.855134	2.336958
6	18.600057	0.901507	-0.196874

6	18.078054	1.106701	-1.462040
16	17.339015	1.082525	1.011656
6	16.708378	1.422167	-1.468683
1	18.680336	1.056201	-2.360940
6	16.137800	1.468004	-0.208872
1	16.152879	1.639983	-2.372685
6	-1.294215	3.794836	1.401688
6	-2.700873	3.816364	1.404435
6	-3.265375	3.652786	0.152788
1	-0.695579	3.939169	2.292794
1	-3.291376	3.978983	2.297808
16	-2.007919	3.438182	-1.052912
6	-0.739794	3.613918	0.147916
6	0.645371	3.553568	-0.227399
6	1.210521	3.646902	-1.486004
16	1.897583	3.322568	0.980632
6	2.614632	3.559782	-1.487426
1	0.623764	3.805465	-2.382566
6	3.166421	3.397204	-0.229998
1	3.214868	3.645368	-2.385023
6	-4.653108	3.635135	-0.217339
6	-5.220058	3.753523	-1.473044
16	-5.906829	3.431783	0.994070
6	-6.626007	3.706748	-1.469486
1	-4.632271	3.901666	-2.370708
1	-7.226809	3.815288	-2.364211
6	-8.561422	3.476302	0.165859
6	-7.177595	3.550981	-0.211001
16	-9.809163	3.192976	-1.035675
6	-9.128478	3.591844	1.421965
1	-8.544723	3.783101	2.314094
6	-10.530620	3.480338	1.425989
1	-11.132399	3.578043	2.321303
6	-11.079429	3.276000	0.173122
6	4.549192	3.287594	0.142656
6	5.124589	3.405045	1.394655
16	5.783276	2.952527	-1.059668
6	6.523254	3.255145	1.394582
1	4.550232	3.625422	2.286159
6	7.060719	3.017978	0.142689
1	7.131353	3.349108	2.286035
6	-12.459628	3.132090	-0.195911
6	-13.036311	3.202245	-1.451182
16	-13.688606	2.811938	1.015739
6	-14.431796	3.027989	-1.446960
1	-12.465200	3.405764	-2.348753
6	-14.966126	2.818898	-0.188363
1	-15.040840	3.084398	-2.340917
6	8.435174	2.832329	-0.229737
6	9.006882	2.861068	-1.488851
16	9.662495	2.510443	0.982995
6	10.398113	2.654405	-1.487138
1	8.436168	3.058051	-2.388138
6	10.933737	2.461387	-0.226716
1	11.003890	2.677385	-2.384812
6	12.301758	2.241517	0.149478
6	12.883191	2.323953	1.401971
16	13.506284	1.795675	-1.046929
6	14.264401	2.060719	1.406629
1	12.327277	2.599319	2.289858
6	14.783143	1.768161	0.157946
1	14.876484	2.113044	2.298776
6	-16.336835	2.619488	0.188783
6	-16.909897	2.674524	1.446726
16	-17.557342	2.238959	-1.014078
6	-18.296520	2.441509	1.451214
1	-16.343450	2.908481	2.339837
6	-18.827964	2.200891	0.196752
1	-18.903029	2.478816	2.347878
6	-20.190500	1.941142	-0.171942
6	-20.772050	1.967714	-1.427115
16	-21.387089	1.511250	1.038463
6	-22.146915	1.674577	-1.423708
1	-20.220905	2.224118	-2.323637
6	-22.661014	1.414338	-0.165594
1	-22.759135	1.682775	-2.317203
6	-24.008462	1.094584	0.210160
6	-24.584433	1.095450	1.468331
16	-25.190467	0.609770	-0.994008
6	-25.944291	0.739722	1.472136
1	-24.041077	1.377418	2.361960
6	-26.452391	0.455466	0.216517
1	-26.551827	0.720398	2.368621
6	-27.785109	0.073093	-0.152668
6	-28.368089	0.052568	-1.407362
16	-28.934816	-0.475745	1.055632
6	-29.708736	-0.369652	-1.405421
1	-27.844626	0.365895	-2.302447
6	-30.194665	-0.685717	-0.148498
1	-30.319857	-0.414475	-2.298512
6	-31.504635	-1.136771	0.225119
6	-32.077790	-1.200402	1.482478
16	-32.634326	-1.727288	-0.982854
6	-33.396674	-1.687803	1.483337
1	-31.564586	-0.872814	2.378463
6	-33.874362	-2.012327	0.225801
1	-33.999358	-1.772997	2.379180
6	-35.164045	-2.521794	-0.146856
6	-35.743766	-2.590040	-1.399858
16	-36.253082	-3.190039	1.058235
6	-37.038657	-3.141194	-1.399396
1	-35.255320	-2.220766	-2.293523
6	-37.488095	-3.511190	-0.145346
1	-37.645306	-3.238125	-2.291329
6	-38.750695	-4.089808	0.228601
6	-39.330285	-4.180968	1.478156
16	-39.796393	-4.823792	-0.975679
6	-40.597725	-4.799469	1.474439
1	-38.867264	-3.779309	2.371454
6	-41.018649	-5.197994	0.222742
1	-41.205844	-4.919976	2.362523
6	-42.252884	-5.844159	-0.160153
6	-42.868091	-5.875006	-1.392426
16	-43.194383	-6.751303	1.009541
6	-44.084643	-6.606191	-1.400360
1	-42.470435	-5.363704	-2.260762
6	-44.395835	-7.129687	-0.177672
1	-44.708610	-6.729362	-2.276686
1	-45.256428	-7.719370	0.101674
1	46.539136	-3.513043	-0.233305

FP[1]

7	1.157340	0.000000	0.000000
6	0.367220	1.123970	0.000000
6	-0.945890	0.711910	0.000000
6	-0.945890	-0.711910	0.000000
6	0.367220	-1.123970	0.000000
1	0.801430	2.111730	0.000000
1	0.801430	-2.111730	0.000000
1	-1.810470	1.359500	0.000000
1	-1.810470	-1.359500	0.000000
1	2.162920	0.000000	0.000000

FP[1]-cation

7	0.000000	0.000000	1.142521
6	0.000000	1.108684	0.352272
6	0.000000	0.685585	-1.015906
6	0.000000	-0.685585	-1.015906
6	0.000000	-1.108684	0.352272
1	0.000000	2.105232	0.771761
1	0.000000	-2.105232	0.771761
1	0.000000	1.351211	-1.866099
1	0.000000	-1.351211	-1.866099
1	0.000000	0.000000	2.154635

FP[2]

6	2.123657	0.044945	-0.000003
6	1.332232	1.176659	-0.000001
6	-0.007266	0.697851	-0.000003
6	0.007266	-0.697851	-0.000003
6	-2.123658	-0.044945	0.000012
6	-1.332232	-1.176659	-0.000001
1	3.199559	-0.040261	-0.000006
1	1.692025	2.194686	-0.000002
1	-3.199559	0.040261	0.000020
1	-1.692024	-2.194686	-0.000002
7	-1.329130	1.088969	-0.000001
7	1.329130	-1.088969	-0.000001
1	-1.672958	2.032765	-0.000004
1	1.672958	-2.032765	-0.000003

FP[2]-cation

6	2.099258	0.069063	-0.000002
6	1.260519	1.218604	-0.000004
6	-0.023199	0.715639	-0.000001
6	0.023199	-0.715639	-0.000001
6	-2.099258	-0.069063	0.000008
6	-1.260519	-1.218604	0.000002
1	3.179139	0.032631	-0.000004
1	1.609781	2.239351	-0.000006
1	-3.179139	-0.032631	0.000012
1	-1.609781	-2.239351	0.000002
7	-1.363110	1.069643	0.000002
7	1.363110	-1.069643	-0.000004
1	-1.739325	2.005969	0.000001
1	1.739325	-2.005969	-0.000006

FP[3]

6	0.799595	0.000453	1.117870
6	-0.540503	0.002895	0.710600
6	-0.540503	0.002895	-0.710600
6	0.799595	0.000453	-1.117870
6	-0.479188	0.004413	-2.952140
6	0.839383	0.001135	-2.536620
1	-0.888267	0.011060	-3.950440
1	1.700741	0.003314	-3.188020
7	-1.316843	0.003718	-1.849400
7	1.632122	-0.054183	0.000000
6	0.839383	0.001135	2.536620
1	1.700741	0.003314	3.188020
6	-0.479188	0.004413	2.952140
7	-1.316843	0.003718	1.849400
1	-0.888267	0.011060	3.950440
1	2.594095	0.237923	0.000000
1	-2.319772	-0.023094	-1.891800
1	-2.319772	-0.023094	1.891800

FP[3]-cation

6	0.000007	-0.816649	1.109695
6	0.000014	0.562930	0.688952
6	0.000014	0.562930	-0.688952
6	0.000007	-0.816649	-1.109695
6	-0.000014	0.484307	-2.910277
6	-0.000014	-0.857644	-2.498494
1	-0.000022	0.877647	-3.915966
1	-0.000017	-1.710697	-3.158453
7	0.000014	1.330673	-1.835142
7	0.000014	-1.638046	0.000000
6	-0.000014	-0.857644	2.498494
1	-0.000017	-1.710697	3.158453
6	-0.000014	0.484307	2.910277
7	0.000014	1.330673	1.835142
1	-0.000022	0.877647	3.915966
1	-0.000031	-2.644701	0.000000
1	-0.000040	2.336191	-1.893159
1	-0.000040	2.336191	1.893159

FP[4]

6	-1.667183	-0.536494	-0.015924
6	-1.973076	0.830164	-0.005644
6	0.252291	0.654042	0.002072
6	-0.252292	-0.654046	-0.002037
6	1.973077	-0.830165	0.005635
6	-3.898266	-0.305353	0.000787
1	-4.924385	-0.638373	-0.007614
6	-3.384109	0.977778	0.004275
1	-3.968207	1.886113	0.013285
6	1.667181	0.536494	0.015925
6	3.384110	-0.977775	-0.004293
6	3.898266	0.305357	-0.000804
1	3.968210	-1.886109	-0.013317
1	4.924386	0.638373	0.007599
7	2.860327	1.224027	-0.005433
7	-0.794016	1.579382	0.062631
7	-2.860330	-1.224027	0.005438
7	0.794018	-1.579384	-0.062618
1	-0.724580	2.505984	-0.325196

1	-2.976505	-2.220638	-0.037986
1	0.724592	-2.505987	0.325206
1	2.976507	2.220639	0.037953

FP[4]-cation

6	-1.642296	-0.554174	-0.000017
6	-1.950743	0.842111	-0.000012
6	0.265001	0.676062	-0.000001
6	-0.265001	-0.676062	-0.000002
6	1.950743	-0.842111	0.000013
6	-3.854005	-0.303063	0.000012
1	-4.886823	-0.617050	0.000019
6	-3.337441	0.996319	0.000009
1	-3.924344	1.901147	0.000011
6	1.642296	0.554174	0.000018
6	3.337441	-0.996319	-0.000006
6	3.854005	0.303063	-0.000010
1	3.924344	-1.901147	-0.000006
1	4.886823	0.617050	-0.000016
7	2.847263	1.229859	0.000008
7	-0.779013	1.579755	-0.000001
7	-2.847263	-1.229859	-0.000010
7	0.779013	-1.579755	0.000002
1	-0.709495	2.582900	-0.000045
1	-2.983133	-2.227201	0.000004
1	0.709495	-2.582900	0.000017
1	2.983133	2.227201	-0.000004

FP[5]

6	2.533419	-0.583427	-0.019366
6	2.940828	0.756297	-0.023463
6	0.708732	0.750133	0.056930
6	1.115405	-0.593250	0.053768
6	-1.114380	-0.591541	-0.010507
6	4.775823	-0.518637	-0.002864
1	5.774467	-0.926730	-0.013819
6	4.358626	0.799189	-0.008369
1	5.008515	1.661729	0.001197
6	-0.708617	0.750659	-0.003973
6	-2.533336	-0.582988	-0.007176
6	-2.941277	0.757140	-0.000314
7	1.819387	1.589515	-0.053653
7	-1.821456	1.593209	0.062049
1	1.830684	2.532935	0.296593
1	-1.823065	2.521041	-0.329730
6	-4.775792	-0.519677	-0.012185
1	-5.774020	-0.928668	-0.021785
6	-4.358929	0.798495	-0.006981
1	-5.009430	1.660564	-0.005114
7	3.672520	-1.358727	0.010474
1	3.716040	-2.354477	-0.116245
7	0.000912	-1.436215	-0.055072
1	-0.011177	-2.347912	0.374523
7	-3.671666	-1.358064	0.001137
1	-3.712912	-2.360881	-0.033164

