

Supporting Information

Quantum-Chemically Informed Machine Learning: Prediction of Energies of Organic Molecules with 10 to 14 Non-hydrogen Atoms

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Table S1. List of 34 molecules of PDS(10-14) that are eliminated by isodesmic reactions.

S. No.	Name of the molecule
1	Octahydro-4,7-methanoindene
2	protoadamantane
3	spiro-4,5-decane
4	E-2,2,5,5-tetramethyl-3-hexene
5	1-methyl adamantane
6	2-methyl adamantane
7	spiro-5,5-undecane
8	2,2-dimethyladamantane
9	diphenylmethane
10	1,3,5-trimethyladamantane
11	1,8-cyclotetradecadiyne
12	trans-anti-trans-tetra-decahydroanthracene
13	1,3,5,7-tetramethyladamantane
14	cyclotetradecane
15	Diamantane
16	1,3-Benzenedicarboxylic acid
17	1,4-Benzenedicarboxylic acid
18	1,4,7,10-Tetraoxa-cyclododecane
19	1-(2,4,6-Trimethylphenyl)ethanone
20	2-(Diacetoxymethyl)furan
21	2-Ethyl-3-oxobutanoic acid ethyl ester
22	1,4-Dimethyl-2,3-diazabicyclo[2.2.2]oct-2-ene
23	1-Hydroxy-2,2,6,6-tetra-methyl-4-piperidinol
24	1-Methyl-2,4-dinitrobenzene
25	Bicyclo[3.3.2]decane
26	3-Aminobenzoic acid
27	2,2,4,4-Tetramethyl-1,3-cyclobutanedione
28	Pentanoic acid propyl ester
29	2,3-Dihydro-1,4-benzodioxin
30	Benzoic acid methyl ester
31	2-Methylnaphthalene
32	(E)-2-Butenoic acid 3-methylbutyl ester
33	1,4-Naphthalenedione
34	Diphenylacetylene

Table S2. Comparison of G4MP2 and experimental enthalpies of formation of the PDS(10-14).
The values shown in the table are in kcal/mol.

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	ΔH_f^0 (298K)		Experiment - G4MP2	G4MP2 - FCHL- Δ
				Experiment	G4MP2		
1	10	C ₁₀ H ₁₂	1,2,3,4-Tetrahydronaphthalene	6.21	4.03	2.18	-0.17
2	10	C ₁₀ H ₁₄	1,2,3,4-Tetramethylbenzene	-8.99	-10.4	1.41	0.41
3	10	C ₁₀ H ₁₄	1,2,3,5-Tetramethylbenzene	-10.61	-12.08	1.47	0.25
4	10	C ₁₀ H ₁₄	1,2,4,6-Tetramethylbenzene	-11.26	-12.79	1.53	0.47
5	10	C ₁₀ H ₁₄	Butylbenzene	-3.13	-4.89	1.76	-0.01
6	10	C ₁₀ H ₁₄	Isobutylbenzene	-5.14	-6.52	1.38	0.34
7	10	C ₁₀ H ₁₄	Sec-Butylbenzene	-4.16	-6.67	2.51	0.10
8	10	C ₁₀ H ₁₄	Tert-Butylbenzene	-5.4	-7.65	2.25	0.07
9	10	C ₁₀ H ₁₆	Adamantane	-32.17	-34.21	2.04	-0.32
10	10	C ₁₀ H ₁₆	Camphene	-6.84	-7.25	0.41	0.23
11	10	C ₁₀ H ₁₆	Limonene	-0.62	-0.91	0.29	0.02
12	10	C ₁₀ H ₁₆	Perhydrotriquinacene	-24.45	-24.16	-0.29	0.09
13	10	C ₁₀ H ₁₆	α -Phellandrene	-2.22	-1.99	-0.23	-0.09
14	10	C ₁₀ H ₁₆	α -Pinene	6.76	4.99	1.78	0.16
15	10	C ₁₀ H ₁₆	α -Terpinene	-4.92	-5.08	0.16	-0.15
16	10	C ₁₀ H ₁₆	β -Pinene	9.25	7.43	1.82	0.20
17	10	C ₁₀ H ₁₈	Bicyclo[5.3.0]decane	-31.26	-29.87	-1.39	-0.05
18	10	C ₁₀ H ₁₈	Cis-3,7,7-Trimethyl-bicyclo[4.1.0]heptane	-16.68	-18.00	1.32	0.11
19	10	C ₁₀ H ₁₈	Cis-Decalin	-40.44	-41.86	1.42	
20	10	C ₁₀ H ₁₈	Trans-3,7,7-Trimethyl-bicyclo[4.1.0]heptane	-17.23	-15.03	-2.2	-0.01
21	10	C ₁₀ H ₁₈	Trans-Decalin	-43.52	-44.56	1.04	-0.01
22	10	C ₁₀ H ₂₀	1-Decene	-29.49	-29.56	0.07	0.43
23	10	C ₁₀ H ₂₀	Butylcyclohexane	-50.98	-51.71	0.73	-0.09
24	10	C ₁₀ H ₂₀	Cyclodecane	-36.88	-36.71	-0.17	0.87

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	ΔH_f^0 (298K)		Experiment - G4MP2	G4MP2 - FCHL- Δ
				Experiment	G4MP2		
25	10	C ₁₀ H ₂₂	2-Methylnonane	-62.12	-59.34	-2.78	0.26
26	10	C ₁₀ H ₂₂	5-Methylnonane	-61.81	-59.72	-2.09	0.35
27	10	C ₁₀ H ₂₂	Decane	-59.63	-58.14	-1.49	0.26
28	10	C ₁₀ H ₈	Azulene	69.1	67.91	1.19	-1.94
29	10	C ₁₀ H ₈	Naphthalene	35.92	32.76	3.17	-0.54
30	10	C ₄ H ₈ N ₄ O ₂	1,4-Dinitrosopiperazine	46.44	47.22	-0.78	0.97
31	10	C ₅ H ₁₀ O ₅	1,3,5,7,9-Pentaoxecane	-186.38	-186.13	-0.24	-0.10
32	10	C ₅ H ₃ NO ₄	5-Nitro-2-furancarboxaldehyde	-35.23	-34.98	-0.25	-0.55
33	10	C ₆ H ₁₀ O ₄	Hexanedioic acid	-206.74	-204.94	-1.8	0.24
34	10	C ₆ H ₁₂ N ₄	1,3,5,7-Tetraazatricyclo-[3.3.1.1 ^{3,7}]decane	47.54	46.85	0.68	1.11
35	10	C ₆ H ₆ N ₂ O ₂	2-Nitroaniline	15.25	13.33	1.92	0.53
36	10	C ₆ H ₆ N ₂ O ₂	3-Nitroaniline	13.96	14.76	-0.8	-0.14
37	10	C ₆ H ₆ N ₂ O ₂	4-Nitroaniline	14.05	13.6	0.46	0.03
38	10	C ₆ H ₉ NO ₃	N,N-Diacetylacetamide	-131.48	-130.67	-0.8	0.82
39	10	C ₇ F ₃ H ₅	(Trifluoromethyl)benzene	-143.19	-143.81	0.62	-0.04
40	10	C ₇ FH ₅ O ₂	4-Fluorobenzoic acid	-118.19	-117.82	-0.37	0.09
41	10	C ₇ H ₁₀ O ₃	2,4,10-Trioxatricyclo-[3.3.1.1 ^{3,7}]decane	-119.31	-121.51	2.2	-0.08
42	10	C ₇ H ₁₆ O ₃	Triethoxymethane	-151.84	-150.83	-1.01	-0.04
43	10	C ₇ H ₆ O ₃	2-Hydroxybenzoic acid	-118.26	-118.36	0.1	0.49
44	10	C ₇ H ₇ NO ₂	1-Methyl-4-nitrobenzene	7.41	5.46	1.95	0.06
45	10	C ₇ H ₇ NO ₂	2-Aminobenzoic acid	-70.75	-73.2	2.45	0.23
46	10	C ₇ H ₇ NO ₂	4-Aminobenzoic acid	-70.91	-71.44	0.53	-0.04
47	10	C ₇ H ₇ NO ₂	Nitromethylbenzene	7.34	7.02	0.32	0.73
48	10	C ₈ H ₁₀ O ₂	1,2-Dimethoxybenzene	-53.37	-50.77	-2.6	-0.20
49	10	C ₈ H ₁₄ O ₂	(E)-2-Butenoic acid 1-methylpropyl ester	-101.6	-102.17	0.56	0.47
50	10	C ₈ H ₁₄ O ₂	(E)-2-Butenoic acid butyl ester	-99.4	-98.65	-0.75	0.37

