Pairing double hybrid functionals with a tailored basis set for an accurate thermochemistry of hydrocarbons

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SUPPLEMENTARY INFORMATION

Table S1. Optimized exponents of the DH-SVPD basis set. These exponents replace the corresponding exponents of the original Def2-SVPD basis set, which are also reported for comparison. All other exponents are kept as in the original basis set.

atom	function	def2-SVPD	DH-SVPD	function	def2-SVPD	DH-SVPD
H	s	0.12194962000	0.4617867850	p	0.11704099050	0.07913402419
C	p	0.15268613795	0.1508036550	d	0.11713185140	0.3229294790

Table S2. Example input for Gaussian code, reporting the optimized DH-SVPD basis set for C and H atoms

#P PBEQIDH/gen Oktane 0 1 C -0.1614620000 4.4569880000 0.0000000000 C -0.8313160000 3.0940090000 0.0000000000 C 0.1614620000 1.9436090000 0.0000000000 C -0.4965940000 0.5746890000 0.0000000000 C 0.4965940000 -0.5746890000 0.0000000000 C -0.1614620000 -1.9436090000 0.0000000000 C 0.8313160000 -3.0940090000 0.0000000000 C 0.1614620000 -4.4569880000 0.0000000000 H -0.8934560000 5.2668790000 0.0000000000 H 0.4730940000 4.5827170000 0.8810000000 H 0.4730940000 4.5827170000 -0.8810000000 H -1.4849260000 3.0045060000 -0.8745100000 H -1.4849260000 3.0045060000 0.8745100000 H 0.8165870000 2.0315690000 -0.8750300000 H 0.8165870000 2.0315690000 0.8750300000 H -1.1515520000 0.4875230000 -0.8750580000 H -1.1515520000 0.4875230000 0.8750580000 H 1.1515520000 -0.4875230000 -0.8750580000 H 1.1515520000 -0.4875230000 0.8750580000 H -0.8165870000 -2.0315690000 -0.8750300000 H -0.8165870000 -2.0315690000 0.8750300000 H 1.4849260000 -3.0045060000 -0.8745100000 H 1.4849260000 -3.0045060000 0.8745100000 H -0.4730940000 -4.5827170000 -0.8810000000 H 0.8934560000 -5.2668790000 0.0000000000 H -0.4730940000 -4.5827170000 0.8810000000	
-H 0 s 3 1.00 13.010701000 0.19682158000e-01 1.9622572000 0.13796524000 0.44453796000 0.47831935000 p 1 1.00 0.80000000000 1.0000000	Standard def2-SVPD exponents and coefficients for H atom
s 1 1.00 0.4617867850E+00 0.1000000000E+01 p 1 1.00 0.7913402419E-01 0.1000000000E+01 ****	DH-SVPD optimized exponents for H atom
-C 0 s 5 1.00 1238.4016938 0.54568832082e-02 186.29004992 0.40638409211e-01 42.251176346 0.18025593888 11.676557932 0.46315121755 3.5930506482 0.44087173314 s 1 1.00 0.40245147363 1.0000000 s 1 1.00 0.13090182668 1.0000000 s 1 1.00 0.67053540256e-01 1.0000000 p 3 1.00 9.4680970621 0.38387871728e-01 2.0103545142 0.21117025112 0.54771004707 0.51328172114 d 1 1.00 0.80000000000 1.0000000	Standard def2-SVPD exponents and coefficients for C atom
p 1 1.00 0.1508036550E+00 0.1000000000E+01 d 1 1.00 0.3229294790E+00 0.1000000000E+01	DH-SVPD optimized exponents for C atom

Table S3. The binding energies(ΔE, kcal/mol) and errors (Er, kcal/mol) of the dimers in the AAA groups