FP[5]-cation

6	2.497775	-0.598659	-0.002083
6	2.914654	0.765553	0.002438
6	0.690992	0.772676	-0.000520
6	1.111241	-0.607301	-0.003228
6	-1.111241	-0.607301	-0.003228
6	4.724811	-0.523214	0.004141
1	5.728144	-0.920981	0.003162
6	4.314978	0.807875	0.005539
1	4.970659	1.664159	0.008943
6	-0.690992	0.772676	-0.000520
6	-2.497775	-0.598659	-0.002083
6	-2.914654	0.765553	0.002438
7	1.807652	1.592373	0.004845
7	-1.807653	1.592372	0.004845
1	1.818250	2.596578	-0.038480
1	-1.818250	2.596578	-0.038479
6	-4.724811	-0.523214	0.004141
1	-5.728143	-0.920981	0.003162
6	-4.314978	0.807875	0.005539
1	-4.970659	1.664159	0.008943
7	3.643475	-1.368222	0.003655
1	3.699337	-2.372476	-0.016114
7	0.000000	-1.436928	-0.041811
1	0.000000	-2.417323	0.183209
7	-3.643475	-1.368222	0.003655
1	-3.699337	-2.372476	-0.016114

FP[6]

6	-3.465712	-0.541725	-0.008939
6	-3.827582	0.811577	-0.005421
6	-1.596078	0.728598	-0.004622
6	-2.048125	-0.599255	-0.008382
6	0.180600	-0.678397	0.055235
6	-5.704802	-0.401692	-0.016407
1	-6.716373	-0.776398	-0.026660
6	-5.242770	0.901494	-0.013359
1	-5.863361	1.785360	-0.014155
6	-0.180600	0.678394	0.055235
6	1.596079	-0.728600	-0.004618
6	2.048125	0.599255	-0.008374
7	-2.679337	1.609469	0.058200
7	0.961284	1.480727	-0.049826
1	-2.648185	2.532917	-0.342843
1	1.001413	2.395761	0.370364
6	3.827582	-0.811577	-0.005416
6	3.465713	0.541723	-0.008930
6	5.242774	-0.901492	-0.013366
1	5.863363	-1.785359	-0.014165
6	5.704803	0.401693	-0.016414
1	4.705048	2.278322	-0.029202
1	6.716373	0.776400	-0.026670
7	4.629786	1.277296	-0.000680
7	-4.629786	-1.277294	-0.000684
1	-4.705054	-2.278320	-0.029186
7	-0.961288	-1.480730	-0.049834
1	-1.001419	-2.395753	0.370382
7	2.679336	-1.609463	0.058192
1	2.648185	-2.532944	-0.342771

FP[6]-cation

6	-3.426721	-0.554752	0.005625
6	-3.792085	0.818420	0.005813
6	-1.569025	0.746540	-0.010599
6	-2.036395	-0.613307	-0.005853
6	0.185990	-0.694482	-0.002160
6	-5.650927	-0.400909	0.007212
1	-6.667195	-0.763901	0.007109
6	-5.193073	0.911885	0.003530
1	-5.816230	1.792213	0.001455
6	-0.185990	0.694482	-0.002160
6	1.569025	-0.746540	-0.010600
6	2.036395	0.613307	-0.005853
7	-2.654954	1.609128	0.024026
7	0.957732	1.483253	-0.046858
1	-2.632111	2.594898	-0.173584
1	0.993197	2.457972	0.199330
6	3.792085	-0.818420	0.005813
6	3.426721	0.554752	0.005624
6	5.193073	-0.911885	0.003533
1	5.816230	-1.792213	0.001460
6	5.650927	0.400909	0.007212
1	4.688625	2.285112	0.007946
1	6.667195	0.763901	0.007110
7	4.598161	1.283474	0.013737
7	-4.598161	-1.283474	0.013738
1	-4.688625	-2.285112	0.007948
7	-0.957732	-1.483253	-0.046857
1	-0.993197	-2.457972	0.199331
7	2.654954	-1.609128	0.024023
1	2.632111	-2.594897	-0.173587

FP[7]

6	4.356232	-0.602915	0.002825
6	4.764976	0.737156	-0.001226
6	2.531939	0.731536	0.011853
6	2.937772	-0.611027	0.013663
6	0.706919	-0.613979	-0.051959
6	6.598995	-0.540521	0.004880
1	7.597030	-0.949981	0.010279
6	6.182358	0.777920	0.003931
1	6.833213	1.639745	0.003661
6	1.115727	0.730400	-0.053559
6	-0.707258	-0.614429	0.026580
6	-1.114793	0.729248	0.035251
7	3.644830	1.574313	-0.057378
7	0.001799	1.567235	0.057899
1	3.648766	2.498433	0.343349
1	-0.010968	2.504408	-0.309363
6	-2.938100	-0.611946	0.000906
6	-2.531557	0.731664	0.008065
6	-4.355730	-0.602813	-0.011690
6	-4.765266	0.737854	-0.007330
1	-3.644946	2.519029	-0.278174
7	-3.645132	1.570232	0.056152
6	-6.598962	-0.540099	-0.006800
1	-7.596982	-0.949539	-0.017346
6	-6.183011	0.778365	-0.005084
1	-6.834113	1.639983	-0.000923
7	5.494151	-1.378357	-0.007891
1	5.534876	-2.381451	0.017541
7	1.821180	-1.455704	0.054104
1	1.830994	-2.366481	-0.377538
7	-1.822263	-1.459848	-0.050519
1	-1.827040	-2.350969	0.422405
7	-5.494216	-1.378053	0.005601
1	-5.534734	-2.380388	-0.041501

FP[7]-cation

6	4.311391	0.615329	0.005451
6	4.724695	-0.740983	0.007279
6	2.500157	-0.747892	-0.015166
6	2.916314	0.622852	-0.009767
6	0.692037	0.626830	-0.004757
6	6.541065	0.542439	0.012867
1	7.542993	0.943048	0.014944
6	6.130781	-0.783878	0.008295
1	6.784495	-1.641845	0.008120
6	1.112819	-0.745571	-0.005425
6	-0.692293	0.626814	-0.013671
6	-1.112329	-0.745951	-0.008507
7	3.616256	-1.572730	0.026766
7	0.000087	-1.576816	-0.051900
1	3.629233	-2.552705	-0.198962
1	0.002041	-2.543818	0.226358
6	-2.916481	0.622543	-0.000771
6	-2.499971	-0.748386	-0.002678
6	-4.310908	0.615258	0.009721
6	-4.725258	-0.741606	0.011143
1	-3.627301	-2.571021	-0.047829
7	-3.616679	-1.569062	0.026451
6	-6.540968	0.542506	0.000956
1	-7.542882	0.943201	0.001375
6	-6.131566	-0.783990	0.004634
1	-6.785750	-1.641576	0.001864
7	5.454934	1.386231	0.017411
1	5.508353	2.390265	0.009056
7	1.807106	1.457528	-0.056875
1	1.808654	2.419667	0.238135
7	-1.806364	1.459670	0.040527
1	-1.811785	2.409488	-0.293535
7	-5.454884	1.386286	-0.001475
1	-5.508147	2.389658	0.036523

FP[8]

6	-5.279195	-0.555611	-0.016250
6	-5.661800	0.792966	-0.014642
6	-3.428510	0.742097	0.005012
6	-3.862146	-0.593156	-0.002632
6	-1.631991	-0.640483	0.038101
6	-7.520740	-0.448022	-0.021615
1	-8.526710	-0.837426	-0.034794
6	-7.078369	0.861901	-0.019325
1	-7.712106	1.736383	-0.018854
6	-2.012600	0.710969	0.044150
6	-0.218249	-0.668360	-0.045830
6	0.218249	0.668361	-0.045834
7	-4.525358	1.603004	0.050769
7	-0.879487	1.527763	0.066690
1	-4.505759	2.550438	-0.286981

1	-0.874954	2.459640	-0.314627
6	2.012600	-0.710966	0.044150
6	1.631988	0.640483	0.038098
6	3.428509	-0.742104	0.005016
6	3.862149	0.593164	-0.002630
1	2.789999	2.354294	0.426848
7	2.763469	1.463255	-0.045484
6	5.661793	-0.792970	-0.014651
6	5.279199	0.555611	-0.016253
6	7.078368	-0.861901	-0.019318
1	7.712111	-1.736381	-0.018849
1	6.493350	2.309407	-0.047189
6	7.520741	0.448015	-0.021619
7	6.433039	1.307888	-0.004284
1	8.526714	0.837424	-0.034799
7	-6.433037	-1.307881	-0.004289
1	-6.493355	-2.309404	-0.047165
7	-2.763472	-1.463250	-0.045490
1	-2.789999	-2.354291	0.426848
7	0.879487	-1.527770	0.066691
1	0.874953	-2.459637	-0.314649
7	4.525361	-1.603006	0.050771
1	4.505763	-2.550439	-0.286974

FP[8]-cation

6	-5.231442	-0.565808	-0.015687
6	-5.616421	0.796731	-0.018471
6	-3.391003	0.756712	0.009238
6	-3.834336	-0.601937	0.004466
6	-1.610332	-0.652954	0.023457
6	-7.460599	-0.447813	-0.013641
1	-8.470156	-0.828623	-0.017822
6	-7.023432	0.868471	-0.015574
1	-7.659112	1.739963	-0.014001
6	-2.000882	0.724864	0.017294
6	-0.224308	-0.681066	0.015723
6	0.224308	0.681066	0.015723
7	-4.489973	1.602027	-0.036944
7	-0.872241	1.536236	0.066882
1	-4.480402	2.598035	0.095703
1	-0.851869	2.491032	-0.251356
6	2.000882	-0.724865	0.017294
6	1.610332	0.652954	0.023458
6	3.391003	-0.756712	0.009238
6	3.834336	0.601937	0.004467
1	2.768661	2.410196	0.302731
7	2.741882	1.462581	-0.036521
6	5.616421	-0.796731	-0.018471
6	5.231442	0.565808	-0.015686
6	7.023432	-0.868471	-0.015574
1	7.659112	-1.739963	-0.014001
1	6.463425	2.315153	-0.054440
6	7.460599	0.447813	-0.013641
7	6.390493	1.313526	-0.007940
1	8.470156	0.828623	-0.017823
7	-6.390493	-1.313526	-0.007939
1	-6.463426	-2.315153	-0.054440
7	-2.741882	-1.462581	-0.036521
1	-2.768661	-2.410196	0.302730
7	0.872241	-1.536236	0.066882
1	0.851869	-2.491032	-0.251355
7	4.489973	-1.602027	-0.036943
1	4.480402	-2.598036	0.095698

FP[12]

6	11.160725	-0.495051	0.038958
6	10.732286	0.819345	0.037040
6	8.917917	-0.578919	0.035592
6	9.314927	0.765587	0.036269
7	10.063866	-1.343481	0.017359
6	7.500934	-0.601753	-0.006138
6	7.081308	0.738678	-0.012302
6	5.269032	-0.623902	-0.014117
6	5.665518	0.724705	-0.022277
7	6.392187	-1.456756	0.050800
6	3.855245	-0.636079	0.020270
6	3.433135	0.705327	0.010666
7	8.187714	1.587136	-0.041970
7	4.542275	1.554575	-0.059435
6	1.623666	-0.659053	-0.064475
6	2.020289	0.689205	-0.067180
6	-0.211397	0.670977	0.044050
6	0.211397	-0.670978	0.044050
6	-2.020289	-0.689206	-0.067180
7	2.747682	-1.489666	0.036164
6	-1.623666	0.659052	-0.064474
7	-0.895966	-1.517764	-0.078284
6	-3.433135	-0.705328	0.010660
6	-3.855245	0.636078	0.020264
6	-5.665518	-0.724705	-0.022274
6	-5.269032	0.623901	-0.014114
7	-4.542275	-1.554576	-0.059438
6	-7.081308	-0.738678	-0.012310
6	-7.500934	0.601754	-0.006146
6	-9.314927	-0.765586	0.036276
6	-8.917916	0.578920	0.035596
7	-8.187715	-1.587134	-0.041969
6	-10.732286	-0.819343	0.037047
1	-11.375169	-1.687137	0.036369
6	-11.160725	0.495052	0.038961
1	-12.162362	0.895214	0.059489
7	0.895966	1.517763	-0.078282
7	-2.747682	1.489665	0.036162
7	-6.392186	1.456756	0.050797
7	-10.063865	1.343483	0.017357
1	11.375169	1.687139	0.036361
1	12.162362	-0.895212	0.059484
1	10.113688	-2.344648	0.079129
1	8.172971	2.537621	0.286607
1	6.402307	-2.363551	-0.389150
1	4.542274	2.481528	0.334016
1	2.775189	-2.399446	-0.396546
1	0.906478	2.450812	0.299555
1	-0.906478	-2.450812	0.299557
1	-2.775186	2.399445	-0.396548
1	-4.542273	-2.481527	0.334017
1	-6.402304	2.363550	-0.389156
1	-8.172969	-2.537624	0.286591
1	-10.113687	2.344649	0.079140

