

## Supporting Information

### Benchmark Calculations for Bond Dissociation Energies and Enthalpy of Formations of Chlorinated and Brominated Polycyclic Aromatic Hydrocarbons

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**Table S1.** Predicted BDEs of C-Cl and C-Br bond using various theoretical methods. (kcal mol<sup>-1</sup>)

No.	G4	CBS-QB3	G3	G3MP2	M06-2X/6-311++G(d,p)	ωB97X-D/6-311++G(d,p)	B2PLYP-D3/6-311++G(d,p)
1 (Cl)	96.65	101.25	98.7	100.07	94.62	94.04	92.96
2 (Cl)	97.12	101.25	99.46	100.88	95.46	94.37	93.48
3 (Cl)	95.81	100.67	98.99	100.36	94.67	94.12	93.09
4 (Cl)	96.15	101.63	99.29	100.7	94.96	94.44	93.35
5 (Cl)	94.95	99.3	97.81	97.94	94.82	93.99	93.59
6 (Cl)	94.67	99.02	97.6	97.7	94.95	94.38	93.7
7 (Cl)	102.55	99.64	99.07	99.6	95.08	94.18	95.46
8 (Cl)	102.25	99.28	98.9	99.57	94.86	94.33	95.22
9 (Cl)	102.49	100.21	97.66	97.73	94.9	93.74	95.93

10 (Cl)	99.98	99.45	103.86	107.28	94.47	93.67	93.43
11 (Cl)	99.95	99.85	99.7	100.44	94.73	93.82	93.46
12 (Cl)	100.26	100.15	100.2	100.93	95.13	94.66	93.94
13 (Cl)	100.11	100	99.9	100.63	94.97	94.49	93.9
14 (Cl)	92.31	92.46	91.64	92.31	86.25	85.63	86.07
15 (Cl)	92.43	104.97	104.1	106.73	96.05	95.39	94.45
16 (Cl)	91.44	104.11	102.85	105.52	95.01	94.47	93.59
17 (Cl)	91.47	103.97	103	105.65	94.88	94.44	93.45
18 (Cl)	91.47	103.98	102.76	105.4	94.66	93.99	93.45
19 (Cl)	63.81	68.43	67.48	69.72	64.95	62.97	63.2
20 (Cl)	96.29	103.27	102.91	103.61	98.94	98.75	98.32
21 (Cl)	92.94	102.15	101.99	104.23	95.57	94.91	94.42
22 (Cl)	91.8	98.38	97.74	97.77	94.27	93.74	93.07
23 (Cl)	93.02	102.51	102.09	104.31	95.6	94.83	94.47
24 (Cl)	69.17	71.29	70.83	73.19	68.92	66.23	68.16
25 (Cl)	94.13	100.51	99.08	99.17	96.54	95.95	95.23
26 (Cl)	92.32	102.82	97.36	97.45	94.52	93.94	93.27
27 (Cl)	93.81	104.28	98.75	98.88	95.95	95.19	94.73
1 (Br)	82.6	89.51	85.08	85.95	80.04	81.15	81.44
2 (Br)	83.13	89.63	85.91	86.77	80.88	81.45	81.95
3 (Br)	81.65	89.12	85.45	86.3	80.12	81.23	81.56
4 (Br)	86.86	89.98	85.76	86.66	80.45	81.62	81.9
5 (Br)	80.96	87.4	84.32	83.86	80.03	80.87	81.88
6 (Br)	75.49	87.57	84.18	83.75	80.43	81.59	82.31
7 (Br)	88.52	87.83	85.63	85.56	80.5	81.45	84.16
8 (Br)	88.16	87.8	85.54	85.6	80.36	81.52	83.85
9 (Br)	88.24	87.77	84.07	83.47	79.82	80.45	84.2
10 (Br)	85.87	87.6	90.36	93.17	79.71	80.62	81.81
11 (Br)	85.76	87.93	86.13	86.28	79.57	80.53	81.63
12 (Br)	86.2	88.64	86.78	86.97	80.57	81.81	82.48

13 (Br)	86.02	88.5	86.49	86.67	80.27	81.49	82.23
14 (Br)	77.45	79.79	77.49	77.57	70.5	71.67	73.69
15 (Br)	78.66	93.36	90.92	92.97	81.51	82.59	83.01
16 (Br)	77.31	92.72	89.4	91.55	80.49	81.71	82.22
17 (Br)	77.32	92.52	89.57	91.69	80.16	81.48	81.96
18 (Br)	77.26	91.94	89.13	91.16	79.68	80.77	81.61
19 (Br)	51.61	60.67	55.76	57.36	51.4	51.1	52.8
20 (Br)	82.65	91.93	89.86	89.99	84.73	86.24	87.14
21 (Br)	78.97	90.74	88.74	90.41	81.03	82.08	82.96
22 (Br)	77.7	86.92	84.32	83.81	79.62	80.84	81.56
23 (Br)	79.09	91.04	88.8	90.43	81.03	81.98	83.02
24 (Br)	57.01	62.34	58.81	60.57	54.93	53.74	57.4
25 (Br)	80.41	89.2	85.97	85.47	82.24	83.32	83.97
26 (Br)	78.23	91.36	83.93	83.49	79.91	81.01	81.78
27 (Br)	79.92	92.85	85.46	84.99	81.46	82.42	83.38

**Table S2.** Predicted  $\Delta_f H_{298}$  of the studied Cl- and Br- PAHs using various theoretical methods.

(kcal mol<sup>-1</sup>)

No.	G4	CBS- QB3	G3	G3MP2	M06- 2X/cc- pVTZ	$\omega$ B97X- D/ cc- pVTZ	B2PLYP- D3/ cc- pVTZ	GA
1 (Cl)	12.81	11.99	18.48	16.60	11.46	14.58	15.46	12.7
2 (Cl)	8.59	3.55	11.48	9.77	3.32	6.68	8.33	4.71
3 (Cl)	9.54	3.43	11.54	9.87	4.13	6.92	8.87	4.71
4 (Cl)	9.74	4.51	11.79	10.11	4.30	7.11	9.10	4.71
5 (Cl)	27.85	28.29	36.76	33.98	27.50	32.66	31.38	27.92
6 (Cl)	27.88	28.28	36.70	33.92	27.03	31.90	30.99	27.92
7 (Cl)	35.25	47.54	58.52	54.74	47.09	54.09	50.49	43.14
8 (Cl)	35.20	47.62	58.61	54.78	47.09	53.63	50.37	43.14

9 (Cl)	35.67	47.90	58.95	16.60	47.95	55.26	51.09	43.14
10 (Cl)	30.06	42.32	53.28	9.77	41.32	48.15	45.26	40.94
11 (Cl)	30.27	42.45	53.38	9.87	41.13	48.10	45.26	40.94
12 (Cl)	29.87	42.11	53.06	10.11	40.62	47.09	44.68	40.94
13 (Cl)	29.79	25.04	52.94	33.98	40.59	47.06	44.56	40.94
14 (Cl)	36.28	31.24	59.92	33.92	47.75	54.67	51.44	40.94
15 (Cl)	24.96	20.00	47.15	54.74	35.66	40.06	41.22	35.09
16 (Cl)	26.08	21.22	48.37	54.78	36.67	40.93	42.18	35.09
17 (Cl)	26.11	37.47	48.39	55.19	36.76	40.93	42.24	35.09
18 (Cl)	26.24	37.50	48.41	49.63	37.25	41.80	42.59	35.09
19 (Cl)	21.11	38.96	49.70	49.70	38.99	43.23	43.84	33.33
20 (Cl)	44.44	55.44	64.15	49.70	56.00	61.01	58.99	44.97
21 (Cl)	43.93	54.91	63.54	49.39	55.43	60.70	58.42	44.63
22 (Cl)	45.13	55.97	64.64	49.28	56.49	61.67	59.58	44.63
23 (Cl)	44.51	55.32	64.03	56.31	55.97	61.41	59.10	44.63
24 (Cl)	13.29	30.57	40.98	44.04	30.16	33.55	35.05	20.57
25 (Cl)	17.89	29.02	39.14	44.04	28.89	32.47	34.34	21.76
26 (Cl)	18.97	30.11	40.20	45.24	29.82	33.31	35.22	21.76
27 (Cl)	18.71	28.75	39.96	45.25	29.77	33.51	35.16	21.76
1 (Br)	24.76	21.63	29.96	45.32	24.16	25.22	23.86	22.01
2 (Br)	15.97	15.79	22.88	61.07	15.99	17.34	16.68	14.02
3 (Br)	21.60	13.75	22.94	60.44	16.75	17.54	17.25	14.02
4 (Br)	16.94	16.22	23.18	61.48	16.92	17.67	17.42	14.02
5 (Br)	39.75	38.10	48.13	60.90	40.33	43.46	39.85	37.23
6 (Br)	39.70	37.65	47.99	36.66	39.66	42.44	39.27	37.23
7 (Br)	65.19	57.29	69.84	37.72	59.83	64.61	58.62	52.45
8 (Br)	65.24	57.02	69.85	37.45	59.65	64.17	58.59	52.45
9 (Br)	65.87	58.28	70.43	28.59	61.13	66.31	59.58	52.45
10 (Br)	60.15	52.11	64.67	21.73	54.11	58.90	53.64	50.25
11 (Br)	60.42	52.31	64.83	21.79	54.38	59.10	53.86	50.25

12 (Br)	59.90	51.54	64.36	22.01	53.29	57.68	53.01	50.25
13 (Br)	59.84	51.44	64.24	45.94	53.34	57.73	53.04	50.25
14 (Br)	67.11	58.85	71.93	45.75	61.61	66.41	60.69	50.25
15 (Br)	53.88	45.77	58.21	66.67	48.25	50.57	49.41	44.4
16 (Br)	55.37	46.77	59.70	66.63	49.30	51.45	50.45	44.4
17 (Br)	55.40	46.83	59.70	67.34	49.62	51.68	50.66	44.4
18 (Br)	55.57	47.47	59.93	61.62	50.25	52.70	51.13	44.4
19 (Br)	48.43	44.65	59.30	61.75	50.05	52.26	50.47	44.24
20 (Br)	71.14	64.70	75.07	61.75	68.19	71.28	66.98	56.96
21 (Br)	70.95	64.24	74.67	61.23	68.05	71.27	66.66	53.94
22 (Br)	72.28	65.34	75.94	61.13	69.23	72.32	67.97	53.94
23 (Br)	71.46	64.71	75.21	68.92	68.60	71.96	67.29	53.94
24 (Br)	39.74	37.44	50.88	55.68	42.31	43.87	42.80	31.48
25 (Br)	45.89	38.25	50.13	55.68	41.22	42.77	42.35	31.07
26 (Br)	47.35	39.50	51.52	57.09	42.54	43.96	43.58	31.07
27 (Br)	46.88	39.21	51.12	57.10	42.31	43.98	43.30	31.07

### optimized geometry at M06-2X/6-311++G(d,p) level

#### PAH Radical

No. 1

C	0.	1.3208	0.
C	-1.20923	0.63016	0.
C	-1.22059	-0.76799	0.
C	0.	-1.39708	0.
C	1.22059	-0.768	0.
C	1.20923	0.63017	0.
H	0.	2.40406	0.
H	-2.14665	1.17483	0.
H	-2.15252	-1.32107	0.
H	2.15252	-1.32106	0.

H	2.14666	1.17482	0.
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No. 2

C	1.15386	1.17974	-0.00001
C	-0.23951	1.15192	0.
C	-0.94058	-0.0601	0.00001
C	-0.15202	-1.19146	0.
C	1.21851	-1.23075	0.
C	1.88732	-0.0018	-0.00001
H	1.66861	2.13306	-0.00001
H	-0.79859	2.0826	0.
H	1.76519	-2.16668	0.
H	2.97087	0.02498	-0.00001
C	-2.44582	-0.12214	0.00001
H	-2.81094	-0.65342	-0.88111
H	-2.81093	-0.65341	0.88113
H	-2.87477	0.88042	0.00001

No. 3

C	-1.313	1.0692	0.00192
C	0.07629	1.15343	-0.00925
C	0.87732	0.00897	-0.01162
C	0.2508	-1.24566	-0.00928
C	-1.12115	-1.27514	0.00274
C	-1.94544	-0.17711	0.00857
H	-1.9093	1.97489	0.00138
H	0.55105	2.12871	-0.01809
H	-3.02541	-0.26155	0.0143
C	2.38059	0.11431	0.00969
H	2.7492	0.1355	1.03892
H	2.84212	-0.73776	-0.49142

H	2.7171	1.02736	-0.4835
H	0.84279	-2.15508	-0.01826

No. 4

C	-1.26979	1.21529	0.00277
C	0.12809	1.20336	-0.00812
C	0.84015	0.00268	-0.01074
C	0.13177	-1.20145	-0.00822
C	-1.26489	-1.21851	0.00281
C	-1.90249	-0.00232	0.0089
H	-1.819	2.14962	0.00213
H	0.66915	2.14442	-0.01685
C	2.34806	0.00126	0.00841
H	2.72233	-0.10995	1.02975
H	2.7484	-0.82421	-0.58246
H	2.74799	0.93339	-0.39275
H	0.67676	-2.14047	-0.01696
H	-1.811	-2.15465	0.00232

No. 5

C	2.3886	0.72861	0.
C	1.18932	1.3898	-0.00001
C	-0.035	0.67212	0.
C	0.01398	-0.75429	0.
C	1.26994	-1.41419	0.
C	2.4298	-0.68679	0.
H	-1.32385	2.40558	-0.00001
H	3.31603	1.28883	-0.00001
H	1.15732	2.47415	-0.00001
C	-1.29925	1.32146	0.
C	-1.2245	-1.41049	0.00001

H	1.28875	-2.49756	0.00001
H	3.38761	-1.19302	0.
C	-2.43974	-0.81877	0.
C	-2.46685	0.60498	0.
H	-3.36121	-1.3892	0.00001
H	-3.42238	1.11661	0.

No. 6

C	2.33743	-0.78902	0.
C	1.12447	-1.42413	0.
C	-0.08555	-0.68225	0.
C	-0.01873	0.73938	0.
C	1.25237	1.36986	0.
C	2.40138	0.62464	0.
H	-1.38827	-2.41011	0.
H	3.25406	-1.36648	0.
H	1.07068	-2.50754	0.
C	-1.35298	-1.32539	0.
C	-1.23359	1.48877	0.
H	1.29664	2.45347	0.
H	3.36726	1.11578	0.
C	-2.39359	0.79646	0.
C	-2.51698	-0.59493	0.
H	-3.48625	-1.07876	0.
H	-1.19946	2.57326	0.