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	ΔH_f^0 (298K)		Experiment - G4MP2	G4MP2 - FCHL- Δ
				Experiment	G4MP2		
51	10	C ₈ H ₁₄ O ₂	2-Pentenoic acid isopropyl ester	-102.61	-100.63	-1.98	0.59
52	10	C ₈ H ₁₄ O ₂	2-Pentenoic acid propyl ester	-98.71	-98.35	-0.36	0.34
53	10	C ₈ H ₁₄ O ₂	3-Pentenoic acid isopropyl ester	-101.6	-101.31	-0.3	0.30
54	10	C ₈ H ₁₄ O ₂	3-Pentenoic acid propyl ester	-96.61	-97.08	0.47	0.10
55	10	C ₈ H ₁₄ O ₂	4-Pentenoic acid isopropyl ester	-99.71	-99.72	0	0.32
56	10	C ₈ H ₁₄ O ₂	4-Pentenoic acid propyl ester	-95.1	-95.51	0.41	0.12
57	10	C ₈ H ₁₆ O ₂	2-Eethylhexanoic acid	-133.72	-134.46	0.74	0.12
58	10	C ₈ H ₁₆ O ₂	Butanoic acid 1-methylpropyl ester	-130.33	-129.64	-0.69	0.04
59	10	C ₈ H ₁₆ O ₂	Heptanoic acid methyl ester	-123.3	-122.86	-0.44	0.02
60	10	C ₈ H ₁₆ O ₂	Octanoic acid	-132.48	-132.79	0.31	0.12
61	10	C ₈ H ₁₆ O ₂	Pentanoic acid isopropyl ester	-130.23	-129.47	-0.76	0.21
62	10	C ₈ H ₁₇ NO	Octanamide	-86.69	-85.53	-1.15	-0.01
63	10	C ₈ H ₁₈ N ₂	Di-N-butyldiazene	2.2	3.12	-0.92	-0.29
64	10	C ₈ H ₁₈ N ₂	Di-tert-butyldiazene	-8.63	-9.74	1.11	-0.04
65	10	C ₈ H ₁₈ O ₂	Tert-Butylperoxide	-83.44	-81.02	-2.42	-1.49
66	10	C ₈ H ₄ N ₂	1,2-Benzenedicarbonitrile	87.83	85.99	1.84	-0.49
67	10	C ₈ H ₄ N ₂	1,3-Benzenedicarbonitrile	86.66	84.58	2.09	-0.53
68	10	C ₈ H ₄ N ₂	1,4-Benzenedicarbonitrile	85.35	84.33	1.02	-0.66
69	10	C ₈ H ₅ NO	α -Oxobenzeneacetonitrile	28.08	26.55	1.54	-0.14
70	10	C ₈ H ₈ O ₂	Acetic acid phenyl ester	-66.85	-66.65	-0.2	-0.07
71	10	C ₉ H ₁₀ O	1-Phenyl-1-propanone	-24.07	-26.21	2.14	-0.02
72	10	C ₉ H ₁₄ O	cis-Octahydro-2H-inden-2-one	-59.66	-59.67	0.02	-0.02
73	10	C ₉ H ₁₄ O	Trans-Octahydro-2H-inden-2-one	-59.56	-60.1	0.54	-0.19
74	10	C ₉ H ₁₈ O	2,2,4,4-Tetramethyl-3-pentanone	-82.65	-83.31	0.66	-0.09
75	10	C ₉ H ₁₈ O	2,6-Dimethyl-4-heptanone	-85.47	-85.71	0.24	0.16

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	ΔH_f^0 (298K)		Experiment - G4MP2	G4MP2 - FCHL- Δ
				Experiment	G4MP2		
76	10	C ₉ H ₁₈ O	2-Nonanone	-81.43	-82	0.57	-0.02
77	10	C ₉ H ₁₈ O	5-Nonanone	-82.43	-82.5	0.07	0.01
78	10	C ₉ H ₂₀ O	1-Nonanol	-89.94	-90.88	0.94	0.08
79	10	C ₉ H ₂₁ N	N,N-Dipropyl-1-propylamine	-38.48	-37.92	-0.56	0.16
80	10	CHN ₃ O ₆	Trinitromethane	-0.05	2.07	-2.11	-3.26
81	11	C ₁₀ H ₁₂ O	1-Phenyl-1-butanone	-30.64	-31.17	0.53	-0.09
82	11	C ₁₀ H ₁₆ O	Camphor	-63.93	-65.12	1.19	-0.48
83	11	C ₁₀ H ₁₉ O	Decanenitrile	-21.87	-22.88	1.01	-0.01
84	11	C ₁₀ H ₂₀ O	2,2,5,5-Tetramethyl-3-hexanone	-94.14	-94.11	-0.04	-0.19
85	11	C ₁₀ H ₂₂ O	1-Decanol	-94.74	-96.11	1.37	0.02
86	11	C ₁₀ H ₈ O	1-Naphthol	-7.15	-7.83	0.69	-0.64
87	11	C ₁₀ H ₈ O	2-Naphthol	-7.17	-8.42	1.25	-0.68
88	11	C ₁₁ H ₁₀	1-Methylnaphthalene	27.94	24.81	3.13	-0.71
89	11	C ₁₁ H ₁₄	1,1-Dimethylindane	-0.38	-3.46	3.07	0.01
90	11	C ₁₁ H ₁₄	4,6-Dimethylindane	-1.39	-3.06	1.68	0.43
91	11	C ₁₁ H ₁₄	4,7-Dimethylindane	-1.77	-3.76	1.99	0.56
92	11	C ₁₁ H ₁₆	Pentamethylbenzene	-16.06	-16.86	0.8	0.32
93	11	C ₁₁ H ₂₀	Bicyclo[3.3.3]undecane	-21.27	-19.84	-1.44	0.97
94	11	C ₁₁ H ₂₂	Cycloundecane	-42.88	-41.56	-1.32	0.46
95	11	C ₁₁ H ₂₄	2,2,4,4,5-Pentamethylhexane	-67.16	-65.7	-1.46	0.34
96	11	C ₁₁ H ₂₄	2,2,5,5-Tetramethylheptane	-72.28	-73.65	1.37	0.43
97	11	C ₁₁ H ₂₄	3,3,5,5-Tetramethylheptane	-66.13	-66.12	-0.02	0.77
98	11	C ₁₁ H ₂₄	Undecane	-64.75	-64.39	-0.35	0.09
99	11	C ₄ F ₅ H ₃ O ₂	Pentafluoropropanoic acid methyl ester	-341.37	-340.78	-0.59	2.75
100	11	C ₆ F ₅ H	Pentafluorobenzene	-192.76	-191.57	-1.19	0.14
101	11	C ₇ F ₄ H ₄	1-Fluoro-3-trifluoromethylbenzene	-189.34	-189.33	-0.01	0.00

