Electronic Supplementary Material

High-precision standard enthalpy of formation for polycyclic aromatic hydrocarbons predicting from general connectivity based hierarchy with discrete correction of atomization energy

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Table S1 The experimental values of the standard enthalpy of formation for 30 reference species

No.	Species	Smiles	Chemical Name	Expt. /(kcal · mol^{-1})
1	CH_4	C	Methane	-17.89[1]
2	C_2H_4	C=C	Ethylene	12.54[2]
3	C_2H_6	CC	Ethane	-20.08[2]
4	C_3H_6	CC=C	Propene	4.88[3]
5	C_3H_8	CCC	Propane	-25.02[4]
6	C_4H_6	C=CC=C	1,3-Butadiene	26.00[5]
7	C_4H_8	CC(=C)C	1-Propene, 2-methyl-	-4.28[5]
8	C_4H_8	C/C=C/C	2-Butene, (E)-	-2.58[5]
9	C_4H_8	CCC=C	1-Butene	-0.15[5]
10	C_4H_{10}	CC(C)C	Isobutane	-32.40[5]
11	C_4H_{10}	CCCC	Butane	-30.34[5]
12	C_5H_8	CC(=C)C=C	Isoprene	18.09[6]
13	C_5H_8	C/C=C/C=C	1,3-Pentadiene, (E)-	18.11[6]
14	C_5H_8	C=CCC=C	1,4-Pentadiene	25.41[6]
15	C_5H_{10}	CC=C(C)C	2-Butene, 2-methyl-	-9.92[7]
16	C_5H_{10}	CCCC=C	1-Pentene	-5.19[8]
17	C_5H_{10}	CC/C=C/C	2-Pentene, (E)-	-7.67[9]
18	C_5H_{10}	CCC(=C)C	2-Methyl-1-butene	-8.39[7]
19	C_5H_{10}	CC(C)C=C	1-Butene, 3-methyl-	-6.09[10]
20	C_5H_{12}	CCC(C)C	Butane, 2-methyl-	-36.74[12]

21	C_5H_{12}	CC(C)(C)C	Neopentane	-40.13[12]
22	C_6H_6	C1=CC=CC=C1	Benzene	19.81[13]
23	C_6H_{12}	C1CCCCC1	Cyclohexane	-29.78[14]
24	C_6H_{12}	CC(=C(C)C)C	2-Butene, 2,3-dimethyl-	-16.73[17]
25	$C_{10}H_8$	C1=CC=C2C=CC=CC2=C1	Naphthalene	35.85[14]
26	$C_{14}H_{10}$	C1=CC=C2C=C3C=CC=CC3=CC2=C1	Anthracene	54.83[14]
27	$C_{14}H_{10}$	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	Phenanthrene	48.09[15]
28	$C_{16}H_{10}$	C1=CC=C2C(=C1)C3=CC=CC4=C3C2=CC=C4	Fluoranthene	69.65[14]
29	$C_{20}H_{12}$	C1=CC2=C3C(=C1)C4=CC=CC5=C4C(=CC=C5)C3=CC=C2	Perylene	76.08[14]
30	$C_{24}H_{12}$	C1=CC2=C3C4=C1C=CC5=C4C6=C(C=C5)C=CC7=C6C3=C(C=C2)C=C7	Coronene	70.51[14]