No. 7

C	3.69092	0.63193	0.
C	2.52426	1.33432	0.00001
C	1.25369	0.67229	0.
C	1.22113	-0.76806	-0.00001



C	2.47976	-1.4093	-0.00002
C	3.67976	-0.80439	-0.00001
C	0.04551	1.36902	0.00001
C	-0.00234	-1.43683	-0.00002
C	-1.20617	-0.73111	-0.00001
C	-1.18148	0.70325	0.00001
C	-2.42517	1.41029	0.00002
H	-2.40293	2.49473	0.00003
C	-3.60963	0.73965	0.00002
C	-3.63387	-0.68741	0.
C	-2.47236	-1.39688	-0.00001
H	0.05982	2.45486	0.00002
H	4.64264	1.15049	0.00001
H	2.53724	2.41858	0.00002
H	4.60993	-1.36059	-0.00002
H	-0.01326	-2.52144	-0.00003
H	-4.54502	1.28643	0.00003
H	-4.58716	-1.20221	0.
H	-2.48531	-2.48141	-0.00002

No. 8

C	3.71873	-0.65975	-0.00001
C	2.54339	-1.35512	0.
C	1.28168	-0.6761	0.
C	1.25472	0.76027	-0.00001
C	2.50543	1.4724	-0.00002
C	3.63507	0.74604	-0.00002
C	0.07556	-1.37716	0.00001
C	0.02667	1.4208	-0.00001
C	-1.17851	0.71637	0.
C	-1.15382	-0.71702	0.00001

C	-2.39586	-1.42661	0.00002
H	-2.37171	-2.51107	0.00002
C	-3.58138	-0.75789	0.00002
C	-3.60617	0.66917	0.00001
C	-2.44554	1.38045	0.
H	0.09354	-2.46286	0.00001
H	4.67564	-1.16731	-0.00001
H	2.54728	-2.44032	0.00001
H	0.00789	2.50624	-0.00002
H	-4.51623	-1.30548	0.00002
H	-4.55992	1.18326	0.00001
H	-2.46058	2.46501	0.
H	2.50428	2.55742	-0.00003

No. 9

C	-3.6503	-0.68198	-0.00003
C	-2.47845	-1.37496	-0.00005
C	-1.2213	-0.69265	-0.00003
C	-1.23209	0.7487	0.00003
C	-2.48353	1.44118	0.00005
C	-3.65349	0.7456	0.00003
C	0.	-1.37067	-0.00005
C	0.	1.36643	0.00005
C	1.23208	0.7487	0.00003
C	1.2213	-0.69266	-0.00003
C	2.47845	-1.37497	-0.00005
H	2.4765	-2.45973	-0.00009
C	3.6503	-0.68199	-0.00002
C	3.65348	0.74561	0.00003
C	2.48353	1.44118	0.00005
H	0.	-2.45608	-0.00009

H	-4.59466	-1.21311	-0.00005
H	-2.4765	-2.45973	-0.00009
H	4.59466	-1.21311	-0.00004
H	4.59936	1.27376	0.00005
H	2.47421	2.52458	0.00009
H	-2.47422	2.52458	0.00009
H	-4.59935	1.27376	0.00005

No. 10

C	3.53251	-0.31321	-0.00001
C	2.83291	0.87087	0.00001
C	1.42334	0.87844	0.00002
C	0.71058	-0.34661	-0.00001
C	1.45722	-1.54365	-0.00004
C	2.83451	-1.53108	-0.00004
C	0.70091	2.13152	0.00004
C	-0.74828	-0.33533	0.
C	-1.43236	0.90941	0.00001
C	-0.63211	2.07999	0.00003
C	-2.84128	0.95251	0.00001
C	-3.57195	-0.21214	0.
C	-2.90762	-1.44969	-0.00001
C	-1.53124	-1.50855	-0.00001
H	1.25542	3.06404	0.00005
H	4.61587	-0.30775	-0.00001
H	3.35753	1.82014	0.00003
H	0.94882	-2.49857	-0.00006
H	3.38043	-2.46684	-0.00006
H	-3.3301	1.9196	0.00003
H	-4.6546	-0.17786	0.
H	-3.48222	-2.36826	-0.00002

H	-1.05403	-2.47953	-0.00002
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No. 11

C	3.50361	-0.35643	-0.00007
C	2.81086	0.83103	-0.00001
C	1.40027	0.84911	0.00001
C	0.68441	-0.37207	-0.00003
C	1.42074	-1.57574	-0.00009
C	2.79772	-1.57064	-0.00011
C	0.69205	2.09991	0.00006
C	-0.77117	-0.33932	0.
C	-1.42188	0.92356	0.00005
C	-0.65853	2.14013	0.00007
C	-2.8144	0.9114	0.00007
C	-3.60952	-0.18856	0.00006
C	-2.94868	-1.43683	0.00002
C	-1.57222	-1.50309	-0.00001
H	1.2718	3.01646	0.00008
H	4.58692	-0.35814	-0.00009
H	3.34175	1.77696	0.00002
H	0.90519	-2.52682	-0.00013
H	3.33846	-2.50951	-0.00016
H	-1.19444	3.08171	0.0001
H	-4.69114	-0.12653	0.00008
H	-3.53258	-2.3501	0.00001
H	-1.10548	-2.47872	-0.00003

No. 12

C	-3.49519	-0.28516	0.00001
C	-2.77043	0.88272	-0.00001
C	-1.35982	0.86181	-0.00001

C	-0.67435	-0.37636	0.00001
C	-1.44438	-1.55915	0.00004
C	-2.82072	-1.51705	0.00004
C	-0.61676	2.09091	-0.00001
C	0.78278	-0.38083	-0.00001
C	1.47164	0.85747	0.00001
C	0.73448	2.09007	0.00001
C	2.88957	0.875	0.00001
C	3.53695	-0.31746	-0.00001
C	2.91909	-1.55841	-0.00004
C	1.53671	-1.57551	-0.00004
H	-1.16899	3.0245	-0.00002
H	-4.57813	-0.2584	0.00001
H	-3.27489	1.84304	-0.00003
H	-0.9575	-2.52512	0.00008
H	-3.3858	-2.44151	0.00007
H	1.29051	3.02109	0.00002
H	3.48639	-2.48131	-0.00008
H	1.03601	-2.53483	-0.00008
H	3.41484	1.8242	0.00002

No. 13

C	-3.51916	-0.21332	-0.00005
C	-2.76184	0.93393	-0.00009
C	-1.3523	0.87329	-0.00006
C	-0.70563	-0.38553	0.
C	-1.50748	-1.54657	0.00005
C	-2.8819	-1.46511	0.00002
C	-0.57174	2.07905	-0.00009
C	0.749	-0.43293	0.00003
C	1.48086	0.78032	0.

C	0.77873	2.03413	-0.00005
C	2.89315	0.76163	0.00003
C	3.59336	-0.428	0.00007
C	2.83272	-1.58705	0.00009
C	1.47573	-1.65128	0.00006
H	-1.09429	3.02933	-0.00014
H	-4.60092	-0.15507	-0.00007
H	-3.2393	1.90793	-0.00014
H	-1.04585	-2.52508	0.00011
H	-3.47419	-2.3723	0.00006
H	1.36246	2.94819	-0.00007
H	0.96895	-2.60768	0.00007
H	3.4259	1.70715	0.00001
H	4.67631	-0.44778	0.00009

No. 14

C	-3.52886	-0.3206	-0.00027
C	-2.81955	0.85853	-0.00021
C	-1.40914	0.85154	0.00007
C	-0.72734	-0.38479	0.00028
C	-1.47125	-1.58094	0.00007
C	-2.84764	-1.55076	-0.00018
C	-0.65512	2.0762	0.00009
C	0.72053	-0.38724	0.00048
C	1.43616	0.83733	0.0002
C	0.69814	2.07109	0.00019
C	2.84814	0.81615	-0.00031
C	3.54705	-0.37028	-0.00055
C	2.85363	-1.60225	-0.00015
C	1.49618	-1.54224	0.00078
H	-1.20124	3.01343	-0.00024

H	-4.61215	-0.3037	-0.00045
H	-3.33781	1.81146	-0.0005
H	-0.94158	-2.52748	-0.00022
H	-3.4092	-2.47731	-0.00027
H	1.25427	3.00236	0.00065
H	3.38116	1.76052	-0.0003
H	4.63088	-0.36599	-0.00108
H	3.3901	-2.54373	-0.00043

No. 15

C	2.94213	-1.25018	-0.00001
C	1.57484	-1.50783	0.
C	0.69285	-0.43206	0.00001
C	1.17052	0.88683	0.00001
C	2.53396	1.13861	-0.00001
C	3.41838	0.06098	-0.00002
C	0.01776	1.86491	0.00002
C	-1.18431	0.94983	-0.00003
C	-0.77712	-0.4001	0.00003
C	-1.71461	-1.42911	0.00005
H	-1.39584	-2.46509	0.00007
C	-3.07122	-1.11534	0.00001
C	-3.49839	0.21913	-0.00003
C	-2.52989	1.19667	-0.00005
H	3.64488	-2.07489	0.
H	1.20703	-2.52771	0.00002
H	2.91027	2.15583	-0.00002
H	4.48655	0.24271	-0.00003
H	-3.80909	-1.90944	0.00001
H	-4.5546	0.46117	-0.00007
H	0.03067	2.51161	0.88196

H	0.0307	2.51172	-0.88184
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No. 16

C	2.9397	-1.22273	-0.00016
C	1.57689	-1.50448	-0.0001
C	0.67538	-0.44519	-0.00003
C	1.1312	0.88139	-0.00001
C	2.48962	1.15779	-0.00007
C	3.39343	0.09613	-0.00015
C	-0.04102	1.83572	0.0001
C	-1.22859	0.90018	0.00008
C	-0.79493	-0.4359	0.00003
C	-1.70508	-1.4894	0.00003
H	-1.36501	-2.5194	-0.00001
C	-3.07304	-1.20124	0.00006
C	-3.44137	0.12493	0.00011
C	-2.58793	1.20436	0.00012
H	3.65651	-2.03529	-0.00022
H	1.22838	-2.5312	-0.00011
H	2.84756	2.18166	-0.00006
H	4.45823	0.29651	-0.0002
H	-3.80916	-1.99634	0.00006
H	-0.03788	2.48324	0.88224
H	-0.03794	2.48344	-0.88189
H	-2.94626	2.228	0.00015

No. 17

C	2.9955	-1.15111	-0.00004
C	1.64415	-1.48256	0.
C	0.70551	-0.45599	0.00001
C	1.11072	0.88674	-0.00001



C	2.45849	1.21217	-0.00005
C	3.39993	0.18398	-0.00006
C	-0.09585	1.79691	0.00003
C	-1.24982	0.82013	0.00002
C	-0.76363	-0.49774	0.00002
C	-1.64187	-1.58532	0.00003
H	-1.28649	-2.60966	0.00004
C	-2.97783	-1.26707	0.00003
C	-3.51057	0.00211	0.00001
C	-2.61323	1.07767	0.00001
H	3.74189	-1.93654	-0.00005
H	1.33283	-2.52116	0.00001
H	2.77904	2.24833	-0.00006
H	4.45676	0.42309	-0.00009
H	-0.11269	2.44454	0.88198
H	-0.11272	2.44467	-0.88182
H	-2.98681	2.09643	0.
H	-4.58087	0.17074	0.

No. 18

C	3.00814	-1.211	-0.00016
C	1.65099	-1.51826	-0.00022
C	0.73476	-0.47273	-0.00005
C	1.16173	0.86299	0.00018
C	2.51531	1.16296	0.00023
C	3.43697	0.11655	0.00006
C	-0.02909	1.79507	0.00038
C	-1.20298	0.84074	0.00015
C	-0.73249	-0.48799	-0.00011
C	-1.66947	-1.49211	-0.00032
C	-3.02593	-1.2783	-0.00032

C	-3.47295	0.04998	-0.00008
C	-2.56429	1.10862	0.00015
H	3.7402	-2.00983	-0.0003
H	1.31149	-2.54791	-0.00041
H	2.85558	2.19278	0.00041
H	4.49806	0.33598	0.0001
H	-0.03723	2.44227	0.88275
H	-0.0372	2.44278	-0.88161
H	-2.92364	2.13164	0.00033
H	-4.53782	0.25238	-0.00009
H	-3.73357	-2.09907	-0.0005

No. 19

C	3.01531	-1.2118	0.
C	1.65659	-1.5199	0.00001
C	0.73417	-0.47597	0.00001
C	1.16486	0.86424	0.
C	2.51937	1.1634	-0.00001
C	3.44428	0.11713	-0.00001
C	-0.02882	1.79694	0.00001
C	-1.20617	0.84236	0.00001
C	-0.73026	-0.49253	0.
C	-1.67586	-1.49022	0.
C	-3.03418	-1.28077	-0.00001
C	-3.48114	0.05091	-0.00001
C	-2.56838	1.10822	0.
H	3.74841	-2.01188	0.
H	1.3205	-2.55128	0.00002
H	2.86062	2.19429	-0.00002
H	4.50648	0.33882	-0.00002
H	-0.03713	2.45508	-0.87853

H	-2.92816	2.13251	-0.00001
H	-4.54736	0.25584	-0.00002
H	-3.74485	-2.10054	-0.00001
H	-1.32954	-2.50262	0.00001

No. 20

C	-0.90727	2.32061	-0.00009
C	-1.23678	0.87367	-0.00003
C	-0.0002	0.18325	-0.00001
C	1.08464	1.09564	-0.00005
C	0.43309	2.40653	-0.00006
C	0.13819	-1.19854	0.00004
C	2.36193	0.59557	-0.00004
C	2.53499	-0.81709	0.00001
C	1.47222	-1.69402	0.00004
C	-2.38884	0.12881	0.00002
C	-2.28409	-1.29344	0.00007
C	-1.07381	-1.94816	0.00008
H	-3.19793	-1.87597	0.0001
H	-1.04005	-3.03211	0.00011
H	1.65104	-2.76376	0.00008
H	-1.62114	3.13121	-0.0001
H	3.22935	1.24493	-0.00006
H	3.54387	-1.21232	0.00002
H	-3.36956	0.59105	0.00001

No. 21

C	0.38979	2.44294	-0.00011
C	1.06083	1.13191	-0.00011
C	0.02402	0.1588	-0.00001
C	-1.23333	0.80281	0.00005
C	-0.95169	2.24876	-0.00001

C	0.21567	-1.21812	0.00003
C	-2.35877	0.01423	0.00014
C	-2.20365	-1.40032	0.0002
C	-0.96739	-2.00909	0.00014
C	2.3146	0.61429	-0.00017
C	2.60117	-0.76191	-0.00014
C	1.56531	-1.67599	-0.00004
H	3.62932	-1.10455	-0.00019
H	1.77918	-2.73958	-0.00002
H	-0.8942	-3.09117	0.00017
H	0.89933	3.39534	-0.00018
H	-3.35555	0.44144	0.0002
H	-3.09438	-2.01733	0.00028
H	-1.70295	3.02601	0.00001

No. 22

C	-1.1447	2.14658	-0.00008
C	-1.35846	0.68619	0.
C	-0.06887	0.10216	0.
C	0.91753	1.11303	0.
C	0.18665	2.39531	0.00009
C	0.197	-1.2629	0.
C	2.23648	0.73245	-0.00003
C	2.54446	-0.65811	-0.00003
C	1.57166	-1.63312	-0.00002
C	-2.45395	-0.15061	0.00003
C	-2.16392	-1.52541	0.00003
C	-0.94555	-2.12689	0.00002
H	-0.83233	-3.20572	0.00002
H	1.85043	-2.68107	-0.00002
H	-1.93139	2.88779	-0.00014

H	3.04257	1.45762	-0.00001
H	3.58662	-0.95542	-0.00003
H	0.64982	3.37219	0.00014
H	-3.47558	0.21254	0.00001

No. 23

C	-0.90308	2.22344	0.00013
C	-1.25604	0.79096	0.00001
C	-0.02586	0.09382	0.
C	1.05414	1.00574	0.00001
C	0.44602	2.34961	-0.00009
C	0.11511	-1.2942	-0.00001
C	2.32925	0.49675	0.00004
C	2.50422	-0.91705	0.00003
C	1.44571	-1.79793	0.00001
C	-2.42311	0.06584	-0.00003
C	-2.34145	-1.36308	-0.00005
C	-1.12249	-1.96559	-0.00003
H	1.6192	-2.86721	0.
H	-1.61623	3.03592	0.00021
H	3.20166	1.14078	0.00002
H	3.51379	-1.3107	0.00003
H	0.99748	3.27932	-0.00016
H	-3.39751	0.54223	0.
H	-3.2529	-1.95011	-0.00005

No. 24

C	3.10184	-0.26323	0.00004
C	1.91715	0.68527	0.00001
C	0.72747	-0.07271	0.00001
C	0.97175	-1.4612	0.00001

C	2.4702	-1.69717	0.
C	-0.56065	0.50853	0.
C	-0.09968	-2.31957	0.
C	-1.41218	-1.78176	-0.00001
C	-1.63517	-0.42192	-0.00001
C	1.83222	2.05573	0.
C	0.54823	2.66068	-0.00001
C	-0.61865	1.92484	-0.00001
H	0.48574	3.74442	-0.00002
H	-1.58106	2.42202	-0.00002
H	3.73965	-0.10643	0.8766
H	3.73973	-0.10641	-0.87646
H	2.78492	-2.27376	0.87653
H	2.71899	2.68172	0.
H	0.02679	-3.39736	0.
H	-2.26353	-2.45238	-0.00001
H	-2.64129	-0.05774	-0.00002