Functional	PBEQIDH		PBEQIDHD3(0)		PBEQIDHD3(BJ)		PBE0DH		PBE0DHD3(BJ)		B2PLYP		B2PLYPD3(0)		DSDPBEP86		revDSDPBEP86D3(BJ)	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
Butane	-3.07	-0.26	-4.40	-1.58	-3.66	-0.84	-2.21	0.61	-4.80	-1.98	-2.42	0.40	-4.81	-1.99	-3.13	-0.31	-4.80	-1.98
Butene.	-2.32	0.00	-3.35	-1.02	-3.10	-0.78	-1.64	0.69	-3.64	-1.32	-1.67	0.66	-3.61	-1.29	-2.60	-0.28	-3.64	-1.32
Butyne.	-3.32	0.11	-4.34	-0.92	-4.13	-0.71	-2.62	0.81	-4.56	-1.14	-2.60	0.83	-4.41	-0.99	-2.70	0.72	-4.56	-1.14
Ethane	-1.47	-0.09	-2.09	-0.70	-1.85	-0.46	-1.13	0.26	-2.29	-0.90	-1.10	0.28	-2.26	-0.87	-1.34	0.05	-2.29	-0.90
Ethene	-1.22	0.26	-1.71	-0.24	-1.53	-0.05	-0.97	0.51	-1.83	-0.35	-0.83	0.65	-1.83	-0.35	-1.00	0.47	-1.83	-0.35
Ethyne.	-1.68	-0.15	-1.88	-0.36	-1.85	-0.33	-1.56	-0.04	-1.95	-0.42	-1.44	0.09	-1.92	-0.39	-0.55	0.97	-1.95	-0.42
Hexane.	-4.84	-0.33	-6.94	-2.43	-6.39	-1.89	-3.37	1.13	-7.58	-3.07	-3.85	0.66	-7.69	-3.18	-5.12	-0.61	-7.58	-3.07
Methane	-0.59	-0.06	-0.79	-0.26	-0.71	-0.18	-0.50	0.03	-0.87	-0.34	-0.47	0.06	-0.82	-0.29	-0.42	0.11	-0.87	-0.34
Pentane	-3.96	-0.30	-5.66	-2.00	-5.19	-1.53	-2.82	0.84	-6.20	-2.54	-3.19	0.47	-6.27	-2.61	-4.06	-0.40	-6.20	-2.54
Pentene.	-3.37	-0.20	-4.74	-1.57	-4.46	-1.29	-2.36	0.81	-5.09	-1.92	-2.54	0.63	-5.02	-1.85	-3.66	-0.49	-5.09	-1.92
Pentyne	-4.25	0.20	-5.62	-1.17	-5.35	-0.90	-3.21	1.24	-5.91	-1.46	-3.18	1.27	-5.81	-1.36	-3.82	0.63	-5.91	-1.46
Propane	-2.19	-0.18	-3.10	-1.09	-2.80	-0.79	-1.64	0.37	-3.41	-1.40	-1.76	0.25	-3.39	-1.39	-2.10	-0.09	-3.41	-1.40
Propene.	-2.39	-0.18	-3.24	-1.02	-2.98	-0.77	-1.82	0.40	-3.36	-1.15	-1.71	0.50	-3.22	-1.01	-2.07	0.14	-3.36	-1.15
Propyne	-2.60	-0.26	-3.11	-0.76	-3.03	-0.69	-2.30	0.05	-3.23	-0.89	-2.16	0.18	-3.25	-0.91	-1.44	0.91	-3.23	-0.89
MAD	0.18		1.08		0.80		0.56		1.11		0.49		1.32		0.44		1.35	