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	ΔH_f^0 (298K)		Experiment - G4MP2	G4MP2 - FCHL- Δ
				Experiment	G4MP2		
102	11	C ₇ H ₁₆ O ₄	3,5,7,9-Tetraoxaundecane	-177.1	-173.39	-3.71	0.24
103	11	C ₈ H ₁₅ NO ₂	N,N-Diacetylbutylamine	-113.41	-113.08	-0.33	0.20
104	11	C ₈ H ₄ O ₃	1,3-Isobenzofurandione	-88.77	-90.52	1.76	-0.26
105	11	C ₈ H ₅ N ₃	Pyridinium dicyanomethylide	125.1	121.68	3.41	-0.44
106	11	C ₈ H ₈ O ₃	2-Methoxybenzoic acid	-103.68	-103.1	-0.58	0.07
107	11	C ₈ H ₈ O ₃	3-Methoxybenzoic acid	-106.62	-107.37	0.75	-0.01
108	11	C ₈ H ₈ O ₃	4-Methoxybenzoic acid	-108.01	-108.66	0.66	0.09
109	11	C ₉ H ₁₀ O ₂	2-Ethylbenzoic acid	-81.41	-82.7	1.3	-0.09
110	11	C ₉ H ₁₀ O ₂	3,4-Dihydro-2H-1,5-benzodioxepin	-44.34	-47.86	3.52	-0.11
111	11	C ₉ H ₁₀ O ₂	3-Ethylbenzoic acid	-82.86	-84.71	1.84	-0.02
112	11	C ₉ H ₁₀ O ₂	4-Ethylbenzoic acid	-86.81	-84.87	-1.94	0.02
113	11	C ₉ H ₁₀ O ₂	Acetic acid-3-methylphenyl ester	-74.9	-73.89	-1.01	-0.01
114	11	C ₉ H ₁₆ O ₂	2-Pentenoic acid butyl ester	-105.09	-103.37	-1.72	0.36
115	11	C ₉ H ₁₆ O ₂	3-Pentenoic acid butyl ester	-103.49	-102.1	-1.39	0.13
116	11	C ₉ H ₁₆ O ₂	4-Pentenoic acid 2-methylpropyl ester	-104.37	-102.77	-1.61	0.19
117	11	C ₉ H ₁₆ O ₂	4-Pentenoic acid butyl ester	-102.08	-100.53	-1.55	0.15
118	11	C ₉ H ₁₈ O ₂	Nonanoic acid	-137.98	-137.91	-0.07	0.12
119	11	C ₉ H ₁₈ O ₂	Octanoic acid methyl ester	-127.58	-127.98	0.4	0.01
120	11	C ₉ H ₁₈ O ₂	Pentanoic acid 1-methylpropyl ester	-137	-134.79	-2.21	0.04
121	11	C ₉ H ₂₀ O ₂	Dibutoxymethane	-119.81	-119.25	-0.57	0.05
122	11	C ₉ H ₇ NO	8-Quinolinol	5.5	7	-1.5	-0.38
123	11	C ₉ H ₇ NO	β -Oxobenzenepropanenitrile	16.78	16.64	0.14	-0.09
124	12	C ₁₀ H ₂₀ O ₂	Decanoic acid	-142.18	-143.03	0.85	0.12
125	12	C ₁₀ H ₂₀ O ₂	Nonanoic acid methyl ester	-132.39	-133.11	0.72	0.01
126	12	C ₁₁ H ₁₄ O	3-Methyl-1-phenyl-1-butanone	-38.41	-38.18	-0.23	1.15

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	ΔH_f^0 (298K)		Experiment - G4MP2	G4MP2 - FCHL- Δ
				Experiment	G4MP2		
127	12	C ₁₁ H ₂₁ N	1-Cyclohexylpiperidine	-27.1	-29.64	2.53	0.47
128	12	C ₁₁ H ₂₂ O	2,2,6,6-Tetramethyl-4-heptanone	-100.67	-99.77	-0.9	0.12
129	12	C ₁₁ H ₂₂ O	6-Undecanone	-92.59	-92.77	0.18	-0.01
130	12	C ₁₁ H ₂₄ O	1-Methoxydecane	-91.09	-92.23	1.15	0.01
131	12	C ₁₂ H ₁₀	Acenaphthene	37.28	34.22	3.07	-0.27
132	12	C ₁₂ H ₁₀	Biphenyl	43.36	40.86	2.5	-0.30
133	12	C ₁₂ H ₁₂	1,8-Dimethylnaphthalene	25.98	23	2.98	-0.87
134	12	C ₁₂ H ₁₂	2,3-Dimethylnaphthalene	18.19	16.45	1.74	-0.62
135	12	C ₁₂ H ₁₂	2,7-Dimethylnaphthalene	19	16.43	2.57	-0.59
136	12	C ₁₂ H ₁₆	Cyclohexylbenzene	-3.99	-6.31	2.32	-0.05
137	12	C ₁₂ H ₁₈	(E,E,E)-1,5,9-Cyclododecatriene	24.21	23.6	0.62	0.12
138	12	C ₁₂ H ₁₈	(E,E,Z)-1,5,9-Cyclododecatriene	23.21	22.88	0.32	-0.17
139	12	C ₁₂ H ₁₈	Hexamethylbenzene	-20.75	-20.02	-0.72	-0.68
140	12	C ₁₂ H ₂₂	Bicyclohexyl	-51.55	-51.98	0.43	-0.03
141	12	C ₁₂ H ₂₄	1-Dodecene	-39.53	-41.21	1.68	0.06
142	12	C ₁₂ H ₂₄	Cyclododecane	-55.02	-54.17	-0.85	0.94
143	12	C ₁₂ H ₂₆	3,3,6,6-Tetramethyloctane	-76.05	-76.42	0.36	0.32
144	12	C ₁₂ H ₂₆	Dodecane	-69.24	-68.89	-0.35	0.12
145	12	C ₁₂ H ₈	Acenaphthylene	62.07	58.75	3.32	-0.78
146	12	C ₁₂ H ₈	Biphenylene	99.88	96.32	3.56	-0.35
147	12	C ₄ H ₈ N ₄ O ₄	1,4-Dinitropiperazine	13.93	16.36	-2.43	4.03
148	12	C ₆ F ₅ HO	Pentafluorophenol	-228.68	-227.32	-1.36	0.40
149	12	C ₆ F ₆	Hexafluorobenzene	-228.35	-227.23	-1.12	0.42
150	12	C ₆ H ₄ N ₂ O ₄	1,3-Dinitrobenzene	12.86	12.1	0.76	0.04
151	12	C ₇ F ₅ H ₃	2,3,4,5,6-Pentafluoro-1-methylbenzene	-201.46	-200.81	-0.65	0.01
152	12	C ₈ H ₁₀ O ₄	3,4-Diethoxy-3-cyclobutene-1,2-dione	-114.36	-111.25	-3.11	1.15