No. 25

C	-1.20721	2.14956	0.00004
C	-1.28613	0.63523	0.00005
C	0.02129	0.10861	0.
C	1.00616	1.12816	-0.00007
C	0.31959	2.47967	-0.00008
C	0.31351	-1.26554	0.00001
C	2.28765	0.69562	-0.00011
C	2.66292	-0.65635	-0.0001
C	1.68668	-1.63239	-0.00004
C	-2.34347	-0.23581	0.0001
C	-2.08136	-1.63377	0.00011
C	-0.80387	-2.14319	0.00007

H	-2.92184	-2.31833	0.00016
H	-0.64374	-3.21571	0.00008
H	1.9651	-2.6808	-0.00003
H	3.71068	-0.93478	-0.00014
H	-1.70396	2.56685	0.8785
H	-1.70409	2.56686	-0.87835
H	0.60607	3.06026	-0.87874
H	0.60618	3.06035	0.8785
H	-3.36897	0.11661	0.00014

No. 26

C	-0.03731	2.42617	0.00014
C	-0.83168	1.13499	0.00008
C	0.06356	0.04666	0.
C	1.41259	0.46418	-0.00003
C	1.45832	1.97978	0.00002
C	-0.3484	-1.298	-0.00005
C	2.40591	-0.4874	-0.0001
C	1.96606	-1.81943	-0.00014
C	0.68953	-2.27995	-0.00011
C	-2.17886	0.88411	0.0001
C	-2.62158	-0.46625	0.00005
C	-1.74862	-1.53025	-0.00002
H	-3.68806	-0.66149	0.00007
H	-2.12519	-2.54698	-0.00005
H	0.45317	-3.33848	-0.00015
H	-0.2736	3.03038	0.87862
H	-0.2737	3.03056	-0.8782
H	1.98839	2.3535	-0.87857
H	1.98854	2.35346	0.87853
H	-2.90705	1.68731	0.00016

H	3.46036	-0.2359	-0.00013
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No. 27

C	-0.48359	2.36882	0.00007
C	-1.04857	0.96168	0.00001
C	0.0219	0.04486	0.
C	1.28222	0.68014	0.00001
C	1.06733	2.18181	-0.00001
C	-0.15917	-1.35344	-0.00002
C	2.41881	-0.08535	0.00001
C	2.28857	-1.50956	0.00001
C	1.05043	-2.06611	-0.00001
C	-2.33107	0.47993	-0.00001
C	-2.53716	-0.92752	-0.00004
C	-1.49733	-1.82769	-0.00003
H	-3.55476	-1.30112	-0.00005
H	-1.68883	-2.89374	-0.00005
H	-0.8192	2.92406	0.87854
H	-0.81927	2.9242	-0.87827
H	1.52395	2.64259	-0.87847
H	1.52406	2.64263	0.87838
H	-3.18713	1.14536	-0.00001
H	3.40802	0.35914	0.
H	3.17902	-2.12866	0.

### Cl-PAHs

No. 1

C	2.26351	0.00001	0.
C	1.56584	1.20352	0.
C	0.17506	1.211	0.



C	-0.50399	-0.00007	-0.00002
C	0.17507	-1.21101	-0.00001
C	1.56596	-1.20345	0.00001
H	3.34634	0.0001	0.
H	2.10283	2.14422	0.
H	-0.37974	2.14037	0.
H	-0.37955	-2.14048	0.
H	2.10289	-2.14418	0.00003
Cl	-2.2495	0.	0.00001

No. 2

C	-2.36554	0.07256	-0.00004
C	-1.47285	1.13765	-0.00003
C	-0.09109	0.93797	0.00004
C	0.35563	-0.38474	-0.00001
C	-0.51667	-1.46457	0.00007
C	-1.8867	-1.23223	0.00004
H	-3.43203	0.26195	-0.00027
H	-1.84868	2.15502	-0.00009
H	-0.11961	-2.47174	0.00018
H	-2.5725	-2.07054	0.00004
C	0.86664	2.096	0.00008
H	1.51512	2.06555	0.8787
H	1.51512	2.06558	-0.87862
H	0.32302	3.04039	-0.00002
Cl	2.07548	-0.70718	-0.00005

No. 3

C	0.65525	1.87734	0.00244
C	1.72555	0.99011	-0.00841
C	1.51022	-0.38821	-0.01143

C	0.19808	-0.86176	-0.00976
C	-0.86033	0.035	0.00066
C	-0.65292	1.4073	0.00744
H	0.8374	2.94542	0.0032
H	2.74112	1.37028	-0.01627
H	-1.49707	2.08437	0.0126
C	2.66568	-1.35493	0.00945
H	2.91085	-1.63623	1.03728
H	2.42573	-2.26811	-0.53702
H	3.55663	-0.91086	-0.43618
H	-0.0025	-1.92679	-0.01812
Cl	-2.49537	-0.5816	0.00072

No. 4

C	-0.3093	1.20808	-0.00254
C	1.08122	1.19796	-0.00903
C	1.79817	0.00196	-0.00951
C	1.08193	-1.19569	-0.00911
C	-0.30751	-1.20737	-0.00253
C	-0.99134	0.00042	0.00117
H	-0.86054	2.13979	-0.00421
H	1.6163	2.14155	-0.01581
C	3.30462	-0.00124	0.01276
H	3.67579	-0.11295	1.03519
H	3.70483	-0.82773	-0.57679
H	3.70642	0.93059	-0.38738
H	1.61853	-2.13862	-0.0158
H	-0.85809	-2.13948	-0.0042
Cl	-2.73824	-0.00105	0.00481

No. 5

C	-2.9168	-0.60795	0.
C	-2.3997	0.65896	0.
C	-0.99716	0.87441	0.
C	-0.12859	-0.25371	0.
C	-0.69189	-1.55565	0.
C	-2.05091	-1.72565	0.
H	-1.1328	3.03019	0.
H	-3.98943	-0.75996	0.
H	-3.05469	1.52352	0.
C	-0.45396	2.1848	0.
C	1.27165	0.00057	0.
H	-0.03423	-2.41484	0.
H	-2.46749	-2.72575	0.00001
C	1.77862	1.27048	0.
C	0.89995	2.37711	0.
H	2.85045	1.42063	0.
H	1.31345	3.37816	0.00001
Cl	2.39102	-1.34071	0.

No. 6

C	3.32675	0.21525	-0.00005
C	2.34466	1.1694	-0.00023
C	0.97553	0.79808	-0.00015
C	0.63448	-0.58072	0.00011
C	1.67354	-1.54744	0.0003
C	2.9863	-1.15883	0.00022
H	0.19393	2.81473	-0.00054
H	4.37014	0.50719	-0.00012
H	2.59865	2.22395	-0.00044
C	-0.0661	1.76187	-0.00034
C	-0.73341	-0.95812	0.00019

H	1.40871	-2.59912	0.00051
H	3.77373	-1.90295	0.00037
C	-1.70121	0.00592	0.00001
C	-1.38015	1.38222	-0.00027
H	-2.17836	2.11304	-0.00042
H	-1.00387	-2.0076	0.00041
Cl	-3.38384	-0.45148	0.00008

No. 7

C	2.89744	1.92988	0.00007
C	1.59235	2.31029	0.00002
C	0.54676	1.33516	-0.00002
C	0.88171	-0.06224	-0.00002
C	2.27626	-0.40005	0.
C	3.24944	0.54899	0.00006
C	-0.79676	1.71078	-0.00005
C	-0.14133	-1.00898	-0.00001
C	-1.48364	-0.62625	0.
C	-1.82181	0.76569	-0.00005
C	-3.20252	1.13949	-0.00006
H	-3.45295	2.19495	-0.00012
C	-4.17943	0.19161	0.
C	-3.84294	-1.19574	0.00007
C	-2.54037	-1.59016	0.00007
H	-1.04717	2.76734	-0.00009
H	3.68827	2.66988	0.00013
H	1.31993	3.35983	0.
H	4.29029	0.25155	0.00012
H	0.10479	-2.06396	-0.00001
H	-5.2228	0.48444	0.00001
H	-4.63648	-1.93339	0.00013

H	-2.2793	-2.64294	0.00012
Cl	2.74262	-2.08109	-0.00005

No. 8

C	2.74023	1.32376	0.
C	1.48365	1.84374	0.00001
C	0.33087	0.99671	0.00001
C	0.52277	-0.42401	-0.00001
C	1.85488	-0.94386	-0.00002
C	2.91141	-0.09124	0.
C	-0.96495	1.51093	0.
C	-0.59133	-1.26353	-0.00002
C	-1.88833	-0.74875	0.
C	-2.08053	0.67218	-0.00001
C	-3.41532	1.18585	-0.00001
H	-3.55571	2.26139	-0.00003
C	-4.48574	0.34508	0.
C	-4.29471	-1.06919	0.00001
C	-3.04003	-1.59724	0.00001
H	-1.10974	2.58704	0.
H	3.61576	1.96032	-0.00001
H	1.3389	2.91852	0.00002
H	-0.44624	-2.33941	-0.00002
H	-5.49293	0.74422	0.00003
H	-5.16005	-1.72136	0.00001
H	-2.8905	-2.67153	0.00002
H	2.01139	-2.01575	-0.00002
Cl	4.54069	-0.71565	0.00001

No. 9

C	-3.64363	-1.19892	-0.00001
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C	-2.45945	-1.86778	0.00003
C	-1.21473	-1.16382	0.00003
C	-1.22995	0.27181	0.00001
C	-2.49632	0.93723	-0.00003
C	-3.6575	0.22598	-0.00004
C	-0.00001	-1.84469	0.00003
C	0.00003	0.9423	0.00001
C	1.22986	0.27175	0.00002
C	1.21464	-1.16387	0.
C	2.45945	-1.86786	-0.00002
H	2.43333	-2.95206	-0.00005
C	3.64357	-1.19904	-0.00003
C	3.65747	0.22595	-0.00001
C	2.4963	0.93721	0.00001
H	-0.00003	-2.93	0.00003
H	-4.58014	-1.7434	-0.00002
H	-2.43337	-2.95198	0.00006
H	4.58013	-1.74344	-0.00004
H	4.60665	0.74841	-0.00002
H	2.51976	2.01831	0.00003
H	-2.51961	2.01832	-0.00003
H	-4.60671	0.74833	-0.00008
Cl	0.0001	2.69118	0.00001

No. 10

C	-3.81676	-0.55532	0.00002
C	-2.73121	-1.3983	0.00009
C	-1.41822	-0.88312	0.00006
C	-1.20625	0.51354	-0.00001
C	-2.33923	1.35433	-0.00012
C	-3.61454	0.83417	-0.0001

C	-0.29809	-1.77742	0.00008
C	0.16011	1.01938	0.00001
C	1.25198	0.11362	-0.00003
C	0.96354	-1.29965	0.
C	2.57165	0.60954	-0.00004
C	2.81583	1.96296	0.
C	1.74331	2.86573	0.00007
C	0.44814	2.40029	0.00008
H	-0.47651	-2.84592	0.00013
H	-4.82245	-0.95788	0.00005
H	-2.86887	-2.47409	0.00016
H	-2.22004	2.42922	-0.00025
H	-4.46687	1.50307	-0.00019
H	3.39677	-0.08978	-0.00008
H	3.83529	2.32893	-0.00001
H	1.93203	3.93251	0.00014
H	-0.36031	3.11832	0.00017
Cl	2.28643	-2.44135	-0.00005

No. 11

C	-4.12081	-0.40627	-0.00001
C	-3.13232	-1.36106	0.00007
C	-1.7703	-0.99348	0.00006
C	-1.41005	0.37348	0.
C	-2.44586	1.33219	-0.00012
C	-3.7695	0.95378	-0.00012
C	-0.74521	-1.99687	0.00009
C	0.00094	0.73782	0.00003
C	0.97758	-0.29081	0.
C	0.56533	-1.66664	0.00003
C	2.34136	0.08642	-0.00002

C	2.73868	1.40071	0.00001
C	1.76263	2.40617	0.00009
C	0.42615	2.08206	0.00011
H	-1.04649	-3.03901	0.00015
H	-5.16438	-0.6978	-0.00001
H	-3.38536	-2.41603	0.00013
H	-2.21217	2.38826	-0.00025
H	-4.5444	1.71115	-0.00023
H	1.32334	-2.43791	0.00001
H	3.79296	1.64548	-0.00001
H	2.07011	3.44495	0.00016
H	-0.30059	2.88209	0.00021
Cl	3.58561	-1.14272	-0.00008

No. 12

C	4.31022	-0.37401	-0.00001
C	3.62165	0.81582	0.00002
C	2.21153	0.83718	0.00002
C	1.49048	-0.38002	-0.00001
C	2.22254	-1.58607	-0.00005
C	3.59965	-1.5852	-0.00005
C	1.50434	2.08733	0.00002
C	0.03537	-0.33874	0.00001
C	-0.61881	0.91523	-0.00001
C	0.1537	2.12674	-0.00001
C	-2.02748	0.97738	-0.00002
C	-2.76194	-0.18073	0.00001
C	-2.13742	-1.43502	0.00005
C	-0.76299	-1.50197	0.00006
H	2.0837	3.00434	0.00003
H	5.39341	-0.37976	0.



H	4.15573	1.75997	0.00005
H	1.70504	-2.53609	-0.00011
H	4.13743	-2.52575	-0.0001
H	-0.3745	3.07371	-0.00003
H	-2.7394	-2.33458	0.00009
H	-0.30066	-2.47993	0.00012
H	-2.52424	1.9401	-0.00004
Cl	-4.50479	-0.10527	-0.00001

No. 13

C	-3.91533	-1.21677	-0.00009
C	-3.62219	0.12632	-0.00023
C	-2.28555	0.57682	-0.00012
C	-1.22903	-0.36416	0.00006
C	-1.55843	-1.73631	0.00025
C	-2.87007	-2.15484	0.00018
C	-1.9938	1.98357	-0.00013
C	0.14466	0.11915	0.00006
C	0.38523	1.51334	0.00012
C	-0.71881	2.43092	0.00005
C	1.71169	1.99143	0.00016
C	2.7825	1.13082	0.00011
C	2.53118	-0.2482	-0.00001
C	1.25316	-0.75262	-0.00003
H	-2.82529	2.67979	-0.00025
H	-4.9453	-1.55276	-0.00017
H	-4.4186	0.86278	-0.00041
H	-0.77597	-2.48364	0.00053
H	-3.09541	-3.21464	0.00036
H	-0.50404	3.49395	0.00011
H	1.12133	-1.82522	-0.00018

H	1.88063	3.06272	0.00023
H	3.8017	1.49476	0.00014
Cl	3.88645	-1.34791	-0.00015

No. 14

C	-3.68732	-0.5265	0.03578
C	-3.16838	0.72966	-0.16581
C	-1.7784	0.95859	-0.12893
C	-0.87621	-0.1213	0.06227
C	-1.44737	-1.38829	0.32328
C	-2.81198	-1.58491	0.30962
C	-1.29526	2.30627	-0.21709
C	0.56406	0.15616	0.04685
C	0.98227	1.5184	0.05641
C	0.0172	2.57461	-0.07726
C	2.34183	1.86961	0.14908
C	3.31756	0.90522	0.19304
C	2.94701	-0.43735	0.08993
C	1.61745	-0.79612	0.00146
H	-2.017	3.10381	-0.3549
H	-4.75768	-0.69135	0.01086
H	-3.82494	1.57613	-0.33587
H	-0.82121	-2.22724	0.57075
H	-3.20567	-2.57204	0.52082
H	0.38323	3.59501	-0.09282
H	2.60252	2.92169	0.17261
H	4.36441	1.1716	0.26865
H	3.69877	-1.21482	0.05167
Cl	1.36722	-2.50866	-0.28727