Functional	M06L		TPSSh		B3LYP		PBE0		M06		CAM-B3LYP		wB97XD		B3LYP-D3	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
Butane	-4.86	-2.04	-1.22	1.60	-1.26	1.56	-1.75	1.07	-4.91	-2.09	-1.82	0.99	-5.79	-2.97	-5.19	-2.37
Butene.	-3.24	-0.92	-0.80	1.52	-0.68	1.64	-1.25	1.08	-3.42	-1.10	-1.17	1.15	-4.13	-1.81	-3.87	-1.55
Butyne.	-4.13	-0.70	-1.66	1.76	-1.46	1.96	-2.26	1.16	-4.60	-1.17	-2.12	1.31	-5.05	-1.63	-4.63	-1.21
Ethane	-2.03	-0.64	-0.73	0.66	-0.61	0.78	-0.92	0.47	-1.92	-0.53	-0.93	0.45	-2.63	-1.24	-2.45	-1.06
Ethene	-1.44	0.04	-0.51	0.96	-0.45	1.03	-0.82	0.65	-1.55	-0.07	-0.74	0.74	-2.04	-0.56	-2.04	-0.56
Ethyne.	-1.19	0.34	-1.22	0.31	-1.13	0.40	-1.52	0.01	-1.44	0.09	-1.44	0.08	-1.88	-0.35	-2.03	-0.50
Hexane.	-7.95	-3.44	-1.73	2.77	-1.48	3.02	-2.56	1.95	-8.09	-3.58	-2.71	1.79	-9.25	-4.74	-8.23	-3.72
Methane	-0.61	-0.08	-0.35	0.18	-0.38	0.15	-0.47	0.06	-0.52	0.01	-0.44	0.09	-0.88	-0.35	-0.88	-0.35
Pentane	-6.31	-2.65	-1.50	2.17	-1.28	2.38	-2.20	1.46	-6.46	-2.80	-2.32	1.34	-7.50	-3.84	-6.75	-3.09
Pentene.	-4.69	-1.52	-1.24	1.93	-1.00	2.17	-1.81	1.36	-4.93	-1.76	-1.79	1.38	-5.72	-2.55	-5.29	-2.12
Pentyne	-5.52	-1.07	-1.81	2.64	-1.55	2.90	-2.59	1.86	-5.87	-1.42	-2.40	2.05	-6.54	-2.09	-5.97	-1.52
Propane	-3.38	-1.37	-0.94	1.07	-0.96	1.05	-1.35	0.66	-3.31	-1.30	-1.39	0.62	-4.02	-2.01	-3.71	-1.70
Propene.	-2.94	-0.73	-0.93	1.28	-0.71	1.50	-1.46	0.76	-3.06	-0.85	-1.35	0.87	-3.72	-1.51	-3.39	-1.18
Propyne	-2.54	-0.20	-1.60	0.74	-1.46	0.88	-2.15	0.20	-2.80	-0.46	-1.98	0.36	-3.41	-1.06	-3.46	-1.11
MAD	1.12		1.40		1.53		0.91		1.23		0.95		1.91		1.57	

Table S4. The binding energies(ΔE, kcal/mol) and errors (Er, kcal/mol) of the dimers in the AAA groups obtained with the cc-pVTZ basis set.