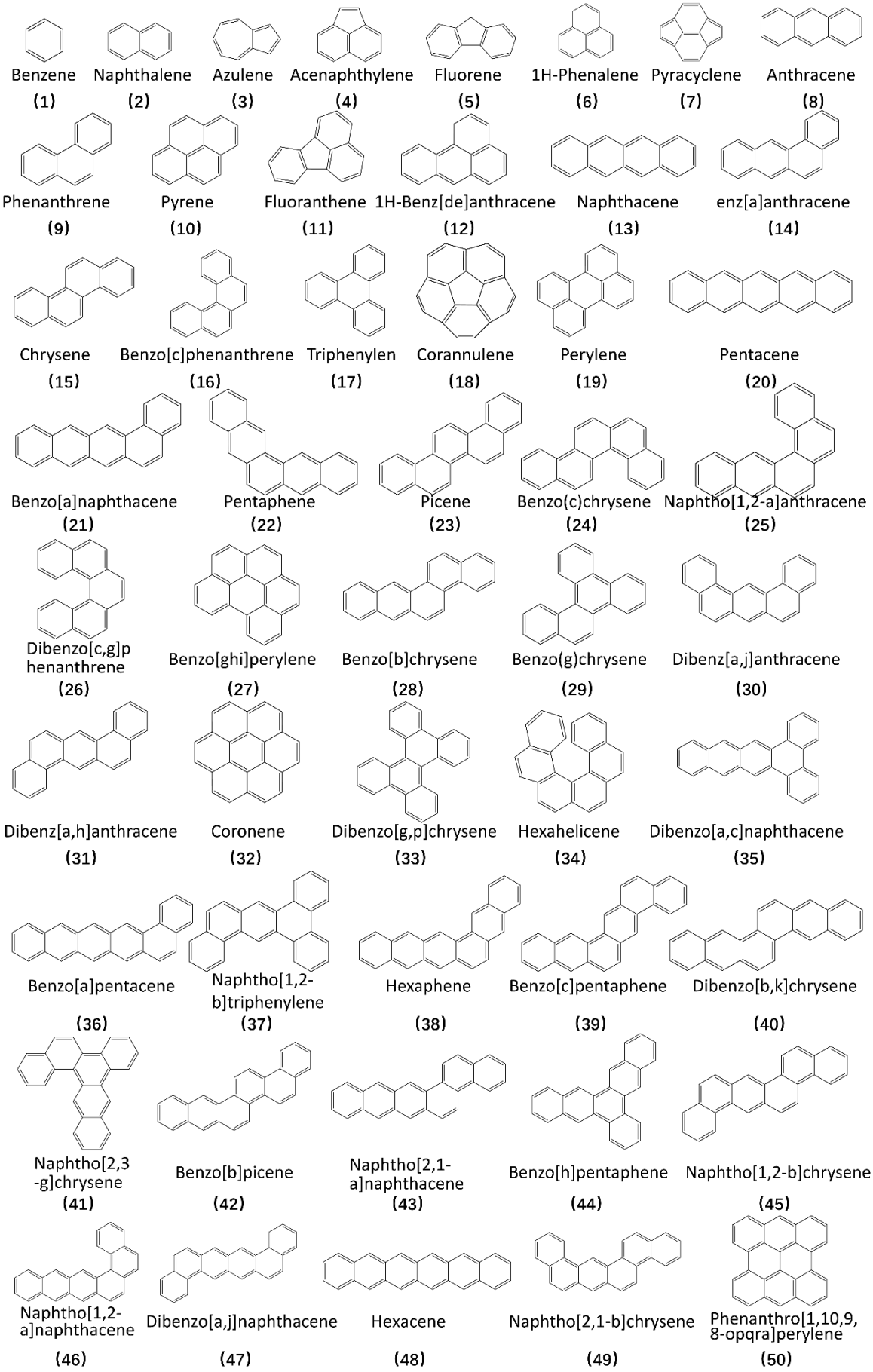
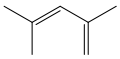


Figure S1 Chemical structures for 50 aromatic molecules.

TABLE S2 Details of fragments in CBH-4 scheme at CCSD(T) and M06-2X

Production				Reactant			
Structure	Molecule	Energy/a.u.		Structure	Molecule	Energy/a.u.	
		CCSD(T)	M06-2X			CCSD(T)	M06-2X
	C_5H_8	-195.2529	-195.0339		C_4H_8	-157.1771	-157.0074
	C_6H_{10}	-234.5603	-234.2991		C_4H_6	-155.9464	-155.7708
	C_6H_{10}	-234.5615	-234.2997		C_5H_{10}	-196.4852	-196.2727
	C_6H_{10}	-234.5573	-234.2955		C_5H_8	-195.2596	-195.0411
	C_7H_{12}	-273.8699	-273.565		C_6H_{12}	-235.7883	-235.5335
	C_8H_{12}	-311.9476	-311.5946		C_6H_{10}	-234.5666	-234.3054
	C_8H_{14}	-313.1678	-312.8209		C_4H_8	-157.1749	-157.005
	C_8H_{12}	-311.9424	-311.5898		C_5H_{10}	-196.4808	-196.2679
	C_9H_{14}	-351.2544	-350.8589				
	C_9H_{14}	-351.2524	-350.8571				
	$C_{10}H_{16}$	-390.5577	-390.1191				

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