No. 15

C	-3.80596	0.56723	-0.00001
C	-2.58921	1.24117	0.00013
C	-1.41453	0.49607	0.00014
C	-1.45337	-0.90565	0.
C	-2.66856	-1.57317	-0.00018
C	-3.8461	-0.82734	-0.00019
C	-0.05172	-1.46996	0.00021
C	0.79533	-0.22484	0.00007
C	-0.00804	0.92556	0.0001
C	0.55927	2.1946	-0.00001
H	-0.06229	3.08242	0.00001
C	1.94663	2.30474	-0.00012
C	2.75767	1.17169	-0.00011
C	2.17061	-0.08951	-0.00002
H	-4.73218	1.12945	0.00001
H	-2.56083	2.32499	0.00026
H	-2.70581	-2.65701	-0.0003
H	-4.80321	-1.33526	-0.00032
H	2.41101	3.28349	-0.00019
H	3.83646	1.26032	-0.0002
H	0.14729	-2.08871	0.88096
H	0.14755	-2.08947	-0.87992
Cl	3.1747	-1.5161	-0.00002

No. 16

C	-3.85838	1.10052	-0.00042
C	-2.5134	1.45699	-0.00036
C	-1.55536	0.44855	0.00001
C	-1.93618	-0.90062	0.0001
C	-3.27768	-1.25175	0.00014
C	-4.23819	-0.24186	-0.00012

C	-0.71364	-1.79034	0.00032
C	0.41935	-0.79026	0.
C	-0.08714	0.51686	0.0003
C	0.776	1.60711	0.00053
H	0.39394	2.62162	0.00081
C	2.14871	1.38465	0.0004
C	2.63367	0.07983	-0.00004
C	1.78569	-1.02285	-0.00023
H	-4.61944	1.87198	-0.0006
H	-2.22139	2.50147	-0.00052
H	-3.57881	-2.29403	0.00021
H	-5.29074	-0.50028	-0.00021
H	2.84664	2.21207	0.00055
H	-0.68204	-2.4361	0.88293
H	-0.68196	-2.4372	-0.88146
H	2.1957	-2.0256	-0.00053
Cl	4.36102	-0.18205	-0.00029

No. 17

C	3.30045	-1.74921	0.00019
C	1.91168	-1.67263	0.0005
C	1.31403	-0.41684	0.00013
C	2.0922	0.74988	-0.0002
C	3.47633	0.66844	-0.00052
C	4.07643	-0.58946	-0.00035
C	1.20236	1.9722	0.00015
C	-0.18378	1.37118	0.00023
C	-0.10323	-0.02856	0.00022
C	-1.25086	-0.81376	0.
H	-1.20634	-1.89585	0.
C	-2.4771	-0.16335	-0.00013

C	-2.57839	1.2248	0.00002
C	-1.41949	1.9985	0.00024
H	3.78603	-2.71778	0.00031
H	1.31072	-2.57525	0.0008
H	4.08521	1.56613	-0.00086
H	5.15704	-0.66921	-0.00057
H	1.37378	2.59631	0.88263
H	1.3737	2.5971	-0.88177
H	-1.49604	3.08016	0.00025
H	-3.55661	1.68791	-0.00006
Cl	-3.94066	-1.11628	-0.00021

No. 18

C	-2.99009	1.37976	-0.0004
C	-1.59828	1.39581	-0.00047
C	-0.91273	0.18171	-0.00017
C	-1.62632	-1.02839	0.00012
C	-3.01208	-1.0372	0.00022
C	-3.69395	0.1775	-0.00004
C	-0.6807	-2.20287	0.00046
C	0.67429	-1.53896	-0.00003
C	0.52673	-0.13978	0.00009
C	1.67693	0.64397	0.00009
C	2.93629	0.05513	-0.00015
C	3.05701	-1.33003	-0.00038
C	1.92219	-2.13824	-0.0003
H	-3.53296	2.3175	-0.00059
H	-1.06723	2.33652	-0.00074
H	-3.55831	-1.97425	0.00043
H	-4.77747	0.18814	-0.00003
H	-0.81756	-2.83423	0.88371

H	-0.81801	-2.83558	-0.88173
H	2.01581	-3.21827	-0.00043
H	4.04439	-1.77534	-0.00063
H	3.81487	0.68768	-0.00019
Cl	1.58945	2.38808	0.00035

No. 19

C	3.01531	-1.2118	0.
C	1.65659	-1.5199	0.00001
C	0.73417	-0.47597	0.00001
C	1.16486	0.86424	0.
C	2.51937	1.1634	-0.00001
C	3.44428	0.11713	-0.00001
C	-0.02882	1.79694	0.00001
C	-1.20617	0.84236	0.00001
C	-0.73026	-0.49253	0.
C	-1.67586	-1.49022	0.
C	-3.03418	-1.28077	-0.00001
C	-3.48114	0.05091	-0.00001
C	-2.56838	1.10822	0.
H	3.74841	-2.01188	0.
H	1.3205	-2.55128	0.00002
H	2.86062	2.19429	-0.00002
H	4.50648	0.33882	-0.00002
H	-0.0343	2.40435	-0.88085
H	-2.92816	2.13251	-0.00001
H	-4.54736	0.25584	-0.00002
H	-3.74485	-2.10054	-0.00001
H	-1.32954	-2.50262	0.00001
Cl	-0.03782	2.79601	1.44894

## No. 20

C	-1.01079	-1.70621	0.00003
C	0.43438	-1.42094	0.00006
C	0.56275	-0.01259	-0.00005
C	-0.70721	0.59838	-0.00004
C	-1.66367	-0.52049	-0.00015
C	1.76598	0.67956	-0.00006
C	-0.78655	1.96666	0.00006
C	0.42914	2.70706	0.00009
C	1.66651	2.09935	0.00001
C	1.58467	-2.16985	0.00012
C	2.83968	-1.49387	-0.00001
C	2.94463	-0.12118	-0.00011
H	3.74422	-2.09077	0.
H	3.92104	0.35079	-0.0001
H	2.56714	2.70394	0.00001
H	-1.47189	-2.68273	0.00008
H	-1.73983	2.48325	0.00007
H	0.37357	3.78912	0.00013
H	1.56282	-3.25377	0.00019
Cl	-3.37143	-0.29029	0.

## No. 21

C	-0.57398	2.06472	0.00007
C	-0.68101	0.59779	-0.00002
C	0.64223	0.1005	0.00004
C	1.55642	1.17756	-0.00001
C	0.73849	2.40449	0.00001
C	0.99675	-1.24156	0.00004
C	2.89819	0.88239	-0.00001
C	3.29899	-0.48395	-0.00005

C	2.39181	-1.52083	-0.00001
C	-1.68735	-0.33142	-0.00008
C	-1.38081	-1.72092	0.
C	-0.0812	-2.17116	0.00007
H	-2.20376	-2.42441	-0.00001
H	0.11674	-3.23735	0.00004
H	2.73882	-2.54834	-0.00002
H	-1.41556	2.74211	0.00018
H	3.65423	1.65987	-0.00003
H	4.35865	-0.7105	-0.00006
H	1.13137	3.41149	-0.00012
Cl	-3.35833	0.15067	-0.00002

No. 22

C	0.9813	2.46799	0.00004
C	0.01598	1.35133	0.
C	0.78891	0.16881	-0.00001
C	2.16385	0.48636	0.
C	2.23759	1.96123	-0.00005
C	0.26883	-1.11765	-0.00001
C	3.06522	-0.54896	0.00001
C	2.56803	-1.88423	0.00002
C	1.22212	-2.17586	0.00001
C	-1.35052	1.23608	0.00001
C	-1.90239	-0.07568	-0.00001
C	-1.14969	-1.22575	-0.00002
H	-1.63787	-2.19274	-0.00002
H	0.8876	-3.20737	0.00001
H	0.71671	3.51605	0.00007
H	4.1359	-0.37816	0.00001
H	3.28169	-2.6997	0.00002



H	3.15312	2.53619	-0.00006
H	-2.01685	2.09018	0.00002
Cl	-3.64563	-0.20744	0.

No. 23

C	2.45174	1.69272	0.00001
C	0.98796	1.51171	-0.00003
C	0.7683	0.11706	0.00004
C	2.00387	-0.56899	0.00004
C	3.04657	0.47551	0.00005
C	-0.47546	-0.50399	0.00002
C	1.9829	-1.94126	-0.00003
C	0.72311	-2.60474	-0.00004
C	-0.47481	-1.9259	-0.00001
C	-0.1098	2.33609	-0.00006
C	-1.40608	1.75244	-0.00001
C	-1.58461	0.38828	0.00003
H	-1.41273	-2.46759	-0.00004
H	2.95759	2.64796	-0.00001
H	2.89471	-2.52821	-0.00003
H	0.71072	-3.68818	-0.00009
H	4.11099	0.28734	0.00003
H	-0.02009	3.41651	-0.00012
H	-2.27988	2.39183	0.00001
Cl	-3.20256	-0.26078	0.00002

No. 24

C	3.10184	-0.26323	0.00004
C	1.91715	0.68527	0.00001
C	0.72747	-0.07271	0.00001
C	0.97175	-1.4612	0.00001

C	2.4702	-1.69717	0.
C	-0.56065	0.50853	0.
C	-0.09968	-2.31957	0.
C	-1.41218	-1.78176	-0.00001
C	-1.63517	-0.42192	-0.00001
C	1.83222	2.05573	0.
C	0.54823	2.66068	-0.00001
C	-0.61865	1.92484	-0.00001
H	0.48574	3.74442	-0.00002
H	-1.58106	2.42202	-0.00002
H	3.73965	-0.10643	0.8766
H	3.73973	-0.10641	-0.87646
H	2.76278	-2.23297	0.87876
H	2.71899	2.68172	0.
H	0.02679	-3.39736	0.
H	-2.26353	-2.45238	-0.00001
H	-2.64129	-0.05774	-0.00002
Cl	2.95146	-2.57841	-1.44547

No. 25

C	0.82441	2.43591	0.00004
C	1.5751	1.11817	0.00002
C	0.64123	0.06263	0.00014
C	-0.68726	0.5331	0.0001
C	-0.6874	2.04248	0.00017
C	0.995	-1.29463	0.00009
C	-1.68599	-0.39737	-0.00003
C	-1.37927	-1.78385	0.00001
C	-0.0785	-2.22555	0.00009
C	2.91072	0.81061	-0.00014
C	3.29964	-0.55687	-0.00011
C	2.38413	-1.58415	0.00002

H	4.35751	-0.7938	-0.00022
H	2.71927	-2.61541	-0.00001
H	0.12834	-3.28981	0.00006
H	-2.19934	-2.49118	-0.00005
H	1.07992	3.03191	-0.87863
H	1.08059	3.0322	0.87832
H	-1.21053	2.43002	0.87746
H	-1.21014	2.43018	-0.87728
H	3.67134	1.58334	-0.00026
Cl	-3.35811	0.10116	-0.0001

No. 26

C	-2.38687	1.84989	0.
C	-2.15196	0.35233	-0.00001
C	-0.76477	0.11055	-0.00019
C	-0.00995	1.30073	-0.0001
C	-0.95899	2.48225	-0.00014
C	-0.19423	-1.17109	-0.00017
C	1.35675	1.22288	0.00008
C	1.94402	-0.07008	-0.00003
C	1.22379	-1.23829	-0.00018
C	-3.00631	-0.71961	0.0002
C	-2.4559	-2.02996	0.00011
C	-1.09957	-2.26404	-0.00009
H	-3.13398	-2.87585	0.00025
H	-0.71932	-3.27921	-0.00008
H	1.73527	-2.19283	-0.00017
H	-2.95851	2.15594	0.87879
H	-2.95949	2.15572	-0.87824
H	-0.79822	3.11078	-0.87854
H	-0.79878	3.11052	0.87855

H	-4.08261	-0.58997	0.00038
H	1.996	2.09715	0.00019
Cl	3.6908	-0.15563	0.00012

No. 27

C	3.09621	-0.25521	-0.00004
C	1.91046	0.68903	-0.00003
C	0.72334	-0.07137	-0.00011
C	0.97433	-1.45802	-0.00004
C	2.4723	-1.68608	-0.00007
C	-0.55924	0.50177	-0.00008
C	-0.091	-2.31878	0.00011
C	-1.40619	-1.78382	0.00006
C	-1.63134	-0.42923	-0.00005
C	1.82066	2.05602	0.00009
C	0.53303	2.6559	0.00006
C	-0.62829	1.91792	-0.00004
H	0.46528	3.73778	0.00014
H	-1.59283	2.40967	-0.00002
H	3.72421	-0.09263	0.87854
H	3.72454	-0.09211	-0.8783
H	2.78049	-2.25719	-0.87849
H	2.78066	-2.25676	0.87856
H	2.7049	2.68352	0.00018
H	0.04122	-3.39454	0.0002
H	-2.25735	-2.4534	0.00014
Cl	-3.27392	0.16511	0.

**Br-PAHs**

No. 1

C	2.86724	0.00001	0.
C	2.16991	1.20344	0.
C	0.77876	1.21184	0.
C	0.10023	-0.00003	0.
C	0.77877	-1.21184	0.
C	2.16996	-1.20341	0.
H	3.95021	0.00005	0.00001
H	2.70683	2.14447	0.
H	0.22774	2.14337	0.00001
H	0.22783	-2.14342	0.
H	2.70686	-2.14446	0.
Br	-1.80025	0.	0.

No. 2

C	-2.86907	-0.27453	0.
C	-2.18003	0.93193	0.
C	-0.78406	0.98278	0.00003
C	-0.11018	-0.24029	0.00001
C	-0.77696	-1.45849	-0.00001
C	-2.16656	-1.47356	0.
H	-3.95223	-0.277	0.00001
H	-2.73153	1.86583	-0.00001
H	-0.21113	-2.38118	-0.00003
H	-2.69264	-2.42035	-0.00001
C	-0.05722	2.29799	-0.00001
H	0.58642	2.38538	0.87832
H	0.58641	2.38531	-0.87837
H	-0.76461	3.12683	-0.00003
Br	1.79554	-0.26514	0.

No. 3

C	1.46316	1.87578	0.0023
C	2.43048	0.87784	-0.00867
C	2.0669	-0.46907	-0.01164
C	0.71074	-0.79788	-0.00984
C	-0.24418	0.20936	0.00112
C	0.11088	1.55102	0.00786
H	1.75978	2.91793	0.00291
H	3.48139	1.14564	-0.01682
H	-0.65043	2.31969	0.01326
C	3.11201	-1.55422	0.00969
H	3.3665	-1.82017	1.03922
H	2.75462	-2.45628	-0.48859
H	4.02697	-1.22673	-0.48568
H	0.40062	-1.8361	-0.01845
Br	-2.08684	-0.26289	0.00026

No. 4

C	0.34154	1.20896	-0.00374
C	1.73249	1.19799	-0.00931
C	2.44904	0.00188	-0.00937
C	1.73283	-1.19568	-0.00936
C	0.34298	-1.20779	-0.00376
C	-0.34054	0.00076	-0.0002
H	-0.20525	2.14307	-0.00573
H	2.26782	2.14153	-0.01569
C	3.95536	-0.00158	0.01402
H	4.32514	-0.11347	1.03693
H	4.35583	-0.82825	-0.57505
H	4.35773	0.93024	-0.38553
H	2.26943	-2.1387	-0.01569
H	-0.20344	-2.14212	-0.00574

Br	-2.24141	-0.00056	0.00277
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No. 5

C	0.34154	1.20896	-0.00374
C	1.73249	1.19799	-0.00931
C	2.44904	0.00188	-0.00937
C	1.73283	-1.19568	-0.00936
C	0.34298	-1.20779	-0.00376
C	-0.34054	0.00076	-0.0002
H	-0.20525	2.14307	-0.00573
H	2.26782	2.14153	-0.01569
C	3.95536	-0.00158	0.01402
H	4.32514	-0.11347	1.03693
H	4.35583	-0.82825	-0.57505
H	4.35773	0.93024	-0.38553
H	2.26943	-2.1387	-0.01569
H	-0.20344	-2.14212	-0.00574
Br	-2.24141	-0.00056	0.00277

No. 6

C	3.98593	0.09687	-0.00006
C	3.05619	1.10228	-0.00024
C	1.66927	0.80485	-0.00017
C	1.25576	-0.55366	0.00009
C	2.2412	-1.57484	0.00028
C	3.573	-1.25696	0.00021
H	0.99642	2.86023	-0.00057
H	5.04341	0.33269	-0.00012
H	3.36752	2.14147	-0.00045
C	0.68046	1.82249	-0.00036
C	-0.13071	-0.85795	0.00017