Functional	PBEQIDH		PBEQIDHD3(0)		PBEQIDHD3(BJ)		PBE0DH		PBE0DHD3(BJ)		B2PLYP		B2PLYPD3(0)		DSDPBEP86		revDSDPBEP86	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
Butane	-1.28	1.54	-2.56	0.26	-2.18	0.64	-0.70	2.12	-2.73	0.09	-0.55	2.27	-2.78	0.04	-2.98	-0.16	-2.61	0.21
Butene.	-1.34	0.99	-2.28	0.04	-2.03	0.30	-0.90	1.43	-2.47	-0.15	-0.74	1.58	-2.45	-0.13	-2.65	-0.33	-2.33	0.00
Butyne.	-2.33	1.09	-3.32	0.10	-3.12	0.31	-1.78	1.64	-3.62	-0.19	-1.59	1.84	-3.41	0.02	-3.76	-0.33	-3.40	0.02
Ethane	-0.57	0.82	-1.17	0.22	-0.93	0.46	-0.35	1.04	-1.26	0.13	-0.20	1.19	-1.25	0.14	-1.37	0.02	-1.21	0.18
Ethene	-0.97	0.51	-1.47	0.01	-1.29	0.19	-0.74	0.74	-1.61	-0.14	-0.58	0.90	-1.62	-0.14	-1.71	-0.23	-1.54	-0.07
Ethyne.	-1.41	0.12	-1.61	-0.09	-1.59	-0.06	-1.33	0.20	-1.79	-0.27	-1.15	0.37	-1.65	-0.12	-1.73	-0.21	-1.64	-0.11
Hexane.	-2.11	2.40	-4.16	0.35	-3.63	0.88	-1.11	3.39	-4.42	0.09	-0.96	3.55	-4.60	-0.09	-4.82	-0.32	-4.22	0.28
Methane	-0.20	0.33	-0.38	0.15	-0.30	0.23	-0.15	0.38	2.77	3.30	-0.05	0.48	-0.37	0.16	-0.54	-0.01	-0.38	0.15
Pentane	-1.67	1.99	-3.34	0.32	-2.87	0.79	-0.90	2.76	-3.55	0.11	-0.74	2.92	-3.68	-0.01	-3.88	-0.22	-3.40	0.26
Pentene.	-1.81	1.36	-3.09	0.08	-2.83	0.34	-1.17	2.00	-3.33	-0.16	-1.02	2.15	-3.23	-0.06	-3.56	-0.39	-3.15	0.02
Pentyne	-2.90	1.55	-4.25	0.20	-3.98	0.47	-2.11	2.34	-4.59	-0.14	-1.90	2.55	-4.47	-0.02	-4.85	-0.40	-4.37	0.08
Propane	-0.84	1.16	-1.75	0.25	-1.46	0.55	-0.48	1.52	-1.89	0.12	-0.34	1.67	-1.89	0.11	-2.06	-0.05	-1.80	0.20
Propene.	-1.45	0.77	-2.27	-0.06	-2.02	0.19	-1.05	1.16	-2.43	-0.21	-0.84	1.37	-2.25	-0.04	-2.53	-0.31	-2.27	-0.06
Propyne	-1.93	0.41	-2.44	-0.10	-2.36	-0.01	-1.70	0.65	-2.72	-0.38	-1.45	0.90	-2.53	-0.19	-2.65	-0.31	-2.44	-0.10
MAD		1.07		0.16		0.39		1.53		0.39		1.69		0.09		0.23		0.13

Functional	M06L		TPSSh		B3LYP		PBE0		M06		CAM-B3LYP		wB97XD		B3LYP-D3	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
Butane	-3.19	-0.37	-0.23	2.59	0.00	2.82	-0.42	2.40	-3.42	-0.60	-0.19	2.63	-4.15	-1.33	-3.37	-0.55
Butene.	-2.46	-0.14	-0.48	1.84	-0.18	2.15	-0.76	1.56	-2.66	-0.34	-0.48	1.84	-3.19	-0.86	-2.82	-0.50
Butyne.	-3.36	0.07	-1.05	2.38	-0.76	2.66	-1.50	1.92	-3.45	-0.03	-1.23	2.19	-4.13	-0.70	-3.81	-0.38
Ethane	-1.16	0.23	-0.15	1.24	0.00	1.39	-0.25	1.13	-1.08	0.31	-0.16	1.22	-1.15	0.24	-1.04	0.35
Ethene	-1.26	0.22	-0.35	1.12	-0.07	1.40	-0.62	0.86	-1.32	0.16	-0.51	0.97	-1.82	-0.35	-1.81	-0.34
Ethyne.	-1.07	0.45	-1.03	0.50	-0.88	0.65	-1.30	0.22	-1.12	0.40	-1.14	0.39	-1.57	-0.05	-1.79	-0.26
Hexane.	-5.39	-0.89	-0.29	4.22	0.00	4.50	-0.60	3.90	-5.88	-1.38	0.00	4.50	-5.79	-1.28	-5.47	-0.97
Methane	-0.41	0.12	-0.10	0.43	0.00	0.53	-0.15	0.38	-0.15	0.38	0.00	0.53	-0.57	-0.04	-0.57	-0.04
Pentane	-4.40	-0.74	-0.26	3.41	-0.01	3.66	-0.52	3.14	-4.57	-0.91	0.00	3.66	-4.46	-0.80	-4.42	-0.76
Pentene.	-3.45	-0.28	-0.49	2.68	-0.15	3.02	-0.84	2.33	-3.67	-0.50	-0.51	2.66	-4.39	-1.22	-3.87	-0.70
Pentyne	-4.51	-0.06	-1.12	3.33	-0.50	3.95	-1.68	2.77	-4.58	-0.13	-1.11	3.34	-4.98	-0.53	-4.39	0.06
Propane	-2.16	-0.15	-0.16	1.85	0.00	2.01	-0.31	1.70	-2.19	-0.18	0.00	2.01	-2.78	-0.77	-2.23	-0.23
Propene.	-2.18	0.03	-0.49	1.72	-0.18	2.03	-0.83	1.38	-2.22	-0.01	-0.60	1.62	-2.88	-0.66	-2.58	-0.37
Propyne	-1.82	0.53	-1.11	1.24	-0.87	1.48	-1.59	0.75	-1.92	0.43	-1.33	1.02	-2.76	-0.41	-2.82	-0.47
MAD		0.30		2.04		2.30		1.75		0.41		2.04		0.66		0.43