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	ΔH_f^0 (298K)		Experiment - G4MP2	G4MP2 - FCHL- Δ
				Experiment	G4MP2		
153	12	C ₈ H ₁₄ O ₄	Octanedioic acid	-213.89	-215.27	1.38	0.23
154	12	C ₉ H ₁₁ NO ₂	1-Phenylalanine	-74.78	-75.03	0.25	0.63
155	13	C ₁₀ H ₁₁ NO ₂	N,N-Diacetylaniline	-65.18	-65.89	0.71	0.45
156	13	C ₁₁ H ₁₄ O ₂	2-tert-Butylbenzoic acid	-89.89	-90.26	0.37	-0.64
157	13	C ₁₁ H ₁₄ O ₂	3,5-Diethylbenzoic acid	-97.47	-97.92	0.46	0.82
158	13	C ₁₁ H ₁₄ O ₂	3-tert-Butylbenzoic acid	-95.79	-98.07	2.28	0.04
159	13	C ₁₁ H ₁₄ O ₂	4-tert Butylbenzoic acid	-95.24	-98.14	2.9	0.13
160	13	C ₁₁ H ₂₂ O ₂	Decanoic acid methyl ester	-137.14	-138.23	1.09	0.01
161	13	C ₁₁ H ₂₂ O ₂	Undecanoic acid	-146.89	-148.15	1.26	0.12
162	13	C ₁₁ H ₈ O ₂	1-Naphthalenecarboxylic acid	-53.32	-54.56	1.24	-0.57
163	13	C ₁₁ H ₈ O ₂	2-Naphthalenecarboxylic acid	-55.57	-57.34	1.78	-0.48
164	13	C ₁₂ H ₁₀ O	Diphenylether	12.43	10.58	1.85	-0.35
165	13	C ₁₂ H ₂₄ O	2-Dodecanone	-96.63	-97.34	0.71	0.00
166	13	C ₁₂ H ₂₆ O	1-Dodecanol	-104.35	-106.33	1.98	0.05
167	13	C ₁₂ H ₉ N	9H-Carbazole	50.1	46.82	3.28	-0.40
168	13	C ₁₃ H ₁₂	4-Methylbiphenyl	33.03	31.77	1.26	-0.15
169	13	C ₁₃ H ₁₈	2,3-Dihydro-1,1,4,6-tetramethyl-1H-indene	-16.85	-19.45	2.6	0.33
170	13	C ₁₃ H ₁₈	2,3-Dihydro-1,1,4,7-tetramethyl-1H-indene	-14.94	-18.26	3.32	0.33
171	13	C ₁₃ H ₂₆	Cyclotridecane	-58.89	-59.34	0.45	1.88
172	13	C ₁₃ H ₂₆	Heptylcyclohexane	-69.12	-67.12	-2	-0.12
173	13	C ₁₃ H ₂₈	3,5-Dimethyl-3,5-diethylheptane	-72.01	-71.37	-0.64	0.82
174	13	C ₁₃ H ₂₈	4,4,6,6-Tetramethylnonane	-74.86	-77.25	2.4	0.87
175	13	C ₆ F ₆ H ₈ O	Bis(3,3,3-trifluoropropyl)ether	-383.44	-384.84	1.41	0.41
176	13	C ₇ F ₄ H ₁₄ N ₂	N,N,N',N'-Tetrafluoro-1,1-heptanediamine	-55.33	-56.84	1.52	-0.05
177	13	C ₇ H ₆ N ₂ O ₄	Dinitromethyl benzene	8.29	11.35	-3.05	-0.69

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	ΔH_f^0 (298K)		Experiment - G4MP2	G4MP2 - FCHL- Δ
				Experiment	G4MP2		
178	13	C ₈ H ₁₈ O ₅	3,5,7,9,11-Pentaoxa-tridecane	-216.52	-212.79	-3.73	0.05
179	14	C ₁₂ H ₁₀ N ₂	Cis-Azobenzene	109.49	105.8	3.69	-0.81
180	14	C ₁₂ H ₁₀ N ₂	Trans-Azobenzene	96.58	94.46	2.13	-1.21
181	14	C ₁₂ H ₂₄ O ₂	Dodecanoic acid	-153.44	-153.25	-0.19	0.14
182	14	C ₁₂ H ₂₄ O ₂	Undecanoic acid methyl ester	-141.92	-143.35	1.43	0.01
183	14	C ₁₂ H ₈ N ₂	Benzo-c-cinnoline	94.81	91.5	3.31	-1.10
184	14	C ₁₄ H ₁₀	Anthracene	55.19	50.34	4.84	-1.91
185	14	C ₁₄ H ₁₀	Phenanthrene	49.59	44.88	4.71	-1.14
186	14	C ₁₄ H ₁₂	9,10-Dihydroanthracene	38.17	35.04	3.13	-0.16
187	14	C ₁₄ H ₁₂	Cis-Stilbene	60.3	57.14	3.16	-0.11
188	14	C ₁₄ H ₁₂	Trans-Stilbene	56.43	54.34	2.09	-0.61
189	14	C ₁₄ H ₁₄	1,2-Diphenylethane	34.15	30.24	3.92	-0.10
190	14	C ₁₄ H ₁₆	1,4,5,8-Tetramethyl naphthalene	19.5	15.96	3.54	-1.64
191	14	C ₁₄ H ₁₈	1,2,3,4,5,6,7,8-Octahydro-anthracene	-8.89	-10.32	1.43	-0.25

Table S3. Signed deviations of B3LYP, and ω B97X-D from experimental enthalpies of formation of the PDS(10-14). The values shown in the table are in kcal/mol.