FP[12]-cation

6	11.094378	-0.492824	0.047426
6	10.668680	0.824487	0.050680
6	8.861170	-0.585440	0.039323
6	9.256850	0.766684	0.048742
7	10.010644	-1.346491	0.033090
6	7.455426	-0.607108	-0.005704
6	7.029963	0.747253	-0.008963
6	5.228154	-0.635267	-0.011701
6	5.631230	0.730060	-0.003463
7	6.353156	-1.453327	0.037264
6	3.833458	-0.645928	-0.017921
6	3.404084	0.714301	-0.019595
7	8.135970	1.588084	0.076435
7	4.513353	1.558940	-0.051555
6	1.605993	-0.668880	-0.053621
6	2.012673	0.700486	-0.048226
6	-0.216202	0.681256	-0.024110
6	0.216202	-0.681256	-0.024111
6	-2.012673	-0.700487	-0.048230
7	2.729204	-1.494459	0.004818
6	-1.605993	0.668880	-0.053624
7	-0.891496	-1.523141	-0.085038
6	-3.404084	-0.714301	-0.019594
6	-3.833457	0.645927	-0.017919
6	-5.631230	-0.730060	-0.003463
6	-5.228154	0.635267	-0.011700
7	-4.513354	-1.558941	-0.051556
6	-7.029963	-0.747253	-0.008964
6	-7.455426	0.607108	-0.005704
6	-9.256850	-0.766684	0.048741
6	-8.861170	0.585440	0.039322
7	-8.135970	-1.588084	0.076435
6	-10.668680	-0.824486	0.050682
1	-11.311578	-1.691037	0.052928
6	-11.094378	0.492825	0.047428
1	-12.098866	0.886291	0.057585
7	0.891496	1.523143	-0.085038
7	-2.729204	1.494460	0.004821
7	-6.353156	1.453327	0.037265
7	-10.010644	1.346491	0.033090
1	11.311578	1.691037	0.052926
1	12.098866	-0.886290	0.057583
1	10.070818	-2.347615	0.097581
1	8.139846	2.557110	-0.192637
1	6.369634	-2.419581	-0.240683
1	4.508218	2.495553	0.318107
1	2.744996	-2.428865	-0.370281
1	0.884481	2.483279	0.215100
1	-0.884482	-2.483286	0.215070
1	-2.744997	2.428862	-0.370286
1	-4.508219	-2.495550	0.318118
1	-6.369634	2.419580	-0.240686
1	-8.139846	-2.557109	-0.192644
1	-10.070817	2.347615	0.097586

FP[16]

6	14.802738	-0.520457	0.113355
6	14.379863	0.795698	0.104668
6	12.559705	-0.594980	0.087314
6	12.962360	0.747871	0.089861
6	10.729322	0.730220	0.015575
6	11.143240	-0.612000	0.028336
6	8.911360	-0.624572	0.002182
7	13.702588	-1.364346	0.081658
6	9.313648	0.722335	-0.004607
7	10.030195	-1.462049	0.077693
6	7.497282	-0.630889	0.018637
6	7.081001	0.712324	0.002905
6	5.266112	-0.644832	-0.078783
6	5.668632	0.702261	-0.080337
7	6.385765	-1.479677	0.029248
6	3.853119	-0.651024	0.006324
6	3.436265	0.692225	0.003854
6	1.622410	-0.660431	-0.094187
6	2.023285	0.685661	-0.091379
7	2.742699	-1.498699	-0.117174
6	0.208729	-0.670590	-0.077933
6	-0.208729	0.670593	-0.077942
7	11.839498	1.573885	-0.002554
7	8.194199	1.557008	-0.056183
7	4.547147	1.534087	-0.104491
7	0.901203	1.521332	-0.010098
6	-2.023285	-0.685658	-0.091372
6	-1.622410	0.660434	-0.094196
6	-3.853119	0.651027	0.006313
6	-3.436264	-0.692221	0.003858
6	-5.668631	-0.702260	-0.080330
7	-0.901203	-1.521328	-0.010080
6	-5.266113	0.644834	-0.078791
7	-4.547146	-1.534085	-0.104476
6	-7.081001	-0.712322	0.002904
6	-7.497283	0.630890	0.018621
6	-9.313647	-0.722336	-0.004600
6	-8.911361	0.624572	0.002173
7	-8.194197	-1.557008	-0.056170
6	-10.729322	-0.730222	0.015573
6	-11.143241	0.611998	0.028316
6	-12.962359	-0.747875	0.089865
6	-12.559706	0.594977	0.087301
7	-11.839496	-1.573888	-0.002542
6	-14.379863	-0.795704	0.104669
1	-15.026347	-1.660809	0.109071
6	-14.802740	0.520451	0.113339
1	-15.802402	0.924759	0.145579
7	-2.742699	1.498702	-0.117194
7	-6.385766	1.479679	0.029225
7	-10.030197	1.462049	0.077668
7	-13.702590	1.364341	0.081632
1	15.026349	1.660803	0.109061
1	15.802400	-0.924766	0.145600
1	-11.824868	-2.525450	0.322811
1	-8.193373	-2.483699	0.337980
1	-4.555456	-2.472180	0.260003
1	-0.887356	-2.429750	-0.447058
1	2.726693	-2.405489	0.323194
1	6.411054	-2.391165	-0.399847
1	10.039765	-2.369964	-0.359910
1	13.747573	-2.365504	0.147261
1	11.824872	2.525449	0.322794

1	8.193377	2.483704	0.337955
1	4.555459	2.472187	0.259975
1	0.887356	2.429750	-0.447086
1	-2.726694	2.405497	0.323164
1	-6.411054	2.391163	-0.399880
1	-10.039765	2.369958	-0.359947
1	-13.747576	2.365500	0.147231

FP[16]-cation

6	14.734270	-0.520092	0.034446
6	14.315264	0.798183	0.043217
6	12.497849	-0.599684	0.025101
6	12.900870	0.748573	0.036163
6	10.671331	0.737447	0.013530
6	11.088676	-0.614434	0.006755
6	8.860937	-0.631713	-0.011812
7	13.643126	-1.366825	0.011085
6	9.266488	0.726429	-0.001692
7	9.981674	-1.462968	0.041930
6	7.460515	-0.637027	0.005504
6	7.037534	0.720210	0.012512
6	5.230248	-0.652720	-0.024029
6	5.640776	0.711115	-0.016424
7	6.353076	-1.476982	0.019873
6	3.835479	-0.658483	-0.004547
6	3.410497	0.701267	-0.002681
6	1.606530	-0.672229	-0.043640
6	2.016415	0.692200	-0.038555
7	2.726182	-1.504043	0.019756
6	0.213316	-0.679969	-0.003365
6	-0.213317	0.679969	-0.003363
7	11.782642	1.571622	0.000025
7	8.151834	1.559352	-0.029907
7	4.522997	1.539074	-0.041480
7	0.896954	1.520274	-0.074386
6	-2.016416	-0.692199	-0.038555
6	-1.606530	0.672229	-0.043637
6	-3.835479	0.658484	-0.004545
6	-3.410497	-0.701267	-0.002682
6	-5.640776	-0.711115	-0.016424
7	-0.896954	-1.520273	-0.074389
6	-5.230248	0.652720	-0.024026
7	-4.522997	-1.539074	-0.041483
6	-7.037534	-0.720210	0.012508
6	-7.460515	0.637027	0.005503
6	-9.266488	-0.726429	-0.001697
6	-8.860937	0.631713	-0.011813
7	-8.151834	-1.559352	-0.029913
6	-10.671331	-0.737447	0.013524
6	-11.088676	0.614434	0.006752
6	-12.900870	-0.748574	0.036153
6	-12.497848	0.599684	0.025096
7	-11.782642	-1.571622	0.000015
6	-14.315263	-0.798184	0.043205
1	-14.962600	-1.661616	0.051287
6	-14.734270	0.520091	0.034438
1	-15.736038	0.920338	0.043362
7	-2.726182	1.504043	0.019760
7	-6.353076	1.476982	0.019876
7	-9.981674	1.462968	0.041931
7	-13.643126	1.366824	0.011080
1	14.962600	1.661616	0.051302
1	15.736038	-0.920339	0.043370
1	-11.782691	-2.553694	0.211811
1	-8.154563	-2.501661	0.323091
1	-4.523353	-2.496138	0.267311
1	-0.894244	-2.471359	0.254101
1	2.739041	-2.430144	-0.375910
1	6.366425	-2.437848	-0.275743
1	9.995163	-2.388644	-0.354404
1	13.695586	-2.369593	0.044078
1	11.782691	2.553692	0.211826
1	8.154564	2.501659	0.323103
1	4.523353	2.496138	0.267316
1	0.894244	2.471357	0.254111
1	-2.739041	2.430146	-0.375902
1	-6.366424	2.437850	-0.275735
1	-9.995163	2.388646	-0.354399
1	-13.695587	2.369593	0.044077

P[24]

6	-19.804615	0.612134	-0.650289
6	-20.208314	-0.729806	-0.690255
6	-17.982052	-0.717703	-0.500909
6	-18.391508	0.625414	-0.537629
6	-16.169013	0.632822	-0.335901
7	-20.937740	1.384152	-0.784822
6	-22.036530	0.542832	-0.875787
1	-23.032224	0.949436	-0.959936
6	-21.618739	-0.774328	-0.833154
1	-22.263754	-1.637987	-0.899455
6	-16.571190	-0.712619	-0.382791
7	-17.287671	1.473430	-0.377783
6	-14.766501	0.634519	-0.146464
6	-14.355025	-0.708855	-0.112962
6	-12.533816	0.643106	-0.062094
6	-12.938898	-0.703780	-0.095243
7	-13.657420	1.476570	-0.037796
6	-11.134314	0.648661	0.154674
6	-10.722644	-0.695079	0.188364
6	-8.902013	0.652193	0.228882
6	-9.308205	-0.694259	0.210983
7	-10.015699	1.493050	0.133060
6	-7.493760	0.657092	0.348810
6	-7.081091	-0.688014	0.379105
7	-19.084757	-1.558913	-0.648366
7	-15.456119	-1.553455	-0.305063
7	-11.834316	-1.537273	0.113198
7	-8.195487	-1.531058	0.349882
6	-5.262278	0.662533	0.455445
6	-5.669452	-0.684576	0.446561
6	-3.436364	-0.679948	0.487120
6	-3.849026	0.664532	0.467245
6	-1.618980	0.671755	0.597116
7	-6.377413	1.499269	0.346289
6	-2.025890	-0.674089	0.594114
7	-2.735266	1.510778	0.473368
6	-0.206508	0.672556	0.496318
6	0.206510	-0.672531	0.496390
6	2.025892	0.674126	0.594024

6	1.618984	-0.671719	0.597178
7	0.907872	1.511076	0.611796
6	3.436364	0.679974	0.487011
6	3.849028	-0.664508	0.467279
6	5.669452	0.684602	0.446440
6	5.262281	-0.662508	0.455474
7	4.553116	1.522232	0.521429
6	7.081089	0.688036	0.378962
6	7.493761	-0.657072	0.348810
7	-4.553117	-1.522201	0.521637
7	-0.907869	-1.511039	0.611970
7	2.735269	-1.510755	0.473508
7	6.377417	-1.499253	0.346394
6	9.308202	0.694269	0.210832
6	8.902014	-0.652182	0.228877
6	11.134316	-0.648650	0.154651
6	10.722641	0.695092	0.188200
6	12.938894	0.703771	-0.095411
7	8.195483	1.531080	0.349644
6	12.533817	-0.643113	-0.062120
7	11.834309	1.537282	0.112943
6	14.355020	0.708850	-0.113134
6	14.766503	-0.634525	-0.146495
6	16.571185	0.712596	-0.382960
6	16.169015	-0.632842	-0.335929
7	15.456111	1.553435	-0.305321
6	17.982048	0.717674	-0.501077
6	18.391510	-0.625444	-0.537656
6	20.208310	0.729768	-0.690420
6	19.804618	-0.612170	-0.650315
7	19.084749	1.558874	-0.648620
6	21.618735	0.774282	-0.833323
1	22.263745	1.637938	-0.899713
6	22.036532	-0.542880	-0.875819
1	23.032229	-0.949487	-0.959924
7	10.015703	-1.493046	0.133136
7	13.657425	-1.476570	-0.037736
7	17.287677	-1.473449	-0.377723
7	20.937747	-1.384195	-0.784768
1	20.987008	-2.385755	-0.729451
1	19.111658	2.508633	-0.318545
1	17.251093	-2.378635	-0.819759
1	13.645560	-2.409326	-0.416330
1	10.030161	-2.400836	0.570906
1	6.398431	-2.426517	0.738472
1	2.765421	-2.418326	0.910986
1	-0.923060	-2.443336	0.232475
1	-4.546202	-2.447190	0.123635
1	-8.160778	-2.456083	-0.046568
1	-11.783298	-2.469490	-0.263350
1	-15.508308	-2.461182	0.130141
1	-19.111671	-2.508638	-0.318195
1	-20.986997	2.385717	-0.729606
1	-17.251083	2.378569	-0.819914
1	-13.645552	2.409287	-0.416486
1	-10.030149	2.400886	0.570736
1	-6.398419	2.426575	0.738270
1	-2.765411	2.418398	0.910744
1	0.923059	2.443332	0.232199
1	4.546198	2.447180	0.123331
1	8.160771	2.456062	-0.046907
1	11.783288	2.469459	-0.263704
1	15.508294	2.461208	0.129788