H	1.91982	-2.6108	0.00049
H	4.31823	-2.04349	0.00036
C	-1.04588	0.15635	-0.00002
C	-0.65264	1.51446	-0.00029
H	-1.4064	2.29108	-0.00044
H	-0.45257	-1.89249	0.00037
Br	-2.90234	-0.24577	0.00008

No. 7

C	2.01287	2.69867	0.0001
C	0.659	2.81906	-0.0001
C	-0.17796	1.66018	-0.00014
C	0.41952	0.35174	-0.0001
C	1.85391	0.29118	0.00005
C	2.62447	1.41146	0.00021
C	-1.56814	1.77417	-0.00013
C	-0.40844	-0.77011	-0.00014
C	-1.79892	-0.64915	-0.00011
C	-2.39616	0.65237	-0.00006
C	-3.8224	0.7574	0.00012
H	-4.26835	1.74607	0.0002
C	-4.6012	-0.35873	0.0002
C	-4.00685	-1.65667	0.00008
C	-2.65289	-1.79657	-0.00009
H	-2.01331	2.76442	-0.00017
H	2.6459	3.57764	0.00015
H	0.18803	3.79561	-0.00028
H	3.7034	1.32704	0.00042
H	0.03121	-1.75994	-0.00022
H	-5.68106	-0.26989	0.00035
H	-4.64511	-2.53229	0.0001



H	-2.19672	-2.78049	-0.00021
Br	2.72615	-1.39937	0.00001

No. 8

C	1.98501	1.54377	0.00001
C	0.703	1.99744	0.00003
C	-0.40462	1.09273	0.00002
C	-0.13928	-0.31633	0.00001
C	1.21852	-0.76745	-0.00001
C	2.22981	0.13892	0.00001
C	-1.72499	1.53995	0.00001
C	-1.20858	-1.21197	0.00001
C	-2.53038	-0.76429	0.00001
C	-2.79583	0.64526	-0.00001
C	-4.15522	1.0897	-0.00004
H	-4.3499	2.15675	-0.00008
C	-5.18093	0.1949	-0.00003
C	-4.91714	-1.20788	0.
C	-3.63709	-1.67059	0.00002
H	-1.92385	2.60735	0.
H	2.8234	2.22769	0.00001
H	0.50395	3.06354	0.00005
H	-1.00929	-2.27914	0.00001
H	-6.20718	0.54242	-0.00003
H	-5.74807	-1.9031	0.00001
H	-3.43321	-2.73588	0.00006
H	1.42385	-1.83118	-0.00002
Br	4.03619	-0.44781	-0.00001

No. 9

C	-3.64383	-1.63024	0.
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C	-2.45597	-2.29171	-0.00002
C	-1.21496	-1.58114	0.
C	-1.23165	-0.14419	0.00003
C	-2.5043	0.51066	0.00006
C	-3.66218	-0.20591	0.00005
C	-0.0006	-2.26119	-0.00004
C	0.00006	0.52654	0.00001
C	1.23126	-0.14482	0.00002
C	1.21398	-1.58173	-0.00002
C	2.45482	-2.29281	-0.00004
H	2.42118	-3.37684	-0.00009
C	3.64285	-1.63183	0.
C	3.66179	-0.2074	0.00006
C	2.50418	0.50961	0.00007
H	-0.00086	-3.34655	-0.00008
H	-4.57776	-2.17906	-0.00003
H	-2.42279	-3.37576	-0.00004
H	4.57662	-2.18093	0.00001
H	4.61272	0.31196	0.00011
H	2.53797	1.59008	0.00013
H	-2.53755	1.59109	0.00013
H	-4.61294	0.31367	0.00009
Br	0.00088	2.43455	-0.00004

No. 10

C	-3.79663	-1.72816	0.00002
C	-2.47455	-2.10357	0.00006
C	-1.44958	-1.13453	0.00004
C	-1.77537	0.2396	-0.00001
C	-3.14056	0.59563	-0.00008
C	-4.12863	-0.36357	-0.00007

C	-0.07516	-1.5441	0.00005
C	-0.69786	1.21968	0.00001
C	0.65544	0.79083	-0.00001
C	0.91697	-0.62867	0.00001
C	1.68781	1.75108	-0.00002
C	1.40365	3.09653	0.
C	0.07002	3.52796	0.00004
C	-0.9524	2.60705	0.00005
H	0.15264	-2.60328	0.0001
H	-4.57912	-2.47734	0.00003
H	-2.19994	-3.15296	0.0001
H	-3.43289	1.63706	-0.00017
H	-5.16922	-0.06106	-0.00012
H	2.71608	1.416	-0.00004
H	2.21078	3.81888	-0.00001
H	-0.15784	4.5871	0.00008
H	-1.97201	2.96682	0.00011
Br	2.7135	-1.25959	-0.00002

No. 11

C	-4.6106	-0.72793	-0.00001
C	-3.52412	-1.56928	0.00009
C	-2.21058	-1.05511	0.00008
C	-1.99947	0.34224	-0.00002
C	-3.13395	1.18274	-0.00017
C	-4.40857	0.66193	-0.00015
C	-1.08355	-1.94131	0.00012
C	-0.63493	0.85664	0.00002
C	0.44965	-0.06048	0.
C	0.18373	-1.47242	0.00004
C	1.76314	0.46704	-0.00001

C	2.01188	1.81828	0.00004
C	0.93122	2.71008	0.00012
C	-0.36054	2.23949	0.00012
H	-1.2702	-3.0098	0.00019
H	-5.61639	-1.13033	0.00002
H	-3.66069	-2.64536	0.00016
H	-3.01748	2.25784	-0.00034
H	-5.26102	1.33082	-0.00026
H	1.01882	-2.15935	0.00002
H	3.03033	2.18362	0.00004
H	1.12233	3.77628	0.00002
H	-1.17194	2.95346	0.00023
Br	3.2739	-0.69339	-0.00006

No. 12

C	-4.98367	-0.39312	-0.00004
C	-4.30289	0.80113	-0.00015
C	-2.89284	0.83162	-0.00009
C	-2.16405	-0.38104	0.00002
C	-2.88831	-1.59191	0.00019
C	-4.26529	-1.59994	0.00016
C	-2.19364	2.08627	-0.00006
C	-0.70955	-0.33057	-0.00001
C	-0.06331	0.92738	0.00009
C	-0.84318	2.13417	0.00009
C	1.3453	0.99879	0.00011
C	2.08873	-0.15445	-0.00001
C	1.47081	-1.41292	-0.00017
C	0.09667	-1.48834	-0.00018
H	-2.77877	2.99963	-0.00013
H	-6.06682	-0.40607	-0.00009

H	-4.84296	1.74187	-0.00027
H	-2.36451	-2.53848	0.00041
H	-4.79725	-2.54381	0.00032
H	-0.32082	3.08437	0.00019
H	2.07413	-2.31148	-0.00031
H	-0.35873	-2.4696	-0.00038
H	1.83054	1.9675	0.00021
Br	3.98447	-0.05961	0.00001

No. 13

C	-4.32151	-1.58307	-0.00004
C	-4.20903	-0.21296	-0.00013
C	-2.94409	0.41107	-0.00008
C	-1.77227	-0.38188	0.00002
C	-1.91639	-1.78499	0.00015
C	-3.16078	-2.37432	0.00012
C	-2.8402	1.84374	-0.0001
C	-0.47467	0.27891	0.00002
C	-0.41935	1.69205	0.00007
C	-1.63509	2.45603	0.00001
C	0.83328	2.33905	0.00011
C	2.00865	1.62665	0.0001
C	1.94017	0.22622	0.00001
C	0.73844	-0.44049	-0.00003
H	-3.75607	2.4247	-0.00019
H	-5.29787	-2.05237	-0.00008
H	-5.09628	0.41127	-0.00022
H	-1.04163	-2.42191	0.00031
H	-3.24376	-3.45458	0.00024
H	-1.5626	3.53807	0.00005
H	0.74271	-1.52088	-0.00015

H	0.86098	3.4233	0.00015
H	2.96858	2.12602	0.00014
Br	3.55609	-0.77285	-0.00005

No. 14

C	-3.57663	-1.5065	0.07487
C	-3.53087	-0.16593	-0.22429
C	-2.31717	0.54876	-0.17992
C	-1.10068	-0.12163	0.11219
C	-1.19516	-1.4817	0.48296
C	-2.39748	-2.15571	0.46303
C	-2.33969	1.97322	-0.34928
C	0.14783	0.64621	0.09704
C	0.05191	2.06715	0.04981
C	-1.21826	2.70011	-0.17823
C	1.19127	2.8838	0.17195
C	2.4419	2.33258	0.29664
C	2.58108	0.94353	0.22871
C	1.47196	0.13036	0.10744
H	-3.2886	2.45271	-0.56291
H	-4.51543	-2.04622	0.0447
H	-4.43743	0.37416	-0.47502
H	-0.3239	-2.01284	0.82555
H	-2.42549	-3.19682	0.76215
H	-1.2393	3.78217	-0.24327
H	1.05984	3.95972	0.1526
H	3.32075	2.95724	0.39758
H	3.56577	0.49547	0.23788
Br	1.91496	-1.70089	-0.23019

No. 15

C	-4.37772	0.14379	0.00006
C	-3.2804	0.99892	0.00036
C	-2.00478	0.4449	0.00031
C	-1.82466	-0.94556	-0.00001
C	-2.92152	-1.79424	-0.00022
C	-4.20051	-1.24004	-0.00022
C	-0.35186	-1.28325	0.0001
C	0.2927	0.07833	-0.00005
C	-0.68247	1.08826	-0.0002
C	-0.32392	2.43086	-0.00016
H	-1.07887	3.20847	-0.00026
C	1.0284	2.76022	-0.0001
C	2.00945	1.77079	-0.00007
C	1.62919	0.43192	-0.00005
H	-5.3804	0.55445	0.00011
H	-3.42072	2.07404	0.00062
H	-2.79032	-2.87083	-0.00044
H	-5.06758	-1.89006	-0.0004
H	1.33212	3.80037	-0.00014
H	3.05943	2.03407	-0.00005
H	-0.05935	-1.86438	0.88051
H	-0.05901	-1.86497	-0.87978
Br	2.95752	-0.92831	0.00004

No. 16

C	-4.56085	1.0646	-0.00014
C	-3.22141	1.44065	-0.00002
C	-2.24916	0.44604	0.00011
C	-2.60973	-0.9092	0.00005
C	-3.94572	-1.2795	-0.00009
C	-4.92054	-0.2832	-0.00019

C	-1.37342	-1.77924	0.00024
C	-0.25551	-0.7625	0.00007
C	-0.78268	0.53698	0.00007
C	0.06264	1.64083	0.00015
H	-0.33474	2.64937	0.00016
C	1.4392	1.44059	0.00014
C	1.94455	0.14341	0.00001
C	1.11421	-0.97365	-0.00005
H	-5.33305	1.82471	-0.0002
H	-2.94508	2.48927	0.00003
H	-4.23199	-2.3258	-0.00015
H	-5.969	-0.55724	-0.00031
H	2.11946	2.28223	0.00016
H	-1.33203	-2.42488	0.88277
H	-1.33194	-2.42567	-0.88169
H	1.53567	-1.97163	-0.00012
Br	3.82781	-0.1113	-0.00008

No. 17

C	3.7453	-1.94382	0.
C	2.37071	-1.72979	0.00012
C	1.89999	-0.42085	0.00008
C	2.79053	0.66223	-0.00002
C	4.15994	0.44389	-0.00018
C	4.63257	-0.86728	-0.00017
C	2.02789	1.96731	0.00017
C	0.58838	1.5078	0.00005
C	0.52834	0.10708	0.00013
C	-0.69285	-0.55814	0.0001
H	-0.75311	-1.63933	0.00016
C	-1.84765	0.21345	-0.00001



C	-1.80935	1.60499	-0.0001
C	-0.57755	2.25689	-0.00006
H	4.13172	-2.95601	0.00001
H	1.68438	-2.5691	0.00021
H	4.85435	1.27696	-0.00029
H	5.69994	-1.05361	-0.00029
H	2.26034	2.57141	0.88256
H	2.26056	2.5721	-0.88167
H	-0.54399	3.34073	-0.00014
H	-2.73282	2.1692	-0.0002
Br	-3.53597	-0.66214	-0.00003

No. 18

C	2.76294	-1.96257	-0.00029
C	1.43688	-1.54013	-0.00036
C	1.16504	-0.1714	-0.00019
C	2.22579	0.74971	0.00004
C	3.54408	0.32283	0.00018
C	3.81024	-1.04408	0.
C	1.70416	2.16256	0.00038
C	0.20932	1.96503	-0.00002
C	-0.10092	0.59085	-0.00002
C	-1.44533	0.22621	0.00002
C	-2.44487	1.19382	-0.00014
C	-2.11057	2.54357	-0.00027
C	-0.77524	2.93743	-0.00018
H	2.98148	-3.02393	-0.00045
H	0.63997	-2.26931	-0.0007
H	4.35626	1.04171	0.00032
H	4.83526	-1.39572	0.00006
H	2.03426	2.71809	0.8835

H	2.03493	2.71915	-0.8818
H	-0.5101	3.98877	-0.00025
H	-2.90044	3.28479	-0.00046
H	-3.48236	0.88544	-0.00015
Br	-1.99653	-1.59406	0.00014

No. 19

C	3.01531	-1.2118	0.
C	1.65659	-1.5199	0.00001
C	0.73417	-0.47597	0.00001
C	1.16486	0.86424	0.
C	2.51937	1.1634	-0.00001
C	3.44428	0.11713	-0.00001
C	-0.02882	1.79694	0.00001
C	-1.20617	0.84236	0.00001
C	-0.73026	-0.49253	0.
C	-1.67586	-1.49022	0.
C	-3.03418	-1.28077	-0.00001
C	-3.48114	0.05091	-0.00001
C	-2.56838	1.10822	0.
H	3.74841	-2.01188	0.
H	1.3205	-2.55128	0.00002
H	2.86062	2.19429	-0.00002
H	4.50648	0.33882	-0.00002
H	-0.0343	2.40435	-0.88085
H	-2.92816	2.13251	-0.00001
H	-4.54736	0.25584	-0.00002
H	-3.74485	-2.10054	-0.00001
H	-1.32954	-2.50262	0.00001
Br	-0.03859	2.88116	1.57243

No. 20

C	-0.49133	-1.64805	-0.0001
C	0.96367	-1.4153	0.00002
C	1.14175	-0.01317	-0.00007
C	-0.1058	0.64348	-0.0001
C	-1.1024	-0.4399	-0.00022
C	2.36936	0.63518	-0.00002
C	-0.1342	2.01387	-0.00002
C	1.10752	2.70952	0.00005
C	2.32206	2.05768	0.00002
C	2.08631	-2.20587	0.0001
C	3.36438	-1.57561	0.00005
C	3.51806	-0.20719	-0.00001
H	4.24733	-2.20402	0.00008
H	4.51094	0.22903	0.00004
H	3.24392	2.62913	0.00006
H	-0.98511	-2.6085	-0.00016
H	-1.0682	2.56484	-0.00003
H	1.09125	3.79281	0.00008
H	2.02494	-3.2883	0.00012
Br	-2.95147	-0.12694	0.00005

No. 21

C	-0.05492	2.0265	0.00014
C	-0.12169	0.55689	-0.00003
C	1.21608	0.09746	0.00015
C	2.09904	1.19981	0.00003
C	1.24698	2.40327	0.00024
C	1.6084	-1.23366	0.00014
C	3.44834	0.943	-0.00012
C	3.88795	-0.41153	-0.00029
C	3.01097	-1.47349	-0.0001

C	-1.10032	-0.40143	-0.00015
C	-0.75481	-1.78206	0.00014
C	0.55775	-2.19375	0.00031
H	-1.55362	-2.51257	0.00016
H	0.78626	-3.2539	0.00026
H	3.38649	-2.4908	-0.00014
H	-0.91491	2.68079	0.00028
H	4.18184	1.74166	-0.00018
H	4.9535	-0.60796	-0.0004
H	1.61154	3.42086	0.00011
Br	-2.93468	0.07531	-0.00008

No. 22

C	1.66991	2.46156	0.00004
C	0.67555	1.3706	0.
C	1.41725	0.16847	-0.00001
C	2.80007	0.44943	0.
C	2.91249	1.92194	-0.00005
C	0.86343	-1.10352	-0.00001
C	3.67324	-0.60989	0.00001
C	3.14065	-1.93161	0.00002
C	1.7875	-2.18728	0.00001
C	-0.69398	1.29211	0.00001
C	-1.28017	-0.00504	-0.00001
C	-0.55795	-1.17495	-0.00002
H	-1.06607	-2.13155	-0.00002
H	1.4254	-3.20934	0.00001
H	1.43296	3.51615	0.00007
H	4.74813	-0.46768	0.00001
H	3.83249	-2.76565	0.00003
H	3.84269	2.47272	-0.00005

H	-1.33343	2.16625	0.00002
Br	-3.18086	-0.09977	0.