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	Experiment – B3LYP	Experiment – ω B97X-D
1	10	C ₁₀ H ₁₂	1,2,3,4-Tetrahydronaphthalene	-1.77	-1.07
2	10	C ₁₀ H ₁₄	1,2,3,4-Tetramethylbenzene	0.1	-2.96
3	10	C ₁₀ H ₁₄	1,2,3,5-Tetramethylbenzene	0.95	-2.74
4	10	C ₁₀ H ₁₄	1,2,4,6-Tetramethylbenzene	1.27	-2.49
5	10	C ₁₀ H ₁₄	Butylbenzene	1.24	-1.88
6	10	C ₁₀ H ₁₄	Isobutylbenzene	-1.38	-2.59
7	10	C ₁₀ H ₁₄	Sec-Butylbenzene	-0.27	-1.85
8	10	C ₁₀ H ₁₄	Tert-Butylbenzene	-2.87	-3.48
9	10	C ₁₀ H ₁₆	Adamantane	-10.05	-2.54
10	10	C ₁₀ H ₁₆	Camphene	-11.25	-6.27
11	10	C ₁₀ H ₁₆	Limonene	-4.93	-5.31
12	10	C ₁₀ H ₁₆	Perhydrotriquinacene	-10.46	-2.85
13	10	C ₁₀ H ₁₆	α -Phellandrene	-5.7	-6.33
14	10	C ₁₀ H ₁₆	α -Pinene	-7.93	-4.24
15	10	C ₁₀ H ₁₆	α -Terpinene	-3.34	-5.22
16	10	C ₁₀ H ₁₆	β -Pinene	-8.66	-3.84
17	10	C ₁₀ H ₁₈	Bicyclo[5.3.0]decane	-7.84	-3.6
18	10	C ₁₀ H ₁₈	Cis-3,7,7-Trimethylbicyclo[4.1.0]heptane	-4.07	-1.46
19	10	C ₁₀ H ₁₈	Cis-Decalin	-5.59	-1.34
20	10	C ₁₀ H ₁₈	Trans-3,7,7-Trimethylbicyclo[4.1.0]heptane	-7.91	-5.44
21	10	C ₁₀ H ₁₈	Trans-Decalin	-5.21	-1.95
22	10	C ₁₀ H ₂₀	1-Decene	0.61	-3.63
23	10	C ₁₀ H ₂₀	Butylcyclohexane	-0.46	-2.18

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	Experiment – B3LYP	Experiment – ωB97X-D
24	10	C ₁₀ H ₂₀	Cyclodecane	-3.16	-1.27
25	10	C ₁₀ H ₂₂	2-Methylnonane	-0.48	-5.89
26	10	C ₁₀ H ₂₂	5-Methylnonane	-1.57	-4.99
27	10	C ₁₀ H ₂₂	Decane	1.89	-3.95
28	10	C ₁₀ H ₈	Azulene	0.01	-5.08
29	10	C ₁₀ H ₈	Naphthalene	-0.02	-1.46
30	10	C ₄ H ₈ N ₄ O ₂	1,4-Dinitrosopiperazine	15.49	9.21
31	10	C ₅ H ₁₀ O ₅	1,3,5,7,9-Pentaoxecane	5.32	4.17
32	10	C ₅ H ₃ NO ₄	5-Nitro-2-furancarboxaldehyde	8.79	6.63
33	10	C ₆ H ₁₀ O ₄	Hexanedioic acid	-3.02	2.88
34	10	C ₆ H ₁₂ N ₄	1,3,5,7-Tetraazatricyclo-[3.3.1.1 ^{3,7}]decane	0.47	2.55
35	10	C ₆ H ₆ N ₂ O ₂	2-Nitroaniline	12.01	8.41
36	10	C ₆ H ₆ N ₂ O ₂	3-Nitroaniline	7.31	4.43
37	10	C ₆ H ₆ N ₂ O ₂	4-Nitroaniline	9.98	7.07
38	10	C ₆ H ₉ NO ₃	N,N-Diacetylacetamide	5.85	5.25
39	10	C ₇ F ₃ H ₅	(Trifluoromethyl)benzene	9.04	2.53
40	10	C ₇ FH ₅ O ₂	4-Fluorobenzoic acid	3.04	3.33
41	10	C ₇ H ₁₀ O ₃	2,4,10-Trioxatricyclo-[3.3.1.1 ^{3,7}]decane	-4.53	1.68
42	10	C ₇ H ₁₆ O ₃	Triethoxymethane	6.09	-1.09
43	10	C ₇ H ₆ O ₃	2-Hydroxybenzoic acid	0.33	2.92
44	10	C ₇ H ₇ NO ₂	1-Methyl-4-nitrobenzene	8.26	4.34
45	10	C ₇ H ₇ NO ₂	2-Aminobenzoic acid	4.56	6.22
46	10	C ₇ H ₇ NO ₂	4-Aminobenzoic acid	2.36	4.62
47	10	C ₇ H ₇ NO ₂	Nitromethylbenzene	3.41	2.06
48	10	C ₈ H ₁₀ O ₂	1,2-Dimethoxybenzene	1.47	-1.85

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	Experiment – B3LYP	Experiment – ωB97X-D
49	10	C ₈ H ₁₄ O ₂	(E)-2-Butenoic acid 1-methylpropyl ester	5.32	0.61
50	10	C ₈ H ₁₄ O ₂	(E)-2-Butenoic acid butyl ester	5.11	-0.19
51	10	C ₈ H ₁₄ O ₂	2-Pentenoic acid isopropyl ester	3.27	-2.11
52	10	C ₈ H ₁₄ O ₂	2-Pentenoic acid propyl ester	5.51	0.1
53	10	C ₈ H ₁₄ O ₂	3-Pentenoic acid isopropyl ester	3.34	-0.61
54	10	C ₈ H ₁₄ O ₂	3-Pentenoic acid propyl ester	4.98	0.66
55	10	C ₈ H ₁₄ O ₂	4-Pentenoic acid isopropyl ester	2.25	-0.7
56	10	C ₈ H ₁₄ O ₂	4-Pentenoic acid propyl ester	3.52	0.2
57	10	C ₈ H ₁₆ O ₂	2-Eethylhexanoic acid	0.41	0.54
58	10	C ₈ H ₁₆ O ₂	Butanoic acid 1-methylpropyl ester	4.08	-0.27
59	10	C ₈ H ₁₆ O ₂	Heptanoic acid methyl ester	4.52	0.53
60	10	C ₈ H ₁₆ O ₂	Octanoic acid	2.03	1.19
61	10	C ₈ H ₁₆ O ₂	Pentanoic acid isopropyl ester	4.1	-0.25
62	10	C ₈ H ₁₇ NO	Octanamide	3.83	1.48
63	10	C ₈ H ₁₈ N ₂	Di-N-butyldiazene	6.73	-2.11
64	10	C ₈ H ₁₈ N ₂	Di-tert-butyldiazene	2.48	-3.93
65	10	C ₈ H ₁₈ O ₂	Tert-Butylperoxide	0.31	-7.55
66	10	C ₈ H ₄ N ₂	1,2-Benzenedicarbonitrile	0.72	-3.33
67	10	C ₈ H ₄ N ₂	1,3-Benzenedicarbonitrile	1.04	-2.79
68	10	C ₈ H ₄ N ₂	1,4-Benzenedicarbonitrile	0.11	-3.85
69	10	C ₈ H ₅ NO	α -Oxobenzeneacetonitrile	1.13	-0.996
70	10	C ₈ H ₈ O ₂	Acetic acid phenyl ester	1.39	0.998
71	10	C ₉ H ₁₀ O	1-Phenyl-1-propanone	2.47	0.75