FP[24]-cation

6	-19.745001	0.617052	-0.589190
6	-20.150696	-0.727393	-0.613814
6	-17.926845	-0.720480	-0.433842
6	-18.335912	0.628036	-0.480717
6	-16.114153	0.637798	-0.300259
7	-20.880212	1.388276	-0.713911
6	-21.974996	0.545854	-0.789363
1	-22.971545	0.950591	-0.871971
6	-21.561189	-0.772496	-0.739536
1	-22.208506	-1.634775	-0.790983
6	-16.521054	-0.714188	-0.324899
7	-17.232579	1.474730	-0.345815
6	-14.714838	0.639170	-0.156687
6	-14.301034	-0.713255	-0.112034
6	-12.487902	0.647572	-0.019953
6	-12.898512	-0.708115	-0.039250
7	-13.608739	1.479196	-0.054424
6	-11.091505	0.648884	0.114126
6	-10.675372	-0.706021	0.151997
6	-8.862641	0.656371	0.218314
6	-9.274777	-0.701130	0.203108
7	-9.983425	1.488765	0.201977
6	-7.466191	0.658056	0.324223
6	-7.048111	-0.698606	0.351123
7	-19.033057	-1.555958	-0.558470
7	-15.409192	-1.551094	-0.254496
7	-11.785182	-1.542979	0.021498
7	-8.159952	-1.535528	0.240989
6	-5.235537	0.664978	0.389231
6	-5.648845	-0.694109	0.378757
6	-3.419370	-0.689675	0.471750
6	-3.838538	0.667169	0.460118
6	-1.608497	0.673787	0.460226
7	-6.355857	1.496053	0.392110
6	-2.020011	-0.684549	0.458266
7	-2.726525	1.510124	0.506530
6	-0.210362	0.678146	0.520906
6	0.210367	-0.678108	0.520901
6	2.020017	0.684587	0.458257
6	1.608501	-0.673749	0.460213
7	0.901673	1.516882	0.432591
6	3.419377	0.689710	0.471732
6	3.838541	-0.667135	0.460090
6	5.648851	0.694139	0.378726
6	5.235539	-0.664947	0.389196
7	4.531845	1.526739	0.388932
6	7.048117	0.698631	0.351082
6	7.466192	-0.658032	0.324172
7	-4.531837	-1.526707	0.388952
7	-0.901667	-1.516844	0.432588
7	2.726528	-1.510087	0.506505
7	6.355855	-1.496026	0.392062
6	9.274782	0.701145	0.203055
6	8.862640	-0.656353	0.218257
6	11.091502	-0.648877	0.114055
6	10.675377	0.706030	0.151934

6	12.898515	0.708111	-0.039324
7	8.159961	1.535548	0.240946
6	12.487897	-0.647572	-0.020030
7	11.785191	1.542981	0.021433
6	14.301036	0.713244	-0.112116
6	14.714832	-0.639184	-0.156775
6	16.521055	0.714163	-0.324991
6	16.114145	-0.637820	-0.300352
7	15.409199	1.551075	-0.254581
6	17.926845	0.720447	-0.433942
6	18.335903	-0.628072	-0.480821
6	20.150695	0.727345	-0.613924
6	19.744991	-0.617096	-0.589300
7	19.033062	1.555917	-0.558573
6	21.561187	0.772439	-0.739652
1	22.208510	1.634715	-0.791101
6	21.974986	-0.545913	-0.789482
1	22.971532	-0.950656	-0.872095
7	9.983419	-1.488752	0.201908
7	13.608728	-1.479203	-0.054509
7	17.232566	-1.474759	-0.345916
7	20.880197	-1.388328	-0.714028
1	20.930630	-2.391041	-0.681371
1	19.059109	2.521025	-0.278701
1	17.204784	-2.390570	-0.764483
1	13.594271	-2.421671	-0.405980
1	9.973019	-2.429425	-0.154739
1	6.351097	-2.444664	0.057937
1	2.729152	-2.431272	0.099126
1	-0.906072	-2.462014	0.778159
1	-4.546156	-2.474556	0.725536
1	-8.184797	-2.478994	0.589284
1	-11.817954	-2.485073	0.372892
1	-15.447336	-2.486617	0.114516
1	-19.059097	-2.521066	-0.278598
1	-20.930651	2.390989	-0.681254
1	-17.204805	2.390542	-0.764381
1	-13.594289	2.421666	-0.405891
1	-9.973032	2.429439	-0.154667
1	-6.351105	2.444693	0.057989
1	-2.729154	2.431310	0.099155
1	0.906080	2.462051	0.778166
1	4.546169	2.474587	0.725520
1	8.184812	2.479011	0.589245
1	11.817970	2.485074	0.372829
1	15.447351	2.486597	0.114434

FF1

8	0.000000	0.000000	1.159331
6	0.000000	1.093380	0.346499
6	0.000000	0.717367	-0.958284
6	0.000000	-0.717367	-0.958284
6	0.000000	-1.093380	0.346499
1	0.000000	2.046705	0.849036
1	0.000000	-2.046705	0.849036
1	0.000000	1.373423	-1.815649
1	0.000000	-1.373423	-1.815649

FF[1]-cation

8	0.000000	0.000000	1.173789
6	0.000000	1.080407	0.369321
6	0.000000	0.690349	-0.989428
6	0.000000	-0.690349	-0.989428
6	0.000000	-1.080407	0.369321
1	0.000000	2.043944	0.860740
1	0.000000	-2.043944	0.860740
1	0.000000	1.362698	-1.835254
1	0.000000	-1.362698	-1.835254

FF[2]

6	1.132870	-0.019510	0.000060
6	0.411130	1.141530	-0.000120
6	-0.939840	0.694070	0.000130
6	-0.937790	-0.670810	-0.000070
6	-3.010500	0.042770	0.002240
6	-2.288760	-1.118270	0.001210
1	2.192050	-0.216290	-0.000760
1	0.810980	2.143200	0.000060
1	-4.069690	0.239550	0.003210
1	-2.688610	-2.119940	0.001190
8	-2.211270	1.168520	0.001520
8	0.333630	-1.145270	0.000000

FF[2]-cation

6	2.044882	0.023841	-0.000006
6	1.296260	-1.163841	0.000004
6	-0.006449	-0.705945	0.000003
6	0.006449	0.705945	-0.000003
6	-2.044882	-0.023841	0.000002
6	-1.296260	1.163841	-0.000002
1	3.112523	0.190043	-0.000009
1	1.695494	-2.166601	0.000008
1	-3.112523	-0.190043	0.000004
1	-1.695494	2.166601	-0.000005
8	-1.281733	-1.152147	0.000008
8	1.281733	1.152147	-0.000006

FF[3]

6	-1.131740	-0.054110	0.000000
6	-0.308710	-1.158260	0.000000
6	1.010350	-0.645040	0.000000
6	0.870710	0.725000	0.000000
6	3.006030	0.209040	0.000000
6	2.172170	1.292770	0.000000

1	4.078680	0.113710	0.000000
1	2.470410	2.329260	0.000000
8	2.317850	-0.989220	0.000000
8	-0.440600	1.132420	0.000000
6	-2.474690	-0.515240	0.000000
1	-3.395020	0.047130	0.000000
6	-2.356840	-1.877550	0.000000
8	-1.039790	-2.295610	0.000000
1	-3.083000	-2.672770	0.000000

FF[3]-cation

6	-0.792473	1.066646	0.000000
6	0.573827	0.686512	0.000000
6	0.573828	-0.686513	0.000000
6	-0.792474	-1.066645	0.000000
6	0.484440	-2.836695	0.000000
6	-0.852899	-2.454310	0.000000
1	0.949894	-3.810580	0.000000
1	-1.705267	-3.115755	0.000000
8	1.355395	-1.781878	0.000000
8	-1.641290	0.000002	0.000000
6	-0.852899	2.454311	0.000000
1	-1.705270	3.115752	0.000000
6	0.484440	2.836695	0.000000
8	1.355395	1.781876	0.000000
1	0.949893	3.810581	0.000000

FF[4]

6	1.052880	-0.473010	0.000000
6	0.778610	0.877160	0.000000
6	2.921380	0.732170	0.000000
6	2.461420	-0.579720	0.000000
6	4.604190	-0.724700	0.000000
8	1.910970	1.654770	0.000000
8	-0.092900	-1.189180	0.000000
6	-1.106810	-0.248590	0.000000
1	-2.102530	-0.658480	0.000000
6	-0.631790	1.033630	0.000000
1	-1.223410	1.935370	0.000000
6	4.329920	0.625460	0.000000
8	3.471840	-1.502310	0.000000
6	6.014590	-0.881170	-0.000010
6	6.489610	0.401050	-0.000010
8	5.475700	1.341630	0.000000
1	6.606210	-1.782910	-0.000010
1	7.485330	0.810940	-0.000010

FF[4]-cation

6	1.609952	-0.568584	-0.000002
6	1.891239	0.812846	-0.000002
6	-0.238254	0.674852	0.000000
6	0.238254	-0.674852	0.000000
6	-1.891239	-0.812846	0.000002
8	0.767704	1.588969	-0.000001
8	2.758078	-1.271671	-0.000003
6	3.751193	-0.328218	-0.000004
1	4.754073	-0.725852	-0.000005
6	3.276954	0.972613	-0.000004
1	3.873473	1.871241	-0.000004
6	-1.609952	0.568584	0.000002
8	-0.767704	-1.588969	0.000001
6	-3.276954	-0.972613	0.000005
6	-3.751193	0.328218	0.000002
8	-2.758078	1.271671	0.000003
1	-3.873473	-1.871241	0.000006
1	-4.754073	0.725852	0.000002

FF[5]

6	0.395590	-1.084210	-0.000010
6	1.171450	0.054660	0.000020
6	2.563640	-1.580880	-0.000900
6	1.301900	-2.166410	-0.000890
6	2.689670	-3.804690	-0.000020
8	-0.916450	-0.763580	-0.000010
6	-0.950370	0.619320	0.000030
1	-1.938810	1.046390	0.000280
6	0.299780	1.173800	-0.000030
1	0.532850	2.226790	-0.000020
6	3.474720	-2.656400	-0.000200
8	1.347770	-3.534500	-0.000380
6	3.608110	-4.876620	-0.000560
6	4.859080	-4.298660	-0.000620
6	5.067130	-6.484480	-0.000940
1	5.325890	-7.529680	-0.001150
6	5.819640	-5.342550	-0.000870
8	3.708690	-6.223690	-0.000660
1	6.896620	-5.285800	-0.000980
8	4.815330	-2.924720	-0.000540
8	2.519490	-0.214470	-0.000450

FF[5]-cation

6	-2.447055	0.606085	-0.000264
6	-2.823219	-0.746845	-0.000249
6	-0.687294	-0.761944	-0.000036
6	-1.067433	0.613001	-0.000127
6	1.067433	0.613001	0.000079
8	-3.541495	1.390184	-0.000402
6	-4.601350	0.519490	-0.000472
1	-5.572239	0.988976	-0.000584
6	-4.221294	-0.807689	-0.000386
1	-4.878830	-1.662441	-0.000419
6	0.687294	-0.761944	0.000094
8	0.000000	1.458227	-0.000056
6	2.447055	0.606085	0.000219
6	2.823219	-0.746845	0.000308
6	4.601350	0.519490	0.000432
1	5.572239	0.988976	0.000509
6	4.221294	-0.807689	0.000446
8	3.541495	1.390184	0.000296
1	4.878830	-1.662441	0.000544
8	1.757378	-1.601687	0.000234
8	-1.757378	-1.601687	-0.000111

FF[6]

6	1.120400	-0.277160	0.000000
6	0.608410	1.002490	0.000000

6	2.742400	1.244760	-0.000020
6	2.523650	-0.129290	-0.000020
6	4.658030	0.106790	0.000000
8	0.122030	-1.186640	0.000000
6	-1.044320	-0.442750	0.000000
1	-1.950370	-1.024490	0.000010
6	-0.806520	0.904060	0.000000
1	-1.550020	1.685270	0.000000
6	4.142350	1.399570	0.000000
8	3.685460	-0.855060	-0.000010
6	6.057980	0.261610	-0.000030
6	6.276720	1.635650	-0.000030
6	8.191970	0.503870	-0.000010
6	7.679980	1.783520	-0.000010
8	7.215860	-0.464390	-0.000020
6	9.606900	0.602300	-0.000020
1	10.350390	-0.178910	-0.000020
6	9.844700	1.949110	-0.000020
1	10.750750	2.530860	-0.000020
8	1.584520	1.970750	-0.000010
8	5.114920	2.361420	-0.000020
8	8.678340	2.693000	-0.000020