Table S5. The binding energies(ΔE, kcal/mol) and errors (Er, kcal/mol) of the dimers in the ADIM6 datasets obtained with the DH-SVPD basis set.

	Functional	PBEQIDH		PBE-QIDH-D3(0)		PBE-QIDH-D3(BJ)		PBE0DH		PBE0DH-D3(BJ)		B2PLYP		B2PLYP-D3(0)		DSDPBEP86		revDSDPBEP86D3(BJ)	
		ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
AM2.	AD2.	1.47	0.13	2.05	0.71	1.83	0.49	1.12	-0.22	2.05	0.71	1.10	-0.24	2.12	0.78	1.00	1.00	2.22	0.88
AM3.	AD3.	2.11	0.12	2.98	0.99	2.72	0.73	1.51	-0.48	2.97	0.98	1.58	-0.41	3.19	1.20	1.45	1.45	3.24	1.25
AM4.	AD4.	3.05	0.16	4.35	1.46	3.97	1.08	2.13	-0.76	4.29	1.40	2.33	-0.56	4.65	1.76	2.12	2.12	4.72	1.83
AM5.	AD5.	3.96	0.18	5.64	1.86	5.18	1.40	2.72	-1.06	5.54	1.76	3.05	-0.73	6.12	2.34	2.74	2.74	6.13	2.35
AM6.	AD6.	4.77	0.17	6.87	2.27	6.32	1.72	3.21	-1.39	6.75	2.15	3.64	-0.96	7.47	2.87	3.35	3.35	7.46	2.86
AM7.	AD7.	5.69	0.14	8.12	2.57	7.55	2.00	3.73	-1.82	7.97	2.42	4.24	-1.31	8.95	3.40	3.87	3.87	8.82	3.27
	MAD		0.15		1.64		1.24		0.95		1.57		0.70		2.06		2.42		2.07

Functional		M06L		TPSSh		B3LYP		PBE0		M06		CAM-B3LYP		wB97XD		B3LYP-D3	
		ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
AM2.	AD2.	1.91	0.57	0.34	-1.00	0.25	-1.09	0.89	-0.45	1.68	0.34	0.93	-0.41	2.36	1.02	0.97	0.97
AM3.	AD3.	3.12	1.13	0.30	-1.69	0.26	-1.73	1.09	-0.90	2.99	1.00	1.18	-0.81	3.58	1.59	1.46	1.46
AM4.	AD4.	4.54	1.65	0.36	-2.53	0.41	-2.48	1.50	-1.39	4.39	1.50	1.67	-1.22	5.29	2.40	2.16	2.16
AM5.	AD5.	5.91	2.13	0.37	-3.41	0.52	-3.26	1.86	-1.92	5.87	2.09	2.14	-1.64	6.91	3.13	2.83	2.83
AM6.	AD6.	7.38	2.78	0.30	-4.30	0.50	-4.10	2.11	-2.49	7.32	2.72	2.45	-2.15	8.57	3.97	3.46	3.46
AM7.	AD7.	8.98	3.43	0.10	-5.45	0.35	-5.20	2.29	-3.26	9.05	3.50	2.73	-2.82	10.26	4.71	3.96	3.96
MAD			1.95		3.07		2.98		1.74		1.86		1.51		2.80		2.47

Table S6. The binding energies(ΔE, kcal/mol) and errors (Er, kcal/mol) of the dimers in the ADIM6 datasets obtained with the Def2-QZVP basis set.