S. No.	Number of non- hydrogen atom	Chemical Formula	Name	Experiment – B3LYP	Experiment – ωB97X-D
72	10	C ₉ H ₁₄ O	cis-Octahydro-2H-inden-2-one	-6.13	0.44
73	10	C ₉ H ₁₄ O	Trans-Octahydro-2H-inden-2-one	-4.98	0.74
74	10	C ₉ H ₁₈ O	2,2,4,4,Tetramethyl-3-pentanone	-4.22	-3.55
75	10	C ₉ H ₁₈ O	2,6,Dimethyl-4-heptanone	1.64	-1.61
76	10	C ₉ H ₁₈ O	2-Nonanone	4.3	0.004
77	10	C ₉ H ₁₈ O	5-Nonanone	4.23	-0.52
78	10	C ₉ H ₂₀ O	1-Nonanol	2.16	-1.13
79	10	C ₉ H ₂₁ N	N,N-Dipropyl-1-propylamine	5.28	-2.16
80	10	CHN ₃ O ₆	Trinitromethane	13.73	8.14
81	11	C ₁₀ H ₁₂ O	1-Phenyl-1-butanone	0.85	-1.09
82	11	C ₁₀ H ₁₆ O	Camphor	-11.72	-3.05
83	11	C ₁₀ H ₁₉ O	Decanenitrile	2.75	-2.59
84	11	C ₁₀ H ₂₀ O	2,2,5,5-Tetramethyl-3-hexanone	-4.25	-4.57
85	11	C ₁₀ H ₂₂ O	1-Decanol	2.09	-1.16
86	11	C ₁₀ H ₈ O	1-Naphthol	-3.73	-2.54
87	11	C ₁₀ H ₈ O	2-Naphthol	-2.66	-1.66
88	11	C ₁₁ H ₁₀	1-Methylnaphthalene	-0.74	-2.17
89	11	C ₁₁ H ₁₄	1,1-Dimethylindane	-4.05	-1.9
90	11	C ₁₁ H ₁₄	4,6-Dimethylindane	-0.95	-1.7
91	11	C ₁₁ H ₁₄	4,7-Dimethylindane	-1.2	-1.33
92	11	C ₁₁ H ₁₆	Pentamethylbenzene	-1.17	-4.26
93	11	C ₁₁ H ₂₀	Bicyclo[3.3.3]undecane	-8.82	-3.19
94	11	C ₁₁ H ₂₂	Cycloundecane	-5.56	-2.997
95	11	C ₁₁ H ₂₄	2,2,4,4,5-Pentamethylhexane	-6.25	-6.79

S. No.	Number of non-hydrogen atom	Chemical Formula	Name	Experiment – B3LYP	Experiment – ω B97X-D
96	11	C ₁₁ H ₂₄	2,2,5,5-Tetramethylheptane	-4.81	-5.13
97	11	C ₁₁ H ₂₄	3,3,5,5-Tetramethylheptane	-6.82	-6.41
98	11	C ₁₁ H ₂₄	Undecane	3.65	-3.32
99	11	C ₄ F ₅ H ₃ O ₂	Pentafluoropropanoic acid methyl ester	19.44	8.27
100	11	C ₆ F ₅ H	Pentafluorobenzene	20.56	11.47
101	11	C ₇ F ₄ H ₄	1-Fluoro-3-trifluoromethyl benzene	12.79	4.93
102	11	C ₇ H ₁₆ O ₄	3,5,7,9-Tetraoxaundecane	4.72	-2
103	11	C ₈ H ₁₅ NO ₂	N,N-Diacetylbutylamine	6.51	3.76
104	11	C ₈ H ₄ O ₃	1,3-Isobenzofurandione	2.47	5.41
105	11	C ₈ H ₅ N ₃	Pyridinium dicyanomethylide	10.41	2.35
106	11	C ₈ H ₈ O ₃	2-Methoxybenzoic acid	0.84	1.38
107	11	C ₈ H ₈ O ₃	3-Methoxybenzoic acid	1.94	2.84
108	11	C ₈ H ₈ O ₃	4-Methoxybenzoic acid	2.25	3.15
109	11	C ₉ H ₁₀ O ₂	2-Ethylbenzoic acid	-0.59	0.41
110	11	C ₉ H ₁₀ O ₂	3,4-Dihydro-2H-1,5-benzodioxepin	4.07	4.08
111	11	C ₉ H ₁₀ O ₂	3-Ethylbenzoic acid	0.44	1.43
112	11	C ₉ H ₁₀ O ₂	4-Ethylbenzoic acid	-3.19	-2.21
113	11	C ₉ H ₁₀ O ₂	Acetic acid-3-methylphenyl ester	1.26	-0.2
114	11	C ₉ H ₁₆ O ₂	2-Pentenoic acid butyl ester	4.09	-1.51
115	11	C ₉ H ₁₆ O ₂	3-Pentenoic acid butyl ester	3.06	-1.45
116	11	C ₉ H ₁₆ O ₂	4-Pentenoic acid 2-methylpropyl ester	-0.54	-3.12
117	11	C ₉ H ₁₆ O ₂	4-Pentenoic acid butyl ester	1.5	-2
118	11	C ₉ H ₁₈ O ₂	Nonanoic acid	1.55	0.57

S. No.	Number of non-hydrogen atom	Chemical Formula	Name	Experiment – B3LYP	Experiment – ω B97X-D
119	11	C ₉ H ₁₈ O ₂	Octanoic acid methyl ester	5.26	1.13
120	11	C ₉ H ₁₈ O ₂	Pentanoic acid 1-methylpropyl ester	2.45	-2.04
121	11	C ₉ H ₂₀ O ₂	Dibutoxymethane	6.05	-1.37
122	11	C ₉ H ₇ NO	8-Quinolinol	-1.12	-1.86
123	11	C ₉ H ₇ NO	β -Oxobenzene propanenitrile	-1.73	-2.2
124	12	C ₁₀ H ₂₀ O ₂	Decanoic acid	2.36	1.24
125	12	C ₁₀ H ₂₀ O ₂	Nonanoic acid methyl ester	5.48	1.21
126	12	C ₁₁ H ₁₄ O	3-Methyl-1-phenyl-1-butanone	-1.44	-2.8
127	12	C ₁₁ H ₂₁ N	1-Cyclohexylpiperidine	-1.31	0.66
128	12	C ₁₁ H ₂₂ O	2,2,6,6-Tetramethyl-4-heptanone	-6.75	-5.68
129	12	C ₁₁ H ₂₂ O	6-Undecanone	4.14	-0.89
130	12	C ₁₁ H ₂₄ O	1-Methoxydecane	6.31	-1.02
131	12	C ₁₂ H ₁₀	Acenaphthene	-2.57	-1.45
132	12	C ₁₂ H ₁₀	Biphenyl	-3.04	-2.28
133	12	C ₁₂ H ₁₂	1,8-Dimethylnaphthalene	-1.92	-3.31
134	12	C ₁₂ H ₁₂	2,3-Dimethylnaphthalene	-1.82	-3.82
135	12	C ₁₂ H ₁₂	2,7-Dimethylnaphthalene	-0.3	-2.93
136	12	C ₁₂ H ₁₆	Cyclohexylbenzene	-4.23	-1.93
137	12	C ₁₂ H ₁₈	(E,E,E)-1,5,9-Cyclododecatriene	-7.49	-5.28
138	12	C ₁₂ H ₁₈	(E,E,Z)-1,5,9-Cyclododecatriene	-6.97	-5.5
139	12	C ₁₂ H ₁₈	Hexamethylbenzene	-4.55	-6.93
140	12	C ₁₂ H ₂₂	Bicyclohexyl	-7.13	-3.09
141	12	C ₁₂ H ₂₄	1-Dodecene	3.46	-2.96
142	12	C ₁₂ H ₂₄	Cyclododecane	-5.38	-2.6