FF[6]-cation

6	3.349732	0.567217	0.000010
6	3.679857	-0.793294	0.000008
6	1.543764	-0.738899	-0.000002
6	1.967267	0.619066	0.000002
6	-0.168352	0.692174	0.000004
8	4.468924	1.316165	0.000012
6	5.501351	0.411368	0.000011
1	6.486265	0.850009	0.000014
6	5.078474	-0.899973	0.000009
1	5.706758	-1.776306	0.000009
6	0.168352	-0.692174	0.000003
8	0.928400	1.500373	0.000004
6	-1.543764	0.738899	-0.000006
6	-1.967267	-0.619066	-0.000008
6	-3.679857	0.793294	-0.000005
6	-3.349732	-0.567217	-0.000005
8	-2.586022	1.613440	-0.000005
6	-5.078474	0.899973	-0.000011
1	-5.706758	1.776306	-0.000013
6	-5.501351	-0.411368	-0.000009
1	-6.486265	-0.850009	-0.000010
8	2.586022	-1.613440	0.000002
8	-0.928400	-1.500373	-0.000004
8	-4.468924	-1.316165	-0.000010

FF[7]

6	1.152550	0.062310	0.000860
6	0.288740	1.136570	-0.001630
6	2.258020	1.991980	0.048770
6	2.450390	0.613590	0.047690
6	4.422250	1.463210	0.006120
8	0.463380	-1.099240	0.000520
6	-0.869110	-0.728590	-0.001630
1	-1.565510	-1.549730	-0.013730
6	-1.035560	0.628960	0.001880
1	-1.974910	1.158740	0.000750
6	3.550410	2.548850	0.002040
8	3.773740	0.259400	0.029010
6	5.712770	2.020050	0.081180
6	5.521380	3.399220	0.081330
6	7.684010	2.871420	0.038980
6	6.813270	3.957130	0.034030
8	7.033580	1.665730	0.060670
6	8.975470	3.437300	0.087380
6	8.786880	4.802720	0.086090
6	10.938230	4.365110	0.089850
1	12.013370	4.308240	0.103430
6	10.064960	5.417680	0.082520
8	10.293300	3.141480	0.090080
1	10.324280	6.464480	0.081100
8	0.938740	2.347770	0.021450
8	4.199620	3.753550	0.040330
8	7.459920	5.161070	0.059460

FF[7]-cation

6	0.000000	4.212332	-0.620975
6	0.000000	4.585602	0.725048
6	0.000000	2.448073	0.740674
6	0.000000	2.825697	-0.627028
6	0.000000	0.688085	-0.631705
8	0.000000	5.306041	-1.407147
6	0.000000	6.368927	-0.536910
1	0.000000	7.338283	-1.008476
6	0.000000	5.989445	0.785654
1	0.000000	6.645543	1.641264
6	0.000000	1.069417	0.738656
8	0.000000	1.758564	-1.474940
6	0.000000	-0.688085	-0.631705
6	0.000000	-1.069417	0.738656
6	0.000000	-2.825697	-0.627028
6	0.000000	-2.448073	0.740674
8	0.000000	-1.758564	-1.474940
6	0.000000	-4.212332	-0.620975
6	0.000000	-4.585602	0.725048
6	0.000000	-6.368927	-0.536910
1	0.000000	-7.338283	-1.008476
6	0.000000	-5.989445	0.785654
8	0.000000	-5.306041	-1.407147
1	0.000000	-6.645543	1.641264
8	0.000000	3.518829	1.580959
8	0.000000	0.000000	1.583938
8	0.000000	-3.518829	1.580959

FF[8]

6	-5.158072	0.565732	-0.015743
6	-5.500871	-0.769477	-0.011336
6	-3.353937	-0.734801	0.030830
6	-3.748525	0.600099	0.028317
6	-1.602416	0.641337	-0.039095
8	-6.265525	1.338752	-0.009909
6	-7.325719	0.450652	-0.001133
1	-8.299347	0.910426	-0.009060
6	-6.916455	-0.854366	0.004201
1	-7.552967	-1.724901	0.010932

6	-1.948131	-0.707876	-0.037338
8	-2.690354	1.469583	-0.005350
6	-0.198156	0.667665	0.043929
6	0.198156	-0.667664	0.043929
6	1.948131	0.707876	-0.037334
6	1.602416	-0.641336	-0.039090
8	0.858799	1.536486	0.003162
6	3.353937	0.734801	0.030823
6	3.748525	-0.600099	0.028309
6	5.500872	0.769477	-0.011331
6	5.158072	-0.565732	-0.015738
8	4.408622	1.603836	0.009888
6	6.916455	0.854365	0.004201
1	7.552968	1.724900	0.010931
6	7.325719	-0.450653	-0.001134
1	8.299346	-0.910427	-0.009059
8	-4.408622	-1.603836	0.009888
8	-0.858799	-1.536485	0.003161
8	2.690354	-1.469583	-0.005351
8	6.265525	-1.338753	-0.009908

FF[8]-cation

6	-5.107742	0.576529	-0.000018
6	-5.454423	-0.773961	-0.000017
6	-3.316334	-0.748607	0.000011
6	-3.718748	0.608864	0.000010
6	-1.580946	0.655153	0.000011
8	-6.215938	1.342587	-0.000007
6	-7.263279	0.452488	-0.000004
1	-8.240898	0.906306	-0.000003
6	-6.858797	-0.861162	-0.000008
1	-7.498054	-1.729368	-0.000006
6	-1.935479	-0.719861	0.000010
8	-2.668124	1.477639	0.000008
6	-0.203684	0.680875	-0.000006
6	0.203684	-0.680875	-0.000006
6	1.935479	0.719861	0.000010
6	1.580946	-0.655153	0.000011
8	0.850461	1.545770	0.000005
6	3.316334	0.748607	0.000012
6	3.718748	-0.608864	0.000010
6	5.454423	0.773961	-0.000017
6	5.107742	-0.576529	-0.000018
8	4.371085	1.609574	0.000001
6	6.858797	0.861162	-0.000007
1	7.498054	1.729368	-0.000006
6	7.263279	-0.452488	-0.000003
1	8.240898	-0.906306	-0.000002
8	-4.371085	-1.609574	0.000001
8	-0.850461	-1.545770	0.000005
8	2.668124	-1.477639	0.000009
8	6.215938	-1.342587	-0.000006

FF[12]

6	10.866988	-0.493270	-0.006275
6	10.471035	0.815784	0.009357
6	8.698643	-0.586693	-0.021009
6	9.054745	0.745107	-0.006253
8	9.798298	-1.370659	-0.021563
6	7.289079	-0.607140	0.022974
6	6.907882	0.731894	0.035936
6	5.142963	-0.626676	-0.045400
6	5.502387	0.719438	-0.033624
8	6.222690	-1.465780	-0.017103
6	3.739603	-0.639299	0.044211
6	3.356174	0.700681	0.053069
8	7.971242	1.590255	0.021435
8	4.421984	1.558798	0.014524
6	1.593583	-0.657872	-0.051865
6	1.954027	0.688836	-0.047090
6	-0.191931	0.670172	0.052884
6	0.191932	-0.670173	0.052883
6	-1.954026	-0.688835	-0.047081
8	2.674275	-1.497266	-0.007154
6	-1.593582	0.657872	-0.051855
8	-0.873806	-1.528187	0.004078
6	-3.356174	-0.700680	0.053057
6	-3.739602	0.639299	0.044198
6	-5.502387	-0.719438	-0.033619
6	-5.142964	0.626676	-0.045396
8	-4.421984	-1.558798	0.014522
6	-6.907882	-0.731894	0.035931
6	-7.289079	0.607140	0.022969
6	-9.054745	-0.745107	-0.006250
6	-8.698644	0.586692	-0.021006
8	-7.971243	-1.590255	0.021435
6	-10.471036	-0.815784	0.009359
1	-11.116242	-1.679793	0.022650
6	-10.866988	0.493270	-0.006274
1	-11.836035	0.962579	-0.017862
8	0.873807	1.528187	0.004077
8	-2.674275	1.497267	-0.007155
8	-6.222691	1.465780	-0.017104
8	-9.798298	1.370659	-0.021561
1	11.116241	1.679792	0.022649
1	11.836034	-0.962579	-0.017866

FF[12]-cation

6	-10.798635	0.494618	0.000138
6	-10.407226	-0.819717	0.000102
6	-8.639250	0.593919	0.000079
6	-8.997460	-0.747245	0.000066
8	-9.738921	1.373381	0.000118
6	-7.242713	0.611875	0.000032
6	-6.857324	-0.741908	-0.000006
6	-5.102820	0.636983	0.000023
6	-5.468276	-0.726707	0.000000
8	-6.182733	1.470983	0.000056
6	-3.718313	0.647462	0.000104
6	-3.327068	-0.712086	0.000072
8	-7.920821	-1.593899	0.000018
8	-4.392697	-1.565700	0.000011
6	-1.576909	0.668946	0.000022
6	-1.945277	-0.698807	-0.000006
6	0.196382	-0.680788	-0.000003
6	-0.196383	0.680787	0.000040
6	1.945277	0.698807	-0.000001
8	-2.656972	1.504401	0.000077
6	1.576909	-0.668947	-0.000038

8	0.867646	1.535985	0.000044
6	3.327068	0.712085	-0.000011
6	3.718313	-0.647463	-0.000055
6	5.468276	0.726707	-0.000019
6	5.102820	-0.636983	-0.000054
8	4.392697	1.565699	0.000007
6	6.857324	0.741908	-0.000068
6	7.242713	-0.611875	-0.000107
6	8.997461	0.747246	-0.000043
6	8.639249	-0.593919	-0.000077
8	7.920821	1.593899	-0.000031
6	10.407224	0.819720	-0.000070
1	11.054311	1.682026	-0.000054
6	10.798635	-0.494617	-0.000112
1	11.770248	-0.960276	-0.000131
8	-0.867646	-1.535986	-0.000023
8	2.656972	-1.504402	-0.000071
8	6.182734	-1.470984	-0.000102
8	9.738924	-1.373381	-0.000123
1	-11.054313	-1.682024	0.000100
1	-11.770244	0.960286	0.000179

FF[16]

6	-14.411708	0.515177	-0.012047
6	-14.020604	-0.795170	0.013731
6	-12.243170	0.600685	-0.026238
6	-12.604073	-0.729708	-0.001341
6	-10.457292	-0.724099	0.039562
6	-10.833568	0.616251	0.016129
6	-8.687477	0.627620	-0.049391
8	-13.339939	1.388558	-0.033489
6	-9.051746	-0.717160	-0.027206
8	-9.764149	1.470726	-0.029083
6	-7.284076	0.635672	0.037381
6	-6.905596	-0.705741	0.056863
6	-5.138084	0.645872	-0.055425
6	-5.503438	-0.699647	-0.040033
8	-6.215804	1.489388	-0.018842
6	-3.736551	0.653666	0.046913
6	-3.357579	-0.688355	0.057534
6	-1.590666	0.663962	-0.051852
6	-1.956325	-0.681870	-0.046504
8	-2.668031	1.507446	-0.007166
6	-0.189519	0.671090	0.052932
6	0.189518	-0.671089	0.052933
8	-11.523725	-1.578585	0.032315
8	-7.974553	-1.560120	0.026183
8	-4.426614	-1.542640	0.016262
8	-0.879257	-1.525127	0.004802
6	1.956324	0.681871	-0.046499
6	1.590665	-0.663961	-0.051847
6	3.736550	-0.653665	0.046916
6	3.357578	0.688356	0.057536
6	5.503438	0.699648	-0.040021
8	0.879256	1.525128	0.004803
6	5.138084	-0.645872	-0.055413
8	4.426614	1.542641	0.016269
6	6.905596	0.705742	0.056866
6	7.284076	-0.635671	0.037384
6	9.051747	0.717160	-0.027200
6	8.687477	-0.627620	-0.049384
8	7.974554	1.560120	0.026187
6	10.457293	0.724098	0.039558
6	10.833568	-0.616251	0.016125
6	12.604074	0.729707	-0.001352
6	12.243170	-0.600686	-0.026246
8	11.523726	1.578584	0.032308
6	14.020605	0.795169	0.013714
1	14.668956	1.656689	0.033288
6	14.411709	-0.515178	-0.012064
1	15.379059	-0.987881	-0.027223
8	2.668030	-1.507445	-0.007160
8	6.215803	-1.489388	-0.018834
8	9.764149	-1.470726	-0.029081
8	13.339939	-1.388559	-0.033502
1	-14.668955	-1.656690	0.033308
1	-15.379059	0.987879	-0.027202