No. 23

C	3.08667	1.59443	-0.00007
C	1.61598	1.48597	-0.00003
C	1.3257	0.10393	-0.00001
C	2.52646	-0.6421	0.00002
C	3.61985	0.34919	0.0001
C	0.05146	-0.45439	-0.00001
C	2.4392	-2.01145	0.
C	1.14833	-2.61195	-0.00003
C	-0.0146	-1.87499	-0.00002
C	0.56267	2.36557	0.
C	-0.7618	1.84846	0.00001
C	-1.01034	0.49478	0.
H	-0.97748	-2.37103	-0.00003
H	3.63913	2.52349	-0.00007
H	3.32178	-2.64151	0.00002
H	1.08217	-3.69349	-0.00004
H	4.67374	0.1082	0.00013
H	0.7073	3.44001	-0.00001
H	-1.59823	2.53534	0.00003
Br	-2.81103	-0.10817	0.00001

No. 24

C	3.10184	-0.26323	0.00004
C	1.91715	0.68527	0.00001
C	0.72747	-0.07271	0.00001
C	0.97175	-1.4612	0.00001
C	2.4702	-1.69717	0.

C	-0.56065	0.50853	0.
C	-0.09968	-2.31957	0.
C	-1.41218	-1.78176	-0.00001
C	-1.63517	-0.42192	-0.00001
C	1.83222	2.05573	0.
C	0.54823	2.66068	-0.00001
C	-0.61865	1.92484	-0.00001
H	0.48574	3.74442	-0.00002
H	-1.58106	2.42202	-0.00002
H	3.73965	-0.10643	0.8766
H	3.73973	-0.10641	-0.87646
H	2.76278	-2.23297	0.87876
H	2.71899	2.68172	0.
H	0.02679	-3.39736	0.
H	-2.26353	-2.45238	-0.00001
H	-2.64129	-0.05774	-0.00002
Br	2.99247	-2.65352	-1.56867

No. 25

C	1.33248	2.43799	0.00005
C	2.11401	1.13849	0.00002
C	1.20584	0.06097	0.00012
C	-0.13449	0.49934	0.00012
C	-0.16893	2.00829	0.00016
C	1.59168	-1.28735	0.00008
C	-1.11026	-0.45524	0.00003
C	-0.77091	-1.83479	0.00005
C	0.5407	-2.24372	0.00009
C	3.4567	0.8629	-0.00014
C	3.87796	-0.49478	-0.00013
C	2.98719	-1.54382	-0.00001

H	4.94113	-0.70642	-0.00023
H	3.34666	-2.56674	-0.00004
H	0.77325	-3.30279	0.00006
H	-1.57009	-2.56533	0.00001
H	1.57417	3.03974	-0.87859
H	1.57472	3.03998	0.87839
H	-0.70215	2.38213	0.87747
H	-0.70188	2.38224	-0.87726
H	4.19839	1.65378	-0.00024
Br	-2.94189	0.0501	-0.00006

No. 26

C	-3.04321	1.81652	0.00002
C	-2.77864	0.32407	0.
C	-1.38686	0.11006	-0.00015
C	-0.65578	1.31474	-0.00009
C	-1.62813	2.47731	-0.00011
C	-0.79109	-1.1597	-0.00015
C	0.71263	1.26502	0.00004
C	1.32539	-0.01647	-0.00005
C	0.62866	-1.19922	-0.00017
C	-3.61087	-0.76513	0.00018
C	-3.0344	-2.06442	0.0001
C	-1.67375	-2.27111	-0.00008
H	-3.69552	-2.92365	0.00021
H	-1.27293	-3.27835	-0.00007
H	1.15376	-2.14625	-0.00017
H	-3.6209	2.11118	0.87874
H	-3.6217	2.11099	-0.87825
H	-1.48022	3.10889	-0.87858
H	-1.48063	3.10869	0.87857

H	-4.68963	-0.65744	0.00033
H	1.3301	2.15453	0.00012
Br	3.2284	-0.07367	0.00006

No. 27

C	3.65738	-0.17279	-0.00012
C	2.44165	0.73249	-0.00008
C	1.27857	-0.06475	-0.00025
C	1.57583	-1.44235	-0.00008
C	3.08018	-1.62258	-0.00015
C	-0.02345	0.46637	-0.00018
C	0.54112	-2.3391	0.00025
C	-0.79135	-1.849	0.00013
C	-1.0631	-0.50229	-0.00011
C	2.30992	2.0958	0.00022
C	1.00411	2.65431	0.00013
C	-0.1334	1.88018	-0.00009
H	0.90138	3.73344	0.00031
H	-1.11207	2.34299	-0.00004
H	4.27942	0.01019	0.87867
H	4.28007	0.01135	-0.87821
H	3.40581	-2.18414	-0.87845
H	3.40616	-2.18312	0.87866
H	3.17421	2.75039	0.00041
H	0.70961	-3.40978	0.00046
H	-1.61546	-2.55112	0.0003
Br	-2.87696	0.07035	0.

**Frequencies of Cl-PAHs at M06-2X/6-311++G(d,p) level without scale**

No.1

190.2340

299.1523

417.9241



422.7575	483.9694	624.0565
710.6652	720.4507	766.9422
860.5146	936.9603	998.9136
1017.0345	1018.2436	1059.0558
1108.8581	1127.1400	1180.9412
1201.2001	1320.6177	1344.6692
1491.6247	1522.5492	1665.1296
1668.1485	3189.8064	3198.9842
3210.4988	3220.0530	3222.0138

No.2

153.0039	166.4044	242.3630
254.5619	372.8043	446.2919
450.7072	525.1675	559.4291
696.4242	716.9219	772.1370
820.9578	883.0942	969.7330
1014.5089	1014.5757	1066.1509
1073.4098	1082.7897	1165.3917
1183.9402	1247.6584	1309.2175
1320.3332	1426.4427	1470.4114
1488.1777	1506.2865	1528.6219
1651.7269	1679.4044	3063.0253
3128.1667	3149.6640	3184.7573
3196.5061	3207.3718	3216.3894

No.3

65.3844	174.0008	214.7514
233.5278	388.8149	421.2838
444.5010	525.7343	545.1797
698.7583	705.5258	799.8330
878.1006	902.7060	926.5838
1007.6559	1015.8451	1020.1874
1063.0522	1118.6630	1132.0584

1192.8277	1249.5682	1307.0448
1337.6816	1416.2195	1462.2179
1499.1731	1504.5382	1528.5302
1654.8241	1681.0184	3056.9528
3123.8992	3143.6381	3184.7405
3201.0580	3202.8855	3222.1813

No.4

56.1171	120.2289	251.6492
308.2562	377.6382	384.6613
421.6517	499.3764	645.4515
647.0950	729.5555	824.3372
833.2601	853.5497	970.1813
994.5738	1010.7871	1036.6547
1067.9940	1130.9287	1137.1131
1206.1382	1249.5512	1316.6187
1329.9611	1418.7813	1446.6850
1496.2548	1500.7320	1543.2614
1658.5268	1680.7722	3052.6220
3115.9493	3147.6304	3179.7769
3181.1452	3215.6388	3216.4579

No.5

115.9851	171.7955	222.9097
235.2230	399.3637	419.4715
431.3779	476.8030	520.4688
545.8267	560.7953	638.0188
680.2947	751.7690	785.7092
801.1330	816.8795	847.9995
889.9457	933.6779	983.6757
997.3225	1008.4038	1021.9260
1054.8592	1093.0799	1165.9423
1171.8659	1191.3970	1233.4986

1237.1819	1283.7868	1376.7087
1413.8680	1420.7054	1476.9034
1502.1469	1559.7142	1645.8569
1673.1475	1704.3384	3185.2495
3185.5130	3195.7091	3201.7281
3211.8525	3219.2986	3230.4329

No.6

100.7502	179.1533	217.3406
274.5138	360.4742	405.5756
418.5067	486.4376	523.3486
523.4837	613.3895	647.9133
654.0706	766.5023	780.7556
790.2363	830.6631	866.8456
883.8133	913.6214	955.7112
985.0422	999.0988	1015.7698
1049.8527	1109.5309	1156.0005
1162.4210	1179.4111	1216.8542
1260.6963	1287.6742	1380.7887
1398.5888	1427.4526	1477.2680
1500.0295	1557.0762	1651.3717
1671.1320	1705.8750	3178.8297
3191.6084	3193.9344	3200.9739
3208.5466	3210.0090	3212.7074

No.7

83.6299	91.9828	166.0478
186.8438	246.8975	281.5141
294.3782	378.1615	404.7892
433.4007	455.2796	485.6160
500.8210	542.7456	564.0996
589.7580	624.6105	655.5835
696.4425	739.6082	764.5506

771.5106	798.6868	798.9838
861.6949	868.9285	913.6977
924.7212	926.2344	933.0972
961.5217	998.5604	1002.3932
1014.6477	1034.3820	1075.0071
1145.7721	1153.3930	1184.1801
1192.7121	1200.4654	1260.1042
1296.4252	1306.1803	1346.0660
1369.9339	1399.2890	1444.3122
1455.9564	1474.2069	1498.9219
1521.5295	1605.8246	1633.3759
1659.1826	1703.7556	1712.4354
3179.5349	3183.9069	3185.3069
3190.6936	3200.9102	3204.2742
3211.5260	3217.1521	3219.9437

No.8

57.7377	113.8158	160.2355
168.4657	253.3127	283.7930
317.8270	335.1891	396.5490
422.7103	474.3348	480.6847
490.6412	533.7891	562.4250
612.3823	627.7054	645.9588
719.9436	742.8101	769.8669
778.6397	779.1475	829.8016
841.7915	868.1631	890.4889
919.2144	923.1232	933.3659
949.7112	1001.2129	1005.5140
1019.4877	1034.8013	1094.9194
1143.2334	1150.4374	1183.6841
1195.7538	1211.8373	1284.0871
1296.4784	1300.2545	1334.1873

1368.9677	1391.7503	1443.6355
1466.0508	1475.8916	1495.8060
1522.9265	1606.1925	1633.5189
1655.9717	1702.9917	1711.6066
3178.7904	3181.3891	3183.1200
3188.2908	3192.1493	3200.6774
3208.0069	3216.7838	3232.2952

No.9

79.2749	113.5585	128.5102
234.0033	234.7644	240.5636
292.9577	393.0028	401.7160
419.4108	426.4355	485.6438
499.4484	554.8168	562.8559
594.6118	613.1760	649.4469
682.4587	743.4553	754.1162
778.5858	779.4258	850.1244
862.7174	867.7789	876.6558
919.6751	931.4474	955.9722
1000.9487	1003.9912	1015.9443
1017.1697	1042.8543	1044.2315
1137.1164	1160.0503	1184.9362
1200.4416	1208.3077	1254.0041
1292.8376	1305.1456	1345.0384
1355.6050	1414.9044	1424.7464
1455.5248	1485.1144	1494.4672
1525.6550	1598.2153	1623.8410
1654.5381	1705.7694	1706.1355
3176.9662	3181.6161	3182.1245
3189.8865	3190.1012	3207.1603
3207.3417	3225.1743	3225.7450

No.10

78.5378	93.8967	124.8796
218.8785	238.9778	248.1782
301.8856	359.7519	414.5767
415.0095	445.4766	478.8532
521.1307	556.8247	564.2071
603.2261	616.1842	629.5766
728.5266	734.8052	760.4875
772.5632	775.2183	792.5280
874.2597	875.4415	880.3451
912.3879	958.6835	982.4275
990.7790	1014.3449	1018.2547
1020.6430	1074.2198	1081.5201
1133.4076	1176.0857	1184.0990
1192.2783	1222.7798	1233.2430
1280.8816	1304.2607	1323.5241
1370.0161	1392.4586	1414.1052
1470.6658	1491.0978	1493.4320
1543.2940	1590.4653	1646.6213
1675.4141	1690.7541	1693.8546
3184.7384	3192.6835	3198.1461
3204.1086	3205.4764	3208.7337
3214.8711	3220.6103	3236.8579

No.11

60.9421	103.3810	169.1700
195.9047	237.6776	253.3721
284.6933	401.8335	411.5857
426.0611	481.6479	490.9116
504.4829	525.9649	574.8041
581.0686	600.1696	655.7501
712.3705	724.8994	764.0590
768.4245	808.0702	812.5914

834.6252	847.6176	887.9718
890.9838	921.0345	980.3200
999.0488	1005.6631	1014.9263
1045.9116	1073.1533	1101.1329
1140.3880	1170.5485	1183.9880
1201.2263	1219.3852	1237.3038
1255.8644	1294.5388	1324.3013
1367.2760	1393.4108	1427.7809
1455.0064	1487.6138	1496.4266
1543.6773	1583.3634	1641.2901
1671.1333	1688.6754	1699.7377
3176.6398	3189.0166	3191.5282
3200.0815	3210.8195	3211.4370
3213.4106	3225.4600	3234.3512

No.12

61.2040	96.4012	169.0907
170.1366	230.9358	278.3946
312.3142	360.2415	401.6937
440.2285	463.7259	504.0715
516.6437	528.4965	540.0673
561.1188	622.8432	662.7667
716.0557	737.0865	762.5593
764.2076	776.6224	831.1610
835.7291	870.3209	880.1187
900.6241	914.6332	976.7597
987.6735	1008.1605	1015.1102
1019.3439	1072.8403	1121.3419
1137.7225	1169.4952	1179.8899
1197.1492	1210.5282	1243.9751
1280.1807	1297.4778	1327.6025
1377.6559	1387.2044	1422.8582

1464.1516	1484.0056	1500.1296
1542.3260	1584.3383	1646.3606
1673.1527	1689.8153	1700.1125
3178.4340	3182.2603	3190.0348
3191.5355	3197.5534	3203.9537
3207.1627	3221.1522	3233.4706

No.13

61.4049	102.9398	155.3235
163.2794	244.3921	288.6924
319.4713	352.9428	417.0310
428.8174	436.7092	469.3099
515.7765	529.1797	564.5608
611.1574	631.2852	645.9805
715.9387	730.1887	756.8881
761.5503	782.8287	818.1351
859.3974	870.7329	879.8099
893.1324	895.8371	978.1487
989.8569	1005.9167	1014.0535
1036.3923	1070.8896	1121.1353
1136.1820	1168.3936	1176.5971
1194.7470	1219.8068	1244.7155
1272.7696	1295.1971	1318.8453
1370.5234	1389.3398	1438.9933
1464.7985	1474.3524	1494.6302
1549.8174	1578.6670	1643.1644
1673.9577	1687.8093	1699.2358
3170.4053	3180.8151	3189.3686
3191.4683	3199.7369	3203.2522
3214.9785	3221.0383	3240.6285

No.14

46.1314	90.6400	166.6872
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220.1774	223.6532	259.2592
295.0923	380.7461	411.9527
446.6228	465.1563	500.2160
507.3129	515.5804	554.2106
576.9433	611.2879	660.0036
715.9471	728.8405	761.3527
774.4705	781.6407	798.6444
844.9838	849.9141	889.7740
925.2351	943.2425	987.6227
999.3695	1009.8101	1014.8583
1016.7682	1085.2633	1126.0770
1129.5778	1169.0226	1176.3498
1198.8721	1214.9233	1232.6931
1247.2046	1290.0563	1323.2326
1346.8125	1369.8655	1442.3210
1448.2145	1474.1608	1494.7627
1546.5193	1585.1334	1635.3131
1671.8691	1685.5743	1701.7185
3174.0186	3186.5179	3189.3522
3190.9857	3201.1538	3206.4232
3208.3155	3212.4621	3289.6561