S. No.	Number of non-hydrogen atom	Chemical Formula	Name	Experiment – B3LYP	Experiment – ω B97X-D
143	12	C ₁₂ H ₂₆	3,3,6,6-Tetramethyloctane	-6.24	-6.5
144	12	C ₁₂ H ₂₆	Dodecane	2.41	-3.31
145	12	C ₁₂ H ₈	Acenaphthylene	-4.27	-3.92
146	12	C ₁₂ H ₈	Biphenylene	-1.17	-0.92
147	12	C ₄ H ₈ N ₄ O ₄	1,4-Dinitropiperazine	18.51	13.75
148	12	C ₆ F ₅ HO	Pentafluorophenol	19.89	12.87
149	12	C ₆ F ₆	Hexafluorobenzene	25.07	14.44
150	12	C ₆ H ₄ N ₂ O ₄	1,3-Dinitrobenzene	12.28	7.97
151	12	C ₇ F ₅ H ₃	2,3,4,5,6-Pentafluoro-1-methylbenzene	21.59	11.45
152	12	C ₈ H ₁₀ O ₄	3,4-Dioxy-3-cyclobutene-1,2-dione	6.94	4.9
153	12	C ₈ H ₁₄ O ₄	Octanedioic acid	-0.05	5.58
154	12	C ₉ H ₁₁ NO ₂	1-Phenylalanine	-4.45	0.68
155	13	C ₁₀ H ₁₁ NO ₂	N,N-Diacetylaniline	2.71	3.78
156	13	C ₁₁ H ₁₄ O ₂	2-tert-Butylbenzoic acid	-7.05	-3.45
157	13	C ₁₁ H ₁₄ O ₂	3,5-Diethylbenzoic acid	-1.37	-0.82
158	13	C ₁₁ H ₁₄ O ₂	3-tert-Butylbenzoic acid	-4.09	-0.7
159	13	C ₁₁ H ₁₄ O ₂	4-tert Butylbenzoic acid	-3.24	0.07
160	13	C ₁₁ H ₂₂ O ₂	Decanoic acid methyl ester	5.74	1.33
161	13	C ₁₁ H ₂₂ O ₂	Undecanoic acid	2.67	1.41
162	13	C ₁₁ H ₈ O ₂	1-Naphthalenecarboxylic acid	-3.14	-1
163	13	C ₁₁ H ₈ O ₂	2-Naphthalenecarboxylic acid	-2.49	-0.05
164	13	C ₁₂ H ₁₀ O	Diphenylether	0.56	0.3
165	13	C ₁₂ H ₂₄ O	2-Dodecanone	4.16	-0.56
166	13	C ₁₂ H ₂₆ O	1-Dodecanol	2.52	-1.01
167	13	C ₁₂ H ₉ N	9H-Carbazole	1.44	2.41

S. No.	Number of non-hydrogen atom	Chemical Formula	Name	Experiment – B3LYP	Experiment – ω B97X-D
168	13	C ₁₃ H ₁₂	4-Methylbiphenyl	-3.39	-4.15
169	13	C ₁₃ H ₁₈	2,3-Dihydro-1,1,4,6-tetramethyl-1H-indene	-4.73	-3.21
170	13	C ₁₃ H ₁₈	2,3-Dihydro-1,1,4,7-tetramethyl-1H-indene	-5.4	-2.46
171	13	C ₁₃ H ₂₆	Cyclotridecane	-5.96	-1.05
172	13	C ₁₃ H ₂₆	Heptylcyclohexane	-3.54	-5.67
173	13	C ₁₃ H ₂₈	3,5-Dimethyl-3,5-diethylheptane	-10.84	-7.55
174	13	C ₁₃ H ₂₈	4,4,6,6-Tetramethylnonane	-5.79	-4.57
175	13	C ₆ F ₆ H ₈ O	Bis(3,3,3-trifluoropropyl)ether	21.07	9.44
176	13	C ₇ F ₄ H ₁₄ N ₂	N,N,N',N'-Tetrafluoro-1,1-heptanediamine	25.2	8
177	13	C ₇ H ₆ N ₂ O ₄	Dinitromethyl benzene	6.89	2.85
178	13	C ₈ H ₁₈ O ₅	3,5,7,9,11-Pentaoxatridecane	5.38	-1.23
179	14	C ₁₂ H ₁₀ N ₂	Cis-Azobenzene	4.42	0.97
180	14	C ₁₂ H ₁₀ N ₂	Trans-Azobenzene	5.6	-0.61
181	14	C ₁₂ H ₂₄ O ₂	Dodecanoic acid	1.15	-0.26
182	14	C ₁₂ H ₂₄ O ₂	Undecanoic acid methyl ester	5.98	1.43
183	14	C ₁₂ H ₈ N ₂	Benzo-c-cinnoline	4.4	0.79
184	14	C ₁₄ H ₁₀	Anthracene	-1.95	-2.89
185	14	C ₁₄ H ₁₀	Phenanthrene	-2.64	-2.01
186	14	C ₁₄ H ₁₂	9,10-Dihydroanthracene	-5.94	-2.11
187	14	C ₁₄ H ₁₂	Cis-Stilbene	-3.36	-3.33
188	14	C ₁₄ H ₁₂	Trans-Stilbene	-2.21	-4.62
189	14	C ₁₄ H ₁₄	1,2-Diphenylethane	-2.24	-1.47
190	14	C ₁₄ H ₁₆	1,4,5,8-Tetramethyl naphthalene	-3.19	-4.64
191	14	C ₁₄ H ₁₈	1,2,3,4,5,6,7,8-Octahydro-anthracene	-6.49	-2.81

Table S4. G4 energies for selected aromatic hydrocarbons and non-hydrocarbons molecules in the PDS(10-14) test set. The values shown in the table are in kcal/mol.