FF[16]-cation

6	-14.340155	0.516371	-0.003414
6	-13.952993	-0.797763	0.003624
6	-12.178618	0.606166	-0.004009
6	-12.540781	-0.730788	0.002952
6	-10.399325	-0.731857	0.004943
6	-10.778053	0.619064	-0.001975
6	-8.636917	0.635725	-0.005930
8	-13.275102	1.390854	-0.007997
6	-9.005309	-0.721782	0.000704
8	-9.713824	1.474480	-0.007896
6	-7.247009	0.640767	0.001424
6	-6.863130	-0.715228	0.007439
6	-5.104674	0.655092	-0.007652
6	-5.476049	-0.706518	-0.002619
8	-6.182787	1.494633	-0.006154
6	-3.719470	0.660947	0.005033
6	-3.333462	-0.698039	0.008624
6	-1.576750	0.673203	-0.007625
6	-1.949466	-0.690305	-0.005744
8	-2.653689	1.513705	-0.002758
6	-0.193319	0.679956	0.007704
6	0.193318	-0.679954	0.007675
8	-11.465752	-1.581226	0.008160
8	-7.932500	-1.565335	0.007644
8	-4.402512	-1.548962	0.005329
8	-0.874240	-1.531761	0.001453
6	1.949466	0.690308	-0.005734
6	1.576749	-0.673200	-0.007665
6	3.719469	-0.660945	0.004973
6	3.333462	0.698041	0.008622
6	5.476048	0.706520	-0.002645
8	0.874239	1.531763	0.001505
6	5.104673	-0.655090	-0.007730
8	4.402512	1.548964	0.005350
6	6.863130	0.715229	0.007410
6	7.247008	-0.640767	0.001335
6	9.005309	0.721782	0.000666
6	8.636917	-0.635725	-0.006020
8	7.932501	1.565335	0.007645
6	10.399326	0.731855	0.004897
6	10.778052	-0.619065	-0.002083

6	12.540783	0.730785	0.002880
6	12.178618	-0.606169	-0.004132
8	11.465755	1.581224	0.008135
6	13.952994	0.797759	0.003536
1	14.602771	1.658041	0.008128
6	14.340156	-0.516375	-0.003563
1	15.309316	-0.986655	-0.006379
8	2.653688	-1.513703	-0.002842
8	6.182786	-1.494632	-0.006270
8	9.713824	-1.474481	-0.008031
8	13.275102	-1.390858	-0.008169
1	-14.602770	-1.658045	0.008189
1	-15.309315	0.986652	-0.006198

FF[24]

6	19.335020	-0.616904	-0.042324
6	19.699430	0.712012	0.003157
6	17.552750	0.711480	0.045033
6	17.925430	-0.629358	0.000063
6	15.779330	-0.634198	-0.061970
8	20.429680	-1.407392	-0.063388
6	21.503700	-0.537251	-0.029542
1	22.469800	-1.012182	-0.052949
6	21.116140	0.773561	0.017276
1	21.766780	1.632959	0.049608
6	16.147120	0.709162	-0.018865
8	16.853780	-1.480253	-0.056775
6	14.375940	-0.639795	0.023921
6	14.001080	0.702201	0.064981
6	12.229920	-0.643038	-0.065174
6	12.598800	0.701184	-0.028672
8	13.305460	-1.489757	-0.043807
6	10.828390	-0.648560	0.035556
6	10.453080	0.694231	0.067845
6	8.682500	-0.651782	-0.059149
6	9.051720	0.692945	-0.032505
8	9.757700	-1.498600	-0.029865
6	7.281360	-0.656580	0.043070
6	6.906040	0.686633	0.064789
8	18.621390	1.563109	0.050736
8	15.072270	1.554054	0.047775
8	11.524390	1.546105	0.040476
8	7.977180	1.538283	0.031092
6	5.135560	-0.660248	-0.051866
6	5.504870	0.684747	-0.035828
6	3.359200	0.679174	0.060241
6	3.734470	-0.664257	0.049371
6	1.588730	-0.668492	-0.045376
8	6.210500	-1.506944	-0.016089
6	1.958070	0.676619	-0.040027
8	2.663520	-1.514967	-0.003034
6	0.187620	-0.671753	0.055072
6	-0.187630	0.671746	0.055078
6	-1.958070	-0.676625	-0.040027
6	-1.588730	0.668486	-0.045365
8	-0.883380	-1.522795	0.009193
6	-3.359200	-0.679180	0.060246
6	-3.734470	0.664252	0.049387
6	-5.504870	-0.684752	-0.035834
6	-5.135560	0.660243	-0.051859
8	-4.430250	-1.530538	0.020571
6	-6.906040	-0.686638	0.064789
6	-7.281360	0.656575	0.043079
8	4.430250	1.530532	0.020578
8	0.883380	1.522788	0.009203
8	-2.663520	1.514961	-0.003015
8	-6.210500	1.506940	-0.016075
6	-9.051720	-0.692947	-0.032524
6	-8.682500	0.651780	-0.059154
6	-10.828390	0.648560	0.035542
6	-10.453080	-0.694232	0.067825
6	-12.598800	-0.701182	-0.028734
8	-7.977180	-1.538287	0.031075
6	-12.229920	0.643039	-0.065222
8	-11.524390	-1.546105	0.040429
6	-14.001080	-0.702199	0.064918
6	-14.375940	0.639798	0.023862
6	-16.147120	-0.709158	-0.018990
6	-15.779320	0.634201	-0.062083
8	-15.072270	-1.554051	0.047676
6	-17.552750	-0.711474	0.044915
6	-17.925430	0.629364	-0.000049
6	-19.699430	-0.712005	0.003008
6	-19.335020	0.616910	-0.042462
8	-18.621390	-1.563103	0.050597
6	-21.116130	-0.773554	0.017127
1	-21.766780	-1.632950	0.049451
6	-21.503700	0.537259	-0.029683
1	-22.469790	1.012191	-0.053094
8	-9.757700	1.498599	-0.029870
8	-13.305450	1.489759	-0.043857
8	-16.853780	1.480258	-0.056879
8	-20.429680	1.407400	-0.063522

FF[24]-cation

6	19.266487	0.620933	0.018647
6	19.631468	-0.712182	-0.007598
6	17.488346	-0.716975	-0.015243
6	17.862064	0.630554	0.011385
6	15.719331	0.640172	0.022269
8	20.360680	1.409595	0.034313
6	21.430450	0.538466	0.017332
1	22.397618	1.012269	0.028274
6	21.045766	-0.774978	-0.009433
1	21.697360	-1.633796	-0.026459
6	16.089287	-0.711166	-0.003393
8	16.793777	1.482919	0.032444
6	14.323522	0.641884	0.001831
6	13.945851	-0.709341	-0.023056
6	12.180046	0.649813	0.024283
6	12.552314	-0.704615	0.001527
8	13.256128	1.493073	0.026921
6	10.788142	0.651930	-0.005739
6	10.408803	-0.701808	-0.026293
6	8.644542	0.658716	0.022284
6	9.018102	-0.697582	0.004941
8	9.720246	1.502482	0.019257
6	7.254706	0.661113	-0.011018
6	6.874542	-0.694066	-0.025289
8	18.556798	-1.564987	-0.027657

8	15.017471	-1.557583	-0.028085
8	11.480762	-1.550417	-0.024948
8	7.945987	-1.542989	-0.019368
6	5.111102	0.667074	0.018194
6	5.485330	-0.690261	0.007556
6	3.341766	-0.686159	-0.022398
6	3.722308	0.669770	-0.015178
6	1.578728	0.675046	0.013960
8	6.186094	1.511239	0.010835
6	1.953238	-0.682750	0.010403
8	2.652966	1.519551	0.002534
6	0.190324	0.678081	-0.018932
6	-0.190327	-0.678078	-0.018925
6	-1.953240	0.682754	0.010378
6	-1.578731	-0.675043	0.013959
8	-0.879733	1.527563	-0.005335
6	-3.341768	0.686161	-0.022458
6	-3.722311	-0.669767	-0.015224
6	-5.485332	0.690266	0.007471
6	-5.111104	-0.667070	0.018133
8	-4.412532	1.535365	-0.012725
6	-6.874543	0.694069	-0.025406
6	-7.254707	-0.661109	-0.011117
8	4.412531	-1.535361	-0.012641
8	0.879731	-1.527559	-0.005306
8	-2.652969	-1.519548	0.002521
8	-6.186095	-1.511235	0.010767
6	-9.018104	0.697584	0.004789
6	-8.644543	-0.658714	0.022158
6	-10.788142	-0.651930	-0.005881
6	-10.408804	0.701808	-0.026459
6	-12.552314	0.704615	0.001378
8	-7.945989	1.542991	-0.019513
6	-12.180045	-0.649812	0.024163
8	-11.480763	1.550417	-0.025121
6	-13.945850	0.709339	-0.023231
6	-14.323521	-0.641886	0.001682
6	-16.089286	0.711163	-0.003552
6	-15.719329	-0.640174	0.022141
8	-15.017471	1.557581	-0.028268
6	-17.488344	0.716971	-0.015416
6	-17.862061	-0.630558	0.011239
6	-19.631466	0.712177	-0.007770
6	-19.266484	-0.620937	0.018505
8	-18.556797	1.564982	-0.027848
6	-21.045764	0.774972	-0.009617
1	-21.697358	1.633789	-0.026665
6	-21.430447	-0.538471	0.017171
1	-22.397615	-1.012275	0.028118
8	-9.720246	-1.502480	0.019144
8	-13.256126	-1.493073	0.026803
8	-16.793775	-1.482921	0.032323
8	-20.360677	-1.409599	0.034179

FT1

16	0.000000	0.000000	1.159331
6	0.000000	1.093380	0.346499
6	0.000000	0.717367	-0.958284
6	0.000000	-0.717367	-0.958284
6	0.000000	-1.093380	0.346499
1	0.000000	2.046705	0.849036
1	0.000000	-2.046705	0.849036
1	0.000000	1.373423	-1.815649
1	0.000000	-1.373423	-1.815649

FT[1]-cation

16	-1.227805	-0.001274	0.000000
6	-0.002526	1.217458	0.000000
6	1.317173	0.689350	0.000000
6	1.318600	-0.686617	0.000000
6	0.000000	-1.217459	0.000000
1	-0.278460	2.265255	0.000000
1	-0.273757	-2.265827	0.000000
1	2.197444	1.319321	0.000000
1	2.200176	-1.314760	0.000000

FT[2]

6	1.118300	-0.574490	0.000000
6	-0.068230	-1.245390	0.000000
6	-1.170260	-0.342560	0.000000
6	-0.807580	0.997290	0.000000
6	-3.096150	1.229220	0.000000
6	-1.909620	1.900120	0.000000
1	2.114320	-0.992460	0.000000
1	-0.146280	-2.324880	0.000000
1	-4.092170	1.647190	0.000000
1	-1.831570	2.979610	0.000000
16	-2.905620	-0.510420	0.000000
16	0.927770	1.165150	0.000000

FT[2]-cation

6	-2.264513	-0.062430	0.000000
6	-1.435256	1.076250	0.000000
6	-0.103343	0.702952	0.000000
6	0.103343	-0.702952	0.000000
6	2.264513	0.062430	0.000000
6	1.435256	-1.076250	0.000000
1	-3.347003	-0.056629	0.000000
1	-1.822571	2.086535	0.000000
1	3.347003	0.056629	0.000000
1	1.822571	-2.086535	0.000000
16	1.435256	1.561325	0.000000
16	-1.435256	-1.561325	0.000000

FT[3]

6	3.201190	0.991620	0.000000
6	2.667590	-0.290940	0.000000
6	1.246390	-0.290940	0.000000
6	0.712790	0.991620	0.000000
6	-1.234760	-0.235160	0.000000
6	-0.709830	1.023500	0.000000

1	-2.276660	-0.519280	0.000000
1	-1.311490	1.923210	0.000000
16	-0.014590	-1.489000	0.000000
16	1.956990	2.234450	0.000000
6	4.623810	1.023500	0.000000
1	5.225480	1.923210	0.000000
6	5.148750	-0.235160	0.000000
16	3.928580	-1.489010	0.000000
1	6.190640	-0.519280	0.000000

FT[3]-cation

6	-0.928496	1.232106	0.000000
6	0.395503	0.690563	0.000000
6	0.395503	-0.690563	0.000000
6	-0.928496	-1.232106	0.000000
6	0.334666	-3.143012	0.000000
6	-0.954532	-2.624532	0.000000
1	0.603760	-4.191017	0.000000
1	-1.841727	-3.243438	0.000000
16	1.599096	-1.958881	0.000000
16	-2.178802	0.000000	0.000000
6	-0.954532	2.624532	0.000000
1	-1.841727	3.243438	0.000000
6	0.334666	3.143012	0.000000
16	1.599096	1.958881	0.000000
1	0.603760	4.191017	0.000000

FT[4]

6	0.667900	1.092380	0.000000
6	-0.718000	0.987350	0.000000
6	0.060980	3.345730	0.000000
6	1.115280	2.439660	0.000000
6	1.894260	4.798030	0.000000
16	-1.506680	2.558960	0.000000
16	1.409370	-0.481260	0.000000
6	-0.164310	-1.245960	0.000000
1	-0.221400	-2.324370	0.000000
6	-1.194960	-0.352510	0.000000
1	-2.237980	-0.641360	0.000000
6	0.508360	4.693010	0.000000
16	2.682950	3.226430	0.000000
6	2.371220	6.137900	0.000000
6	1.340580	7.031350	0.000000
16	-0.233110	6.266650	0.000000
1	3.414240	6.426750	0.000000
1	1.397670	8.109760	0.000000