No.15

81.4181	110.6483	145.3660
201.0768	246.8032	266.5808
274.2724	398.2064	429.7673
444.9732	476.7305	511.1465
540.3478	565.7075	589.9805
636.6344	686.1693	704.0825
740.6220	776.1502	807.7316
810.6231	836.3870	863.1333
891.3423	929.9100	940.2957

982.5756	997.1470	1011.3603
1050.8362	1061.2115	1090.9521
1133.3142	1158.9644	1170.4754
1176.7056	1195.4480	1203.7136
1227.1966	1244.9030	1308.9752
1326.1571	1349.2844	1376.6982
1444.3356	1477.2098	1496.2005
1522.2053	1529.0026	1647.8293
1660.6253	1689.8404	1693.9865
3058.0102	3093.4212	3178.3644
3181.5618	3186.9371	3194.0885
3210.4939	3216.4592	3219.5944

No.16

57.3228	133.5620	161.9191
179.9023	239.8045	274.8854
327.6764	355.6310	425.4047
436.6269	497.5450	507.3391
512.9377	560.0973	582.8693
650.2011	684.4004	709.7572
747.1785	768.9933	782.0713
838.0866	844.4991	881.9427
891.7284	894.8273	950.8412
974.4827	984.6623	1008.7144
1028.4731	1056.2452	1106.6407
1127.9957	1152.1237	1169.0930
1172.1778	1196.9975	1212.7487
1232.4274	1263.2002	1304.1910
1323.4513	1335.5968	1369.1244
1450.5796	1464.3232	1495.4962
1513.5012	1531.7529	1647.5991
1657.7468	1685.5042	1688.4424

3071.5284	3109.5022	3173.4898
3188.4389	3191.1821	3197.2779
3198.2297	3209.4055	3212.6023

No.17

78.0776	108.8805	148.1580
184.3948	257.6896	304.4868
304.6997	349.3958	426.4043
439.6316	466.2299	493.3347
510.9413	599.7978	601.4136
640.1805	690.2154	703.8469
747.1941	787.3166	790.8765
824.5225	825.4124	872.2928
897.3087	903.4267	940.8553
977.6041	990.6435	1012.3347
1038.2112	1060.2459	1108.6300
1128.3312	1148.2865	1160.5958
1173.9092	1189.8869	1216.1952
1230.9081	1266.0770	1293.1211
1325.9506	1346.0316	1367.7230
1446.0630	1462.4458	1493.9913
1525.4438	1529.1627	1649.3349
1660.2315	1684.7514	1694.7466
3049.5999	3086.5077	3179.1889
3187.6690	3196.4267	3202.7941
3206.3444	3208.5832	3212.4954

No.18

74.6748	106.7980	171.2060
197.3497	232.9177	286.9606
290.0437	381.7569	427.2351
465.1269	476.6248	520.2357
532.6833	553.0088	577.6472

641.8566	671.5320	710.0272
752.4193	780.6481	789.5474
792.3564	843.1348	888.5712
920.5466	921.2166	956.9421
984.8193	997.9556	1015.1904
1026.1162	1067.1865	1102.6889
1135.1390	1157.4627	1167.2153
1179.1844	1192.0051	1201.5647
1229.8601	1260.5875	1286.1934
1327.6706	1349.2956	1378.6830
1444.0504	1472.6962	1493.6448
1519.4705	1527.6898	1647.2575
1660.4510	1684.2609	1689.7485
3046.5927	3084.4169	3181.1119
3182.3977	3192.5599	3200.5267
3205.5162	3229.8243	3239.5369

No.19

68.6742	110.0141	118.6214
166.4583	205.5097	294.2662
325.8555	421.2666	426.9609
441.0152	483.4467	515.4126
569.6222	589.5784	632.7832
658.0952	707.2638	757.2460
758.4478	767.5168	797.3646
824.2314	859.3396	889.3642
900.3972	900.6284	976.3494
977.4686	1011.0276	1012.5490
1028.2749	1054.5335	1056.7273
1120.9371	1136.6793	1172.6324
1177.3859	1196.1365	1211.4906
1228.3898	1242.1414	1261.3475

1319.7165	1321.5583	1335.4625
1382.6270	1491.0162	1492.9954
1522.7792	1531.6381	1654.8300
1662.0476	1685.1212	1685.4175
3117.7034	3201.2349	3201.8993
3207.3551	3208.4239	3216.4947
3217.2519	3227.3265	3227.6554

No.20

104.2941	161.3106	174.8223
217.8741	291.1719	361.0096
408.9384	454.5949	458.4793
528.8848	540.4478	574.8271
586.2404	632.3688	666.8848
689.0428	764.4206	773.1543
779.3832	818.1015	829.0932
850.7172	937.5130	944.0639
952.8931	1005.7133	1014.4088
1036.8850	1061.5136	1066.1809
1110.9271	1169.4883	1205.4840
1217.7150	1249.0676	1282.9200
1298.2073	1398.9930	1420.5619
1453.8057	1486.0424	1511.1944
1534.7751	1583.2081	1678.7308
1695.2669	1706.1089	3173.0337
3185.3848	3189.9697	3197.7054
3212.6928	3216.2214	3230.3340

No.21

85.9428	189.1966	200.9940
226.4472	271.2124	353.1190
393.3683	461.0675	506.9626
513.1726	540.8398	585.3809

612.5636	613.7127	681.4433
690.4938	709.0101	736.7979
780.5896	811.6054	843.0459
865.7643	916.8518	939.0643
963.8153	986.0565	1006.8403
1034.1762	1051.2483	1105.7832
1116.7541	1150.7937	1174.9255
1208.7351	1246.8772	1259.2039
1334.7581	1372.1350	1424.2306
1450.4741	1480.7646	1509.4315
1528.8262	1572.9647	1673.7635
1686.7082	1697.9461	3172.5804
3191.2578	3191.6424	3209.7502
3210.5573	3226.7940	3252.0856

No.22

96.1599	188.6922	216.0255
227.5151	267.6486	356.3224
377.8347	445.2867	471.9157
495.6943	554.0551	601.0949
601.3387	613.5121	670.6256
702.5466	737.5686	754.6673
784.0892	820.5592	849.2556
882.7904	901.3470	925.4555
949.2649	969.6737	1002.0558
1042.8299	1052.9561	1081.3251
1107.5698	1118.1001	1183.0411
1223.8972	1227.7198	1272.6356
1332.9539	1385.6620	1407.9806
1433.1797	1480.0593	1504.5512
1523.9244	1578.7468	1676.8697
1692.6181	1700.3470	3181.7578

3192.5142	3196.0168	3204.6299
3213.7975	3231.2545	3251.5261

No.23

101.1354	161.0042	209.7955
217.6531	290.6470	363.9325
410.8757	458.4170	463.7850
497.9184	546.2630	585.4029
599.5451	633.0550	672.1016
686.7805	733.5211	750.0679
792.7830	821.1762	828.9335
872.2094	908.4640	951.5369
963.9945	977.5831	1012.5770
1039.4601	1052.3763	1102.6493
1108.6018	1130.8273	1196.1635
1227.1187	1239.9900	1272.6811
1325.8741	1393.4167	1401.7711
1437.5085	1477.5083	1506.4906
1529.1170	1579.9555	1676.3800
1685.2137	1699.4692	3190.1687
3197.0744	3207.5204	3213.6857
3218.2244	3227.3118	3242.4020

No.24

32.8959	135.3671	158.0286
226.1541	260.7149	317.0505
421.7096	457.3080	469.4747
502.8801	513.5149	547.6960
565.2630	629.1909	663.3988
682.4372	708.6111	771.3556
796.3549	814.7419	835.6668
857.6350	912.6894	937.9962
968.2041	999.3849	1004.6092

1008.4150	1031.8863	1039.6809
1070.8558	1115.4491	1173.5960
1194.9452	1201.0972	1228.8299
1242.6995	1250.0046	1277.1077
1288.6229	1309.9092	1393.7935
1406.8513	1456.7783	1471.8428
1487.0017	1518.4862	1553.5880
1673.2348	1681.9079	1701.8506
3081.8952	3137.5997	3151.8715
3196.7003	3198.8943	3207.6776
3209.9168	3218.8169	3221.6323

No.25

81.9386	93.2232	193.1625
200.5701	218.8809	294.5644
352.2318	448.3074	454.2974
506.8524	509.7718	528.7373
562.3100	598.4784	640.9529
658.8718	692.3605	752.1960
781.2110	824.5826	837.0540
847.5581	898.4279	915.9001
967.8127	984.0552	1004.6742
1022.4036	1030.9965	1054.6112
1112.7742	1153.5450	1175.2606
1177.2248	1206.1367	1244.2866
1245.8943	1248.4689	1283.0580
1312.8591	1379.4077	1404.9831
1453.0328	1469.1296	1478.8083
1497.0948	1515.5064	1548.4743
1670.4205	1683.9746	1697.5814
3064.5940	3090.9483	3101.4523
3130.6351	3169.9282	3190.4218



3191.4558	3207.3352	3207.7691
No.26		
61.7005	105.0390	194.4037
214.4276	225.5236	277.7024
353.6590	443.4526	453.4535
463.2585	528.1277	546.5356
560.3810	589.8390	637.9404
676.8790	724.5128	750.7863
789.9070	834.9539	838.2608
882.2972	886.0971	897.8794
929.2383	971.4879	1004.7140
1026.0841	1043.8050	1052.5793
1088.4336	1119.7535	1178.0754
1184.8626	1221.0848	1239.5132
1243.5648	1247.6293	1284.2421
1309.4221	1388.5571	1403.3037
1423.0657	1469.2863	1483.9507
1499.8561	1507.3053	1548.8865
1669.0335	1679.5748	1697.0312
3062.5152	3084.7332	3098.5487
3125.7097	3183.8380	3194.7288
3198.9099	3205.8165	3221.0874
No.27		
60.3138	102.5863	166.1677
212.4007	220.9121	312.5995
359.9690	456.1641	459.0616
469.2530	492.7615	536.9932
588.9755	593.5383	628.6742
662.5472	722.2954	748.3219
797.5996	819.0629	833.3132
861.6684	879.4963	929.2353

963.6628	972.1659	1006.9484
1027.4309	1037.5218	1059.6652
1105.8315	1132.8253	1177.7032
1189.8630	1232.5525	1242.9126
1243.6115	1245.7923	1278.6103
1301.0339	1376.2743	1402.7078
1433.2093	1470.1104	1475.1467
1499.2282	1513.3752	1551.9388
1664.4314	1678.9156	1696.2499
3061.1927	3083.4369	3096.6843
3124.1619	3187.2744	3196.3861
3202.3839	3211.4738	3215.7427

**Frequencies Br-PAHs at M06-2X/6-311++G(d,p) level without scale**

No.1

173.5518	258.2871	324.2310
415.0830	472.8159	624.3809
686.6853	703.3062	759.8470
861.1345	938.7062	1004.1473
1012.5382	1021.1920	1057.0916
1108.4147	1110.1315	1181.8799
1205.4915	1322.4903	1345.5044
1489.5968	1519.2199	1660.1839
1667.3702	3188.0458	3196.4730
3209.0572	3219.0158	3220.8277

No.2

131.6707	143.9750	219.0434
234.6614	304.4374	416.3809
444.1775	515.8632	551.8527
675.2711	712.9809	769.8389
818.0488	885.9000	973.4029
1012.0024	1013.6091	1051.0959

1060.0885	1083.0170	1161.8906
1185.1051	1250.7950	1308.3710
1322.7446	1416.2163	1468.5933
1482.7851	1504.3448	1524.8529
1649.0073	1678.7276	3052.5254
3117.2230	3143.5612	3183.1963
3193.5760	3207.6397	3223.1377

No.3

59.0330	162.4725	200.1990
212.2744	318.0040	385.8092
439.6834	522.3758	534.0039
681.5412	697.4478	793.3639
856.6297	899.9390	925.5187
1006.3504	1011.8113	1018.1197
1065.2005	1108.1785	1131.2476
1192.2901	1242.6117	1301.5166
1332.0920	1416.2773	1457.4506
1496.3518	1502.3123	1522.3830
1644.3351	1671.3492	3064.4867
3129.8391	3153.1978	3199.9857
3216.8072	3218.5600	3238.2988

No.4

53.6473	109.3758	218.7227
294.4263	299.3760	369.1853
417.7685	491.9157	606.5229
645.5363	713.6765	816.2292
829.4140	853.3472	968.2872
997.6545	1011.0139	1031.2477
1066.5131	1112.7676	1139.3834
1209.7849	1248.9237	1318.9848
1331.7170	1418.6439	1443.8839

1496.2007	1499.9981	1539.0162
1657.7945	1676.5222	3052.6654
3116.1420	3147.9701	3178.9708
3180.4280	3215.6699	3216.6577

No.5

112.1199	168.7847	186.7960
232.8998	310.5357	418.7151
425.9634	475.1001	521.9614
537.7518	551.3561	630.0264
666.9601	754.3168	780.5216
803.2293	818.0134	835.6211
890.0504	928.2235	969.3552
998.4106	1014.1457	1022.3172
1057.8648	1093.7303	1164.6107
1170.5228	1193.1519	1228.4398
1236.6593	1290.6016	1378.6262
1413.0739	1422.2645	1477.8103
1501.2363	1559.6872	1644.4767
1675.9134	1706.3932	3179.1182
3193.5189	3202.9241	3203.9494
3208.7359	3217.5251	3240.7531

No.6

94.6966	177.3032	181.2692
264.1226	277.4350	402.4762
406.1687	484.7804	514.9338
522.5732	591.1872	638.3108
640.6660	762.8810	773.9273
789.2193	828.4935	849.2607
883.5818	913.4832	949.3889
983.8313	998.6133	1016.0543
1048.9271	1098.2027	1155.6542

1163.4552	1179.8964	1217.3299
1261.3754	1288.1889	1379.1311
1397.0415	1426.6896	1475.5504
1495.7764	1554.8806	1650.2424
1665.4713	1702.7963	3176.8593
3188.0460	3190.2219	3197.6953
3203.9187	3208.6125	3212.1632

No.7

60.4758	87.9977	128.9486
170.2726	240.6736	263.5292
276.1572	322.1255	397.9390
409.1401	440.4966	474.8254
497.2272	542.0698	544.9002
582.8767	624.3579	654.5436
678.4965	732.4357	760.1297
765.6113	792.2028	800.2780
855.2324	856.9822	901.9176
910.6045	924.6166	927.6742
938.9666	995.9776	1006.9960
1016.9089	1031.5214	1071.1679
1141.0126	1154.1273	1183.3617
1195.2265	1199.9930	1259.0468
1297.8251	1306.3812	1345.0714
1365.5580	1397.2367	1436.6811
1451.2433	1469.9618	1497.9779
1519.1174	1599.0314	1624.6180
1657.1062	1698.7819	1710.9896
3161.8480	3169.7835	3171.9916
3175.4270	3195.5044	3201.5898
3211.7291	3219.4075	3225.2196

No.8

59.7494	110.9325	134.9719
167.0903	236.8685	249.2261
299.5842	312.5668	393.0857
414.7195	450.7661	478.2475
487.8712	529.5141	552.5560
604.4337	624.1841	643.3617
701.4460	739.8101	767.1415
776.3194	777.7187	821.9216
838.4763	867.4233	889.9430
917.8203	922.1714	931.6659
938.8489	997.8385	1002.7631
1016.3859	1033.4615	1084.9741
1142.4827	1149.0993	1184.6328
1193.5444	1211.0874	1284.1250
1294.8604	1300.0139	1333.8202
1366.2459	1390.1434	1442.9809
1464.5516	1473.4362	1492.7572
1520.5545	1605.4324	1632.4394
1653.5825	1698.5057	1710.7754
3178.3029	3180.7911	3182.6900
3186.9986	3190.3538	3200.2583
3207.4995	3212.0025	3222.0334