S. No.	Chemical Formula	Type	Number of non- hydrogen atom	Name	G4 Deviation	G4MP2 Deviation
1	C ₁₀ H ₁₂	Hydrocarbons	10	1,2,3,4-Tetrahydronaphthalene	1.04	2.18
2	C ₁₀ H ₁₄	Hydrocarbons	10	1,2,3,4-Tetramethylbenzene	0.43	1.41
3	C ₁₀ H ₁₄	Hydrocarbons	10	1,2,3,5-Tetramethylbenzene	0.60	1.47
4	C ₁₀ H ₁₄	Hydrocarbons	10	1,2,4,6-Tetramethylbenzene	0.69	1.53
5	C ₈ H ₄ N ₂	Non- hydrocarbons	10	1,2-Benzene-dicarbonitrile	1.70	1.84
6	C ₈ H ₁₀ O ₂	Non- hydrocarbons	10	1,2-Dimethoxybenzene	-2.42	-2.60
7	C ₈ H ₄ N ₂	Non- hydrocarbons	10	1,3-Benzene-dicarbonitrile	2.01	2.09
8	C ₈ H ₄ N ₂	Non- hydrocarbons	10	1,4-Benzene-dicarbonitrile	0.93	1.02
9	C ₇ H ₇ NO ₂	Non- hydrocarbons	10	1-Methyl-4-nitrobenzene	2.49	1.95
10	C ₉ H ₁₀ O	Non- hydrocarbons	10	1-Phenyl 1-propanone	1.39	2.14
11	C ₇ H ₇ NO ₂	Non- hydrocarbons	10	2-Aminobenzoic acid	2.62	2.45
12	C ₇ H ₆ O ₃	Non- hydrocarbons	10	2-Hydroxybenzoic acid	0.32	0.10
13	C ₆ H ₆ N ₂ O ₂	Non- hydrocarbons	10	2-Nitroaniline	2.91	1.92
14	C ₇ H ₇ NO ₂	Non- hydrocarbons	10	4-Aminobenzoic acid	0.77	0.53
15	C ₆ H ₆ N ₂ O ₂	Non- hydrocarbons	10	4-Nitroaniline	1.56	0.46
16	C ₈ H ₈ O ₂	Non- hydrocarbons	10	Acetic acid phenyl ester	-0.27	-0.20
17	C ₈ H ₅ NO	Non- hydrocarbons	10	α-Oxobenzene acetonitrile	1.09	1.54
18	C ₁₀ H ₁₄	Hydrocarbons	10	Butylbenzene	0.66	1.76
19	C ₁₁ H ₁₄	Hydrocarbons	11	1,1-Dimethylindane	2.08	3.07
20	C ₈ H ₄ O ₃	Non- hydrocarbons	11	1,3-Isobenzofurandione	1.91	1.76

S. No.	Chemical Formula	Type	Number of non-hydrogen atom	Name	G4 Deviation	G4MP2 Deviation
21	C ₁₀ H ₈ O	Non-hydrocarbons	11	1-Naphthol	-0.75	0.69
22	C ₁₀ H ₁₂ O	Non-hydrocarbons	11	1-Phenyl 1-butanone	-0.24	0.53
23	C ₇ F ₄ H ₄	Non-hydrocarbons	11	1-Fluoro-3-trifluoromethyl-benzene	-0.15	-0.01
24	C ₁₁ H ₁₀	Hydrocarbons	11	1-Methylnaphthalene	1.32	3.13
25	C ₉ H ₁₀ O ₂	Non-hydrocarbons	11	2-Ethylbenzoic acid	0.95	1.30
26	C ₈ H ₈ O ₃	Non-hydrocarbons	11	2-Methoxybenzoic acid	-0.26	-0.58
27	C ₉ H ₁₀ O ₂	Non-hydrocarbons	11	Acetic acid 3-methylphenyl ester	-0.99	-1.01
28	C ₉ H ₇ NO	Non-hydrocarbons	11	β -Oxobenzene propanenitrile	-0.38	0.14
29	C ₆ H ₄ N ₂ O ₄	Non-hydrocarbons	12	1,3-Dinitrobenzene	2.67	0.76
30	C ₁₂ H ₁₂	Hydrocarbons	12	1,8-Dimethyl naphthalene	1.15	2.98
31	C ₉ H ₁₁ NO ₂	Non-hydrocarbons	12	1-Phenylalanine	0.02	0.25
32	C ₇ F ₅ H ₃	Non-hydrocarbons	12	2,3,4,5,6-Pentafluoro-1-methylbenzene	-0.09	-0.65
33	C ₁₂ H ₁₂	Hydrocarbons	12	2,3-Dimethyl naphthalene	0.08	1.74
34	C ₁₂ H ₁₂	Hydrocarbons	12	2,7-Dimethyl naphthalene	0.96	2.57
35	C ₁₂ H ₁₀	Hydrocarbons	12	Acenaphthene	1.34	3.07
36	C ₁₂ H ₈	Hydrocarbons	12	Acenaphthylene	1.18	3.32
37	C ₁₂ H ₁₀	Hydrocarbons	12	Biphenyl	0.54	2.50
38	C ₁₂ H ₈	Hydrocarbons	12	Biphenylene	1.38	3.56
39	C ₆ F ₆	Non-hydrocarbons	12	Hexafluoro benzene	-0.56	-1.12
40	C ₁₂ H ₁₈	Hydrocarbons	12	Hexamethyl benzene	-1.77	-0.72
41	C ₁₁ H ₈ O ₂	Non-hydrocarbons	13	1-Naphthalene carboxylic acid	0.02	1.24
42	C ₁₃ H ₁₈	Hydrocarbons	13	2,3-Dihydro-1,1,4,6-tetramethyl-1H-indene	1.90	2.60

S. No.	Chemical Formula	Type	Number of non-hydrogen atom	Name	G4 Deviation	G4MP2 Deviation
43	C ₁₃ H ₁₈	Hydrocarbons	13	2,3-Dihydro-1,1,4,7-tetramethyl-1H-indene	2.48	3.32
44	C ₁₁ H ₈ O ₂	Non-hydrocarbons	13	2-Naphthalene carboxylic acid	0.68	1.78
45	C ₁₁ H ₁₄ O ₂	Non-hydrocarbons	13	2-tert-Butylbenzoic acid	-0.03	0.37
46	C ₇ H ₆ N ₂ O ₄	Non-hydrocarbons	13	Dinitromethyl benzene	-0.56	-3.05
47	C ₁₂ H ₁₀ O	Non-hydrocarbons	13	Diphenylether	0.36	1.85
48	C ₁₀ H ₁₁ NO ₂	Non-hydrocarbons	13	N,N-Diacetylaniline	1.22	0.71
49	C ₁₄ H ₁₈	Hydrocarbons	14	1,2,3,4,5,6,7,8-Octahydro-anthracene	0.38	1.43
50	C ₁₄ H ₁₄	Hydrocarbons	14	1,2-Diphenylethane	1.66	3.92
51	C ₁₄ H ₁₆	Hydrocarbons	14	1,4,5,8-Tetramethyl-naphthalene	1.69	3.54
52	C ₁₄ H ₁₀	Hydrocarbons	14	Anthracene	2.24	4.84
53	C ₁₂ H ₈ N ₂	Non-hydrocarbons	14	Benzo-c-cinnoline	1.78	3.31
54	C ₁₄ H ₁₀	Hydrocarbons	14	Phenanthrene	2.17	4.71