FT[4]-cation

6	0.354604	1.746147	0.000000
6	-1.033112	2.044565	0.000000
6	-0.606163	-0.382957	0.000000
6	0.606163	0.382957	0.000000
6	1.033112	-2.044565	0.000000
16	-2.048929	0.608969	0.000000
16	1.311163	3.207416	0.000000
6	-0.140684	4.152738	0.000000
1	-0.058822	5.231147	0.000000
6	-1.311163	3.414690	0.000000
1	-2.296089	3.861565	0.000000
6	-0.354604	-1.746147	0.000000
16	2.048929	-0.608969	0.000000
6	1.311163	-3.414690	0.000000
6	0.140684	-4.152738	0.000000
16	-1.311163	-3.207416	0.000000
1	2.296089	-3.861565	0.000000
1	0.058822	-5.231147	0.000000

FT[5]

6	-0.633660	1.112650	0.000000
6	-1.211380	-0.151850	0.000000
6	-2.900950	1.669220	0.000000
6	-1.597200	2.154030	0.000000
6	-3.283050	3.972380	0.000000
16	1.102450	1.001620	0.000000
6	1.011410	-0.745840	0.000000
1	1.927990	-1.316830	0.000000
6	-0.268820	-1.216580	0.000000
1	-0.519740	-2.269390	0.000000
6	-3.864930	2.708960	0.000000
16	-1.530180	3.906840	0.000000
6	-4.248700	5.011820	0.000000
6	-5.553210	4.531230	0.000000
6	-5.977650	6.792530	0.000000
1	-6.477790	7.749610	0.000000
6	-6.543730	5.551500	0.000000
16	-4.228300	6.751350	0.000000
1	-7.612480	5.380810	0.000000
16	-5.618080	2.773730	0.000000
16	-2.968760	-0.083810	0.000000

FT[5]-cation

6	0.486745	2.621479	0.000000
6	-0.822401	3.160342	0.000000
6	-0.832040	0.692869	0.000000
6	0.488229	1.231864	0.000000
6	0.488229	-1.231864	0.000000
16	1.686693	3.887762	0.000000
6	0.425357	5.080571	0.000000
1	0.700356	6.126214	0.000000
6	-0.852356	4.563183	0.000000
1	-1.743598	5.175924	0.000000
6	-0.832040	-0.692869	0.000000
16	1.736957	0.000000	0.000000
6	0.486745	-2.621479	0.000000
6	-0.822401	-3.160342	0.000000
6	0.425357	-5.080571	0.000000
1	0.700356	-6.126214	0.000000
6	-0.852356	-4.563183	0.000000
16	1.686693	-3.887762	0.000000
1	-1.743598	-5.175924	0.000000
16	-2.075044	-1.930433	0.000000
16	-2.075044	1.930433	0.000000

FT[6]

6	-1.222120	0.382040	0.000000
6	-0.782530	-0.937020	0.000000

6	-3.260110	-0.757130	0.000000
6	-2.636720	0.486810	0.000000
6	-5.110040	0.668620	0.000000
16	0.123630	1.484430	0.000000
6	1.248290	0.143940	0.000000
1	2.308120	0.351180	0.000000
6	0.632720	-1.073390	0.000000
1	1.166820	-2.014700	0.000000
6	-4.673230	-0.652930	0.000000
16	-3.782460	1.815400	0.000000
6	-6.523150	0.772820	0.000000
6	-7.146540	-0.471120	0.000000
6	-9.000730	0.952710	0.000000
6	-8.561140	-0.366350	0.000000
16	-7.668860	2.101400	0.000000
6	-10.415980	1.089080	0.000000
1	-10.950080	2.030390	0.000000
6	-11.031560	-0.128250	0.000000
1	-12.091390	-0.335490	0.000000
16	-2.114400	-2.085710	0.000000
16	-6.000810	-1.799710	0.000000
16	-9.906900	-1.468740	0.000000

FT[6]-cation

6	3.568441	0.761496	0.000000
6	3.568441	2.172742	0.000000
6	1.281439	1.242113	0.000000
6	2.280092	0.229619	0.000000
6	0.000378	-0.711480	0.000000
16	5.195037	0.134825	0.000000
6	5.820776	1.755770	0.000000
1	6.892372	1.898005	0.000000
6	4.856808	2.737016	0.000000
1	5.081477	3.794960	0.000000
6	-0.000378	0.711480	0.000000
16	1.618193	-1.393221	0.000000
6	-1.281439	-1.242113	0.000000
6	-2.280091	-0.229619	0.000000
6	-3.568441	-2.172742	0.000000
6	-3.568441	-0.761496	0.000000
16	-1.954016	-2.862257	0.000000
6	-4.856808	-2.737016	0.000000
1	-5.081477	-3.794960	0.000000
6	-5.820776	-1.755770	0.000000
1	-6.892372	-1.898005	0.000000
16	1.954016	2.862257	0.000000
16	-1.618193	1.393221	0.000000
16	-5.195037	-0.134825	0.000000

FT[7]

6	0.286480	-1.247940	0.000000
6	1.203840	-0.203060	0.000000
6	2.298170	-2.433000	-0.000010
6	0.909510	-2.522090	0.000000
6	1.999660	-4.749590	0.000000
16	-1.344190	-0.641940	0.000000
6	-0.753880	1.005200	0.000000
1	-1.467340	1.815820	0.000000
6	0.607750	-1.087740	0.000000
1	1.150950	-2.023820	0.000000
6	2.920730	-3.705530	0.000000
16	0.339830	-4.181510	0.000000
6	2.622870	-6.021140	0.000020
6	4.012340	-5.932750	0.000020
6	3.715600	-8.247380	0.000020
6	4.636730	-7.204380	0.000020
16	2.055030	-7.681050	0.000010
6	4.340980	-9.520370	0.000010
6	5.728830	-9.435420	0.000010
6	5.484470	-11.722960	0.000010
1	5.688090	-12.783470	0.000010
6	6.383870	-10.697330	0.000010
16	3.820970	-11.180470	0.000010
1	7.456510	-10.841450	0.000010
16	2.867510	-0.773630	0.000000
16	4.581050	-4.272890	0.000010
16	6.297050	-7.770950	0.000020

FT[7]-cation

6	4.558264	-0.528517	0.000005
6	5.094758	0.773422	0.000005
6	2.624480	0.783459	0.000003
6	3.161216	-0.528869	0.000004
6	0.693680	-0.533387	0.000001
16	5.822808	-1.727014	0.000008
6	7.021294	-0.467100	0.000008
1	8.065777	-0.744930	0.000010
6	6.503493	0.804875	0.000007
1	7.113071	1.698279	0.000007
6	1.234384	0.780820	0.000001
16	1.931899	-1.778030	0.000003
6	-0.693680	-0.533387	-0.000001
6	-1.234384	0.780820	-0.000002
6	-3.161216	-0.528869	-0.000003
6	-2.624480	0.783459	-0.000004
16	-1.931899	-1.778030	-0.000001
6	-4.558264	-0.528517	-0.000005
6	-5.094758	0.773422	-0.000006
6	-7.021294	-0.467100	-0.000006
1	-8.065777	-0.744930	-0.000006
6	-6.503493	0.804875	-0.000007
16	-5.822808	-1.727014	-0.000006
1	-7.113071	1.698279	-0.000008
16	3.863989	2.024820	0.000003
16	0.000000	2.027754	-0.000001
16	-3.863989	2.024820	-0.000006

FT[8]

6	0.606490	1.127610	0.000000
6	-0.772090	0.945760	0.000000
6	-0.126550	3.344380	0.000000
6	0.977000	2.496550	0.000000
6	1.624500	4.890380	-0.000010
16	1.434250	-0.402460	0.000000
6	-0.094870	-1.252820	0.000000
1	-0.092020	-2.332700	0.000000
6	-1.173790	-0.418080	0.000000
1	-2.199030	-0.764690	0.000000

6	0.243530	4.711670	-0.000010
16	2.498870	3.369440	0.000000
6	1.993300	6.257210	-0.000010
6	0.889520	7.106490	-0.000010
6	2.639290	8.652030	-0.000030
6	1.258320	8.473310	-0.000020
16	3.514730	7.131230	-0.000020
6	3.009370	10.019310	-0.000040
6	1.905820	10.867150	-0.000040
6	3.654910	12.417940	-0.000060
6	2.276330	12.236090	-0.000050
16	4.530830	10.892740	-0.000050
6	4.056610	13.781780	-0.000070
1	5.081850	14.128390	-0.000080
6	2.977690	14.616520	-0.000080
1	2.974850	15.696400	-0.000090
16	-1.648010	2.470950	0.000000
16	-0.631910	6.232470	-0.000010
16	0.383950	9.994260	-0.000030
16	1.448570	13.766150	-0.000070

FT[8]-cation

6	-5.550228	0.419929	-0.000026
6	-6.031090	-0.900875	-0.000029
6	-3.561553	-0.807137	-0.000018
6	-4.151641	0.478473	-0.000020
6	-1.685514	0.587074	-0.000008
16	-6.863254	1.564065	-0.000032
6	-8.010061	0.255496	-0.000039
1	-9.064929	0.490291	-0.000044
6	-7.439166	-0.991845	-0.000036
1	-8.009628	-1.910743	-0.000039
6	-2.170183	-0.745748	-0.000011
16	-2.975658	1.777612	-0.000014
6	-0.297639	0.644734	-0.000002
6	0.297639	-0.644734	0.000001
6	2.170183	0.745748	0.000011
6	1.685514	-0.587074	0.000008
16	0.885833	1.940858	0.000005
6	3.561553	0.807137	0.000017
6	4.151641	-0.478473	0.000020
6	6.031090	0.900875	0.000030
6	5.550228	-0.419929	0.000027
16	4.748337	2.098888	0.000024
6	7.439166	0.991845	0.000037
1	8.009628	1.910743	0.000041
6	8.010061	-0.255496	0.000041
1	9.064929	-0.490291	0.000047
16	-4.748337	-2.098888	-0.000023
16	-0.885833	-1.940858	-0.000005
16	2.975658	-1.777612	0.000013
16	6.863254	-1.564065	0.000032

FT[12]

6	11.964133	-0.363158	0.000100
6	11.416025	0.886056	0.000085
6	9.484889	-0.466462	0.000033
6	9.995543	0.826950	0.000049
16	10.768551	-1.640503	0.000067
6	8.067021	-0.493749	-0.000005
6	7.512250	0.782698	-0.000019
6	5.587762	-0.541207	-0.000020
6	6.096262	0.755330	-0.000023
16	6.851036	-1.758461	-0.000003
6	4.172670	-0.566934	-0.000023
6	3.616495	0.710357	-0.000034
16	8.728638	2.046764	0.000018
16	4.833828	1.974008	-0.000038
6	1.692785	-0.612801	-0.000045
6	2.201739	0.684139	-0.000048
6	-0.278168	0.638718	-0.000031
6	0.278168	-0.638718	-0.000031
6	-2.201739	-0.684139	-0.000048
16	2.955661	-1.831135	-0.000027
6	-1.692785	0.612801	-0.000045
16	-0.939079	-1.902707	-0.000041
6	-3.616495	-0.710357	-0.000033
6	-4.172670	0.566934	-0.000022
6	-6.096262	-0.755330	-0.000022
6	-5.587762	0.541207	-0.000019
16	-4.833828	-1.974008	-0.000038
6	-7.512250	-0.782698	-0.000018
6	-8.067021	0.493749	-0.000004
6	-9.995543	-0.826950	0.000049
6	-9.484889	0.466462	0.000034
16	-8.728638	-2.046764	0.000018
6	-11.416025	-0.886056	0.000085
1	-12.000845	-1.796692	0.000101
6	-11.964133	0.363158	0.000101
1	-13.011107	0.627753	0.000120
16	0.939079	1.902707	-0.000041
16	-2.955661	1.831135	-0.000027
16	-6.851036	1.758461	-0.000002
16	-10.768551	1.640503	0.000068
1	12.000845	1.796692	0.000101
1	13.011107	-0.627753	0.000119

FT[12]-cation

6	-11.887816	-0.365554	-0.000088
6	-11.344702	0.890435	-0.000093
6	-9.420487	-0.472211	-0.000063
6	-9.930476	0.831202	-0.000078
16	-10.705323	-1.645869	-0.000067
6	-8.013953	-0.497874	-0.000050
6	-7.456491	0.792798	-0.000056
6	-5.543548	-0.550391	-0.000028
6	-6.056010	0.762806	-0.000043
16	-6.807053	-1.768101	-0.000027
6	-4.147126	-0.574485	-0.000018
6	-3.584225	0.721094	-0.000025
16	-8.672789	2.056227	-0.000076
16	-4.800411	1.986678	-0.000043
6	-1.675018	-0.623078	-0.000001
6	-2.190217	0.693741	-0.000015
6	0.282142	0.648588	0.000001
6	-0.282142	-0.648588	0.000008
6	2.190218	-0.693741	0.000026
16	-2.936395	-1.843919	0.000001
6	1.675019	0.623078	0.000011