No.9

67.2861	106.8431	114.0554
185.2256	209.8424	233.5387
289.0449	329.1623	397.0529
406.3719	416.2409	483.3114
498.5234	546.2225	558.6589
589.5275	613.5879	648.8453
671.9946	744.2603	751.4184
776.2131	777.2132	828.1395

858.6370	864.4115	873.9023
921.3392	930.3889	933.0421
998.1938	1001.7376	1014.2709
1015.0148	1044.4068	1046.0161
1136.9462	1159.8800	1184.0551
1201.1901	1209.1174	1253.2439
1289.3293	1301.7040	1340.5950
1348.4830	1414.3521	1420.7653
1451.6669	1484.9230	1493.0242
1525.0904	1596.5113	1620.4872
1654.9057	1703.8295	1706.2289
3176.7232	3182.0109	3182.3865
3189.1485	3189.5133	3208.6037
3208.7263	3225.9573	3226.7228

No.10

78.9267	96.3222	119.1479
176.1965	227.6006	238.8442
295.6254	295.9794	415.3015
415.7273	444.2366	471.8935
517.8775	552.7157	561.9679
598.5586	600.1531	628.8311
727.3568	732.3561	758.9412
759.0351	771.4509	788.8921
865.6236	877.1509	883.3325
913.2783	936.9148	983.7233
990.4032	1010.3985	1015.6201
1021.2566	1072.4357	1081.8738
1130.4259	1173.4987	1183.1654
1191.7980	1222.4383	1228.8546
1282.5411	1303.6456	1323.0133
1368.9897	1392.9573	1409.7572

1470.5180	1490.5771	1493.0595
1541.0033	1589.1184	1645.7889
1673.3424	1690.2730	1692.9181
3178.6742	3187.8299	3197.7459
3202.8406	3206.6763	3209.3065
3218.9271	3228.5878	3239.3084

No.11

59.8516	95.9288	157.6652
162.8014	236.1949	250.1189
250.9066	331.9012	410.7936
422.8116	476.1488	476.5631
505.1194	522.3252	568.8490
575.3177	598.2019	647.9859
711.9311	725.4688	765.0816
772.9485	790.5870	807.3447
842.3087	842.9081	888.7153
889.1673	923.3567	985.8051
999.9587	1011.5547	1017.6973
1036.0779	1075.3941	1105.2066
1136.4015	1173.3587	1188.9123
1209.5188	1223.2164	1241.2394
1260.6836	1295.1983	1321.9801
1367.1914	1393.5178	1428.7546
1457.0333	1484.5317	1495.8586
1544.2793	1585.1710	1641.8093
1670.8751	1686.4793	1698.4337
3183.5382	3187.3102	3196.9731
3199.0533	3207.6075	3216.8942
3223.4301	3226.9101	3239.5432

No.12

58.4148	95.2778	145.1751
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162.6317	225.3425	230.0656
302.8134	327.1600	398.5449
438.2548	459.8830	481.3160
505.7442	526.0480	538.1054
560.4160	616.9185	653.3338
713.5250	735.8561	754.6776
763.6180	776.0617	829.7593
836.1218	863.3947	880.3211
900.1309	904.2358	978.0489
989.5541	1007.8808	1015.3218
1018.6621	1072.5875	1117.1526
1133.7971	1170.0713	1182.5006
1198.6376	1209.6907	1243.4067
1279.6676	1298.9355	1327.2298
1376.5962	1387.2624	1421.2627
1463.8235	1483.3696	1498.6514
1541.4869	1581.9478	1645.1516
1669.0144	1688.9713	1699.8380
3179.5980	3181.2567	3187.6824
3189.6284	3196.7977	3204.9394
3206.8623	3221.8213	3234.4862

No.13

69.8013	98.8173	130.4720
158.3090	240.5126	270.9534
282.6431	313.6164	416.1590
422.9344	439.2953	468.5502
514.5354	527.1892	562.8537
607.0996	613.6011	635.1922
715.2465	729.2981	751.0643
764.9903	785.4488	815.2685
860.0043	860.6118	888.8070

894.3758	900.0904	985.0348
991.5015	1008.9711	1015.6015
1033.4038	1073.7832	1116.5755
1130.8506	1169.1652	1176.4021
1193.2176	1219.5184	1245.0489
1273.0819	1295.7908	1321.2980
1375.3883	1388.9565	1436.4906
1467.4499	1475.8779	1494.6757
1548.7150	1577.0868	1645.1176
1671.0404	1689.9031	1701.8987
3179.6926	3183.0158	3185.9995
3201.3822	3204.5054	3207.9513
3208.3639	3223.0276	3242.3938

No.14

54.5050	86.2365	155.2850
188.1351	215.7217	236.7959
287.8501	330.1916	413.8188
423.8553	452.7333	497.2243
504.7689	516.8128	552.6332
573.7358	607.2701	652.5535
714.8665	729.6348	759.9254
763.1076	784.5696	795.5599
839.3672	847.3761	893.8628
924.4024	930.2626	988.3405
994.6459	1004.4488	1015.6395
1016.6759	1085.3259	1120.3857
1126.6734	1169.0985	1175.1605
1198.9787	1215.3978	1233.0482
1246.9927	1293.3207	1324.9033
1345.3693	1371.9181	1440.9704
1446.2662	1472.6177	1496.5353

1545.2157	1581.1785	1632.0007
1667.5679	1686.4475	1702.2695
3179.6753	3184.9140	3186.7551
3196.8912	3198.1218	3199.5934
3206.7568	3210.0586	3270.4144

No.15

71.6947	110.8679	120.9699
184.8732	246.0975	251.8966
276.7822	313.6591	430.3801
438.8763	480.0980	498.9384
534.7265	562.4148	583.3222
637.3555	675.3752	700.3552
741.8321	777.2713	802.0587
809.6038	830.6158	858.5399
892.6048	917.0845	946.0317
983.0595	998.6552	1014.9277
1043.1298	1060.6057	1089.5425
1133.5094	1166.2245	1174.9273
1179.5629	1197.6913	1203.5831
1226.5640	1245.5296	1309.9801
1323.8244	1348.9454	1374.7666
1451.6184	1472.5096	1491.8775
1521.3200	1526.7880	1639.9821
1662.8645	1680.2065	1691.2623
3073.1834	3109.2370	3177.9055
3182.8263	3190.3812	3200.3686
3204.8317	3215.7866	3222.6100

No.16

56.0820	132.6609	140.8487
173.1578	223.9344	237.8060
310.9216	322.1446	421.3274

434.1348	479.9217	494.0170
506.8282	558.8364	578.2602
649.1727	670.8203	706.0376
743.8887	766.0940	780.7948
835.9875	845.5827	877.0861
880.5586	893.5161	949.7434
975.3622	984.7983	1008.3794
1026.1891	1056.6793	1099.7363
1127.3815	1154.6831	1167.9252
1171.6365	1194.1079	1212.2863
1232.2048	1262.0898	1305.1892
1322.9551	1335.3930	1368.9846
1449.3852	1462.8073	1494.2541
1513.4845	1529.9467	1645.9288
1657.3791	1682.4419	1688.6704
3068.1277	3105.8235	3175.0812
3188.7870	3190.0273	3191.6721
3199.8032	3210.1386	3217.9442

No.17

68.1966	107.7896	117.9632
179.4522	261.2524	264.8453
285.5092	303.6409	421.7576
436.3126	448.7222	493.3320
506.8783	588.3403	595.9374
639.0995	673.7062	702.8777
747.5909	783.9074	786.3544
823.6369	833.4633	864.8238
887.9983	903.2888	945.3965
977.6836	990.8064	1011.7163
1036.2408	1058.0988	1096.7462
1129.9090	1154.1640	1173.6787

1178.5747	1198.0377	1217.9918
1231.9649	1266.8881	1292.2437
1323.2363	1348.6049	1367.6643
1452.1316	1460.4983	1494.1473
1521.1490	1529.0675	1647.6747
1661.6855	1680.8212	1691.6428
3068.6576	3105.2995	3180.7178
3186.3708	3187.0859	3197.7491
3207.4326	3209.9012	3223.0544

No.18

71.0618	102.5918	138.7623
191.9482	241.0300	260.5081
285.7072	321.4030	421.9577
439.4527	477.0840	510.9244
526.2287	553.6404	575.3139
642.7172	661.0645	708.4609
749.4027	776.5317	784.1556
789.1725	842.9101	882.7737
899.5670	919.9462	957.0756
981.1496	995.4202	1014.4543
1024.2587	1068.1346	1102.0130
1132.4656	1158.5358	1166.6266
1182.0323	1195.8913	1200.1848
1232.3033	1259.8754	1286.6672
1324.1726	1349.0040	1372.6538
1452.9528	1469.9627	1490.3251
1516.8136	1525.4379	1637.5655
1657.6509	1681.3323	1685.6210
3061.2921	3100.0726	3175.3943
3182.9707	3194.4922	3202.6253
3209.4740	3221.5731	3228.6296

No.19

63.3826	100.7129	102.4651
152.3402	198.4432	273.7389
292.6639	419.7539	425.4952
444.4281	458.2490	514.1568
569.3506	583.8913	633.0109
654.8318	676.9886	756.5153
758.5861	764.6947	798.6304
802.3696	856.2105	877.1066
900.7015	901.6288	978.2042
978.5760	1012.5954	1014.4028
1028.2149	1055.5501	1057.6296
1121.8940	1137.6949	1171.9817
1178.2288	1183.9799	1191.7043
1216.6137	1227.2079	1258.6084
1322.0911	1322.9933	1335.2166
1382.2608	1490.9658	1493.7702
1523.1247	1531.5679	1654.5842
1661.6441	1684.6531	1684.8755
3135.3089	3200.5598	3201.3288
3206.6382	3207.5991	3215.8608
3216.5817	3227.3048	3227.5940

No.20

99.8908	143.8880	161.3883
217.3368	281.7067	286.9246
402.5952	440.8197	457.9989
524.8097	534.1163	570.0574
584.3606	628.5718	665.1490
689.0027	748.1339	768.7667
779.6640	818.4804	829.2614

854.7549	924.8930	943.6455
955.1568	1006.0535	1014.1895
1035.8633	1058.5450	1063.9499
1110.7121	1170.7201	1205.7566
1217.3518	1249.6446	1281.7254
1294.7686	1397.9529	1419.5089
1454.4121	1485.9030	1510.4511
1534.7042	1580.1130	1676.8119
1695.8262	1704.8147	3174.8773
3187.5315	3192.9620	3198.6934
3208.3149	3218.0358	3231.9017

No.21

79.5221	160.3016	186.9420
225.2259	265.3143	273.5381
390.5227	452.6231	499.6083
504.6471	535.2999	582.1290
596.1460	612.0596	680.4449
687.4484	704.7764	737.8238
779.6443	810.6114	842.0192
861.6538	896.8704	940.0585
968.8587	984.0126	1006.4941
1034.5436	1050.1706	1103.5787
1113.0037	1144.7944	1176.0603
1211.8400	1247.7195	1260.8372
1334.4008	1369.8813	1422.7368
1450.7832	1479.5529	1508.3498
1527.5831	1574.2887	1670.4846
1685.5593	1697.2552	3176.9350
3189.2241	3192.6756	3207.3123
3207.8514	3232.9604	3257.0000

No.22

89.1839	178.9486	188.7436
226.8266	259.3274	264.6012
377.0299	441.9122	472.4978
492.0914	547.1957	592.5283
596.0514	610.2076	670.5054
699.9935	734.9095	738.6221
785.0510	819.3364	840.4315
884.6535	888.4995	935.4680
949.9675	967.8458	1004.4926
1041.1889	1052.4756	1080.5826
1109.2799	1117.1060	1185.0443
1226.6784	1231.8819	1272.7550
1333.4040	1386.3142	1409.1312
1430.3582	1481.1513	1503.2539
1523.2436	1580.4721	1673.8519
1692.7450	1699.7177	3185.5011
3196.5143	3196.6735	3206.6989
3225.7066	3228.0807	3248.4992

No.23

93.1948	160.3301	170.5347
217.0122	280.8610	285.4617
406.1051	455.3368	462.2577
490.8030	536.9749	579.8263
587.7579	627.5744	673.7830
685.8038	732.3985	736.7361
790.5881	818.1580	825.3479
864.1487	896.3516	952.5654
964.5609	975.1192	1009.6921
1038.2756	1047.6785	1096.9158
1104.7355	1130.0934	1191.1864
1228.2548	1240.1737	1271.2777



1325.5414	1392.9841	1398.6950
1432.8976	1475.0993	1503.7353
1526.5366	1579.6806	1678.6714
1680.2301	1697.9868	3188.5569
3196.2653	3202.4014	3215.1471
3215.5326	3227.9951	3248.0435

No.24

32.2224	111.5418	158.3536
216.0148	249.0009	270.2512
420.9626	451.0561	468.4589
494.0000	512.8750	528.9417
554.9963	623.8964	662.8552
664.7159	684.8113	771.5351
794.4497	814.6461	834.4741
853.6462	909.9171	938.8324
958.4224	996.8617	1002.2695
1008.7786	1031.7275	1040.3943
1071.3742	1114.6121	1172.6286
1179.5795	1200.7453	1222.6009
1241.4264	1243.1098	1249.2981
1288.6609	1308.7213	1393.2969
1406.4037	1456.8303	1469.5947
1486.2103	1517.5603	1553.1372
1672.6489	1681.6262	1701.5704
3076.3340	3143.0325	3165.5708
3197.3953	3197.6849	3207.9001
3208.5850	3220.0103	3221.2126

No.25

80.0306	95.0630	154.7358
198.6774	218.8386	273.5758

289.1565	446.9264	447.8648
496.8208	505.1290	525.3185
562.5466	584.2786	636.9287
658.0114	683.4136	751.7587
780.3212	821.5167	836.9961
847.6215	877.2987	916.6052
968.4010	982.9236	1004.9196
1022.4563	1031.7455	1053.5926
1108.4520	1146.6882	1173.7640
1176.2272	1209.4320	1244.4302
1244.7305	1246.1512	1281.9182
1311.4061	1376.0375	1403.5037
1453.3961	1467.7851	1476.3712
1495.9867	1514.4769	1546.9040
1666.3835	1682.4419	1694.4605
3064.8397	3087.8313	3102.1057
3127.8282	3172.7356	3189.3922
3191.0744	3205.2349	3206.9199

No.26

59.3108	96.8199	177.1792
191.8302	225.1314	261.8246
269.9586	441.3550	451.8982
462.3129	520.5922	539.5064
558.4202	582.0156	633.4968
674.8127	706.1853	749.6076
790.3496	832.3929	838.3041
862.9383	884.1219	902.1781
929.9886	970.1928	1006.9217
1025.9011	1041.8758	1051.7722
1088.9919	1116.6682	1178.2098
1185.4713	1225.6373	1239.0497

1244.5674	1247.2684	1284.5171
1309.8451	1388.9104	1400.5471
1422.5366	1469.1172	1483.2682
1499.8577	1506.4294	1547.5426
1666.4923	1678.2928	1695.0564
3061.4147	3088.1383	3097.8809
3128.5808	3183.3618	3193.1229
3202.5459	3208.9323	3226.0390

No.27

64.8880	97.3906	164.8981
174.3429	222.2106	278.4228
305.7950	455.1071	455.5036
468.1524	485.4507	527.4840
579.2455	590.7075	624.8146
661.6143	708.0750	747.2217
796.3927	818.3400	829.6864
857.4082	865.3564	925.0957
959.5441	972.5397	1006.3040
1027.0881	1037.0645	1055.0372
1100.6510	1132.4457	1177.8323
1193.2952	1235.2793	1242.4068
1243.5975	1246.0496	1277.4175
1301.6817	1374.4585	1398.8396
1432.2892	1470.5901	1473.3562
1498.5737	1511.5543	1550.7103
1660.7718	1679.2930	1694.1771
3065.2335	3078.1354	3099.7161
3120.2745	3187.3344	3193.3572
3199.0244	3208.5633	3209.2039