16	0.931619	-1.916533	0.000027
6	3.584225	-0.721094	0.000032
6	4.147126	0.574485	0.000024
6	6.056010	-0.762806	0.000048
6	5.543548	0.550391	0.000033
16	4.800411	-1.986678	0.000051
6	7.456491	-0.792798	0.000055
6	8.013952	0.497874	0.000046
6	9.930475	-0.831202	0.000068
6	9.420487	0.472211	0.000053
16	8.672789	-2.056227	0.000073
6	11.344702	-0.890435	0.000076
1	11.933847	-1.797593	0.000088
6	11.887816	0.365553	0.000067
1	12.936118	0.626800	0.000071
16	-0.931619	1.916533	-0.000017
16	2.936396	1.843919	0.000007
16	6.807053	1.768100	0.000028
16	10.705323	1.645869	0.000050
1	-11.933848	1.797593	-0.000105
1	-12.936119	-0.626800	-0.000096

FT[16]

6	15.854939	-0.417053	-0.000101
6	15.316796	0.836485	-0.000101
6	13.375055	-0.500751	-0.000079
6	13.895896	0.788613	-0.000090
6	11.412424	0.764059	-0.000038
6	11.957034	-0.516780	-0.000049
6	9.477591	-0.544728	-0.000028
16	14.649370	-1.684910	-0.000083
6	9.996290	0.747813	-0.000030
16	10.731209	-1.771892	-0.000045
6	8.062384	-0.559202	-0.000010
6	7.516361	0.722520	0.000000
6	5.582345	-0.585615	0.000001
6	6.101519	0.707374	0.000004
16	6.835584	-1.813836	-0.000007
6	4.167687	-0.600223	0.000020
6	3.621480	0.681730	0.000034
6	1.687637	-0.626275	0.000025
6	2.206924	0.666848	0.000036
16	2.940700	-1.854715	0.000007
6	0.273113	-0.641007	0.000032
6	-0.273113	0.641007	0.000046
16	12.638747	2.018449	-0.000065
16	8.743625	1.976484	-0.000009
16	4.848695	1.936002	0.000026
16	0.953989	1.895403	0.000054
6	-2.206925	-0.666848	0.000034
6	-1.687637	0.626274	0.000047
6	-4.167687	0.600222	0.000055
6	-3.621481	-0.681730	0.000040
6	-6.101519	-0.707375	0.000020
16	-0.953989	-1.895404	0.000022
6	-5.582345	0.585615	0.000041
16	-4.848695	-1.936003	0.000015
6	-7.516361	-0.722520	0.000026
6	-8.062384	0.559202	0.000047
6	-9.996290	-0.747813	-0.000006
6	-9.477591	0.544728	0.000027
16	-8.743625	-1.976484	-0.000015
6	-11.412424	-0.764059	-0.000007
6	-11.957034	0.516780	0.000019
6	-13.895896	-0.788612	-0.000035
6	-13.375055	0.500752	0.000002
16	-12.638747	-2.018449	-0.000053
6	-15.316796	-0.836484	-0.000048
1	-15.908845	-1.742428	-0.000077
6	-15.854939	0.417054	-0.000021
1	-16.899788	0.689918	-0.000025
16	-2.940700	1.854715	0.000063
16	-6.835583	1.813836	0.000066
16	-10.731209	1.771892	0.000053
16	-14.649369	1.684910	0.000023
1	15.908845	1.742429	-0.000112
1	16.899788	-0.689918	-0.000110

ft16-cat

6	15.773775	0.419033	-0.000145
6	15.239778	-0.839279	-0.000147
6	13.302960	0.505136	-0.000104
6	13.823096	-0.791188	-0.000123
6	11.346886	-0.771397	-0.000087
6	11.892763	0.519473	-0.000085
6	9.420308	0.551621	-0.000052
16	14.577745	1.688994	-0.000114
6	9.941625	-0.752684	-0.00007
16	10.674038	1.778754	-0.000058
6	8.018494	0.564170	-0.000035
6	7.468165	-0.730845	-0.000038
6	5.544833	0.593631	-0.000008
6	6.068609	-0.714010	-0.000024
16	6.797412	1.823078	-0.000012
6	4.146766	0.606984	0.000007
6	3.594779	-0.690211	0.000001
6	1.672905	0.634488	0.000024
6	2.197667	-0.674583	0.000011
16	2.924079	1.865335	0.000025
6	0.276222	0.648936	0.000032
6	-0.276223	-0.648936	0.000025
16	12.573144	-2.024955	-0.000116
16	8.695000	-1.985551	-0.000063
16	4.820434	-1.946569	-0.000021
16	0.947976	-1.906453	0.000009
6	-2.197669	0.674583	0.000046
6	-1.672906	-0.634488	0.000033
6	-4.146767	-0.606984	0.000039
6	-3.594779	0.690211	0.000048
6	-6.068610	0.714010	0.000057
16	-0.947978	1.906453	0.000048
6	-5.544833	-0.593631	0.000044
16	-4.820435	1.946569	0.000063
6	-7.468165	0.730845	0.000057
6	-8.018494	-0.564170	0.000045
6	-9.941624	0.752684	0.00006
6	-9.420308	-0.551622	0.000047
16	-8.695000	1.985551	0.00007
6	-11.346885	0.771397	0.000059
6	-11.892762	-0.519472	0.000046

6	-13.823094	0.791188	0.000058
6	-13.302959	-0.505136	0.000045
16	-12.573143	2.024955	0.000071
6	-15.239776	0.839279	0.000057
1	-15.835001	1.742577	0.000066
6	-15.773773	-0.419033	0.000044
1	-16.819515	-0.689734	0.00004
16	-2.924080	-1.865335	0.000026
16	-6.797413	-1.823078	0.000033
16	-10.674038	-1.778754	0.000034
16	-14.577744	-1.688994	0.000032
1	15.835003	-1.742577	-0.000163
1	16.819517	0.689733	-0.000159

FT[24]

6	-21.160450	0.540500	0.000020
6	-21.688640	-0.745880	0.000020
6	-19.205130	-0.735570	0.000010
6	-19.742370	0.548390	0.000010
6	-17.262880	0.562220	0.000010
16	-22.427960	1.731930	0.000020
6	-23.640710	0.470990	0.000020
1	-24.683980	0.749830	0.000030
6	-23.109790	-0.785630	0.000020
1	-23.707040	-1.688140	0.000020
6	-17.788930	-0.727370	0.000010
16	-18.509460	1.796500	0.000010
6	-15.847630	0.568560	0.000010
6	-15.308970	-0.716290	0.000000
6	-13.367560	0.580900	0.000000
6	-13.894090	-0.709150	0.000000
16	-14.613780	1.816220	0.000000
6	-11.952870	0.587350	0.000000
6	-11.414040	-0.697750	0.000000
6	-9.472830	0.599350	-0.000010
6	-9.999460	-0.690850	-0.000010
16	-10.718870	1.834880	0.000000
6	-8.058290	0.605880	-0.000010
6	-7.519470	-0.679330	-0.000010
16	-20.438590	-1.982910	0.000010
16	-16.543360	-1.963210	0.000000
16	-12.648390	-1.944970	0.000000
16	-8.753720	-1.926640	-0.000010
6	-5.578310	0.617700	-0.000010
6	-6.104970	-0.672550	-0.000010
6	-3.625010	-0.660970	-0.000010
6	-4.163820	0.624280	-0.000010
6	-1.683870	0.636000	-0.000010
16	-6.824220	1.853340	-0.000010
6	-2.210540	-0.654270	-0.000010
16	-2.929710	1.871700	-0.000010
6	-0.269400	0.642630	-0.000010
6	0.269400	-0.642630	-0.000010
6	2.210540	0.654270	-0.000010
6	1.683870	-0.636000	-0.000010
16	0.964750	1.890020	-0.000010
6	3.625010	0.660970	-0.000010
6	4.163820	-0.624280	-0.000010
6	6.104970	0.672550	-0.000010
6	5.578310	-0.617700	-0.000010
16	4.859210	1.908320	-0.000010
6	7.519470	0.679330	-0.000010
6	8.058290	-0.605880	-0.000010
16	-4.859210	-1.908320	-0.000010
16	-0.964750	-1.890020	-0.000010
16	2.929710	-1.871700	-0.000010
16	6.824220	-1.853340	-0.000010
6	9.999460	0.690850	-0.000010
6	9.472830	-0.599350	-0.000010
6	11.952870	-0.587350	0.000000
6	11.414040	0.697750	0.000000
6	13.894090	0.709150	0.000000
16	8.753720	1.926640	-0.000010
6	13.367560	-0.580900	0.000000
16	12.648390	1.944970	0.000000
6	15.308970	0.716290	0.000000
6	15.847630	-0.568560	0.000010
6	17.788930	0.727370	0.000010
6	17.262880	-0.562220	0.000010
16	16.543360	1.963210	0.000000
6	19.205130	0.735570	0.000010
6	19.742370	-0.548390	0.000010
6	21.688640	0.745880	0.000020
6	21.160450	-0.540500	0.000020
16	20.438590	1.982910	0.000010
6	23.109790	0.785630	0.000020
1	23.707040	1.688140	0.000020
6	23.640710	-0.470990	0.000020
1	24.683980	-0.749830	0.000030
16	10.718870	-1.834880	0.000000
16	14.613780	-1.816220	0.000000
16	18.509460	-1.796500	0.000010
16	22.427960	-1.731930	0.000020

FT[24]-cation

6	-21.081006	-0.543503	-0.000092
6	-21.608642	0.747122	-0.000098
6	-19.130020	0.740158	-0.000072
6	-19.667659	-0.549979	-0.000078
6	-17.192922	-0.566679	-0.000050
16	-22.348550	-1.734755	-0.000109
6	-23.555251	-0.472543	-0.000121
1	-24.599032	-0.750176	-0.000133
6	-23.027279	0.787048	-0.000115
1	-23.626605	1.687788	-0.000121
6	-17.720427	0.730087	-0.000055
16	-18.439421	-1.800782	-0.000064
6	-15.785874	-0.571342	-0.000036
6	-15.244970	0.721726	-0.000031
6	-13.310326	-0.586044	-0.000009
6	-13.839487	0.713009	-0.000015
16	-14.556077	-1.821830	-0.000022
6	-11.905909	-0.591092	0.000002
6	-11.363933	0.703520	0.000004
6	-9.430423	-0.604739	0.000023
6	-9.960249	0.695425	0.000017
16	-10.675399	-1.841333	0.000015
6	-8.027183	-0.610284	0.000033
6	-7.484842	0.685071	0.000034
16	-20.363399	1.986751	-0.000084

16	-16.479126	1.968748	-0.000043
16	-12.597447	1.951571	-0.000007
16	-8.717639	1.933757	0.000023
6	-5.551859	-0.623105	0.000045
6	-6.081903	0.677529	0.000040
6	-3.606646	0.666494	0.000051
6	-4.149078	-0.629153	0.000051
6	-1.673869	-0.641323	0.000059
16	-6.796157	-1.860245	0.000041
6	-2.203963	0.659469	0.000055
16	-2.917656	-1.878840	0.000057
6	-0.271222	-0.647860	0.000061
6	0.271222	0.647861	0.000058
6	2.203962	-0.659468	0.000063
6	1.673869	0.641324	0.000059
16	0.960569	-1.897274	0.000065
6	3.606645	-0.666493	0.000061
6	4.149078	0.629154	0.000056
6	6.081902	-0.677529	0.000055
6	5.551859	0.623106	0.000052
16	4.838870	-1.915599	0.000062
6	7.484842	-0.685070	0.000049
6	8.027183	0.610284	0.000042
16	-4.838870	1.915600	0.000044
16	-0.960569	1.897275	0.000054
16	2.917656	1.878841	0.000054
16	6.796157	1.860246	0.000043
6	9.960248	-0.695425	0.000037
6	9.430423	0.604739	0.000035
6	11.905909	0.591092	0.000018
6	11.363933	-0.703520	0.000027
6	13.839487	-0.713009	0.000012
16	8.717638	-1.933756	0.000047
6	13.310327	0.586044	0.000010
16	12.597447	-1.951571	0.000025
6	15.244970	-0.721726	-0.000001
6	15.785875	0.571341	-0.000012
6	17.720427	-0.730088	-0.000021
6	17.192923	0.566678	-0.000023
16	16.479126	-1.968748	-0.000004
6	19.130020	-0.740159	-0.000034
6	19.667659	0.549978	-0.000046
6	21.608643	-0.747123	-0.000058
6	21.081006	0.543502	-0.000060
16	20.363399	-1.986753	-0.000039
6	23.027280	-0.787050	-0.000071
1	23.626605	-1.687790	-0.000073
6	23.555251	0.472541	-0.000083
1	24.599033	0.750174	-0.000095
16	10.675399	1.841333	0.000022
16	14.556078	1.821830	-0.000008
16	18.439422	1.800782	-0.000042
16	22.348551	1.734753	-0.000078