	Functional	PBEQIDH		PBE-QIDH-D3(0)		PBE-QIDH-D3(BJ)		PBE0DH		PBE0DH-D3(BJ)		B2PLYP		B2PLYP-D3(0)		DSDPBEP86		revDSDPBEP86D3(BJ)	
		ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
AM2.	AD2.	0.60	-0.74	1.19	-0.15	0.96	-0.38	0.31	-1.03	1.24	-0.10	0.16	-1.18	1.19	-0.15	0.02	0.02	1.21	-0.13
AM3.	AD3.	0.88	-1.11	1.75	-0.24	1.49	-0.50	0.39	-1.60	1.85	-0.14	0.26	-1.73	1.87	-0.12	0.04	0.04	1.79	-0.20
AM4.	AD4.	1.27	-1.62	2.57	-0.32	2.19	-0.70	0.52	-2.37	2.68	-0.21	0.38	-2.51	2.70	-0.19	0.07	0.07	2.61	-0.28
AM5.	AD5.	1.68	-2.10	3.36	-0.42	2.90	-0.88	0.68	-3.10	3.50	-0.28	0.53	-3.25	3.61	-0.17	0.09	0.09	3.41	-0.37
AM6.	AD6.	2.04	-2.56	4.14	-0.46	3.59	-1.01	0.77	-3.83	4.31	-0.29	0.63	-3.97	4.45	-0.15	0.17	0.17	4.20	-0.40
AM7.	AD7.	2.52	-3.03	4.95	-0.60	4.39	-1.16	0.94	-4.61	5.18	-0.37	0.76	-4.79	5.48	-0.07	0.17	0.17	5.02	-0.53
	MAD		1.86		0.37		0.77		2.76		0.23		2.90		0.14		0.09		0.32

Functional		M06L		TPSSh		B3LYP		PBE0		M06		CAM-B3LYP		wB97XD		B3LYP-D3	
		ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
AM2.	AD2.	1.24	-0.10	-0.38	-1.72	-0.63	-1.97	0.12	-1.22	0.97	-0.37	0.03	-1.31	1.57	0.23	0.09	0.09
AM3.	AD3.	2.03	0.04	-0.67	-2.66	-0.96	-2.95	0.04	-1.95	1.92	-0.07	-0.07	-2.06	2.48	0.49	0.25	0.25
AM4.	AD4.	3.03	0.14	-1.05	-3.94	-1.39	-4.28	-0.03	-2.92	2.87	-0.02	-0.15	-3.04	3.70	0.81	0.36	0.36
AM5.	AD5.	3.93	0.15	-1.42	-5.20	-1.79	-5.57	-0.07	-3.85	3.90	0.12	-0.20	-3.98	4.91	1.13	0.52	0.52
AM6.	AD6.	4.98	0.38	-1.83	-6.43	-2.27	-6.87	-0.20	-4.80	4.96	0.36	-0.34	-4.94	6.17	1.57	0.69	0.69
AM7.	AD7.	6.05	0.50	-2.30	-7.85	-2.77	-8.32	-0.30	-5.85	6.27	0.72	-0.43	-5.98	7.52	1.97	0.84	0.84
MAD			0.22		4.64		4.99		3.43		0.28		3.55		1.03		0.46

Table S7. Reaction energies (ΔE, kcal/mol) and errors (Er, kcal/mol) for the IDHC5 set obtained with the DH-SVPD basis set.

Functional	PBEQIDH		PBEQIDHD3(0)		PBEQIDHD3(BJ)		PBE0DH		PBE0DHD3(BJ)		B2PLYP		B2PLYPD3(0)		DSDPBEP86		revDSDPBEP86D3(BJ)	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
Reaction1	-0.97	0.36	-1.96	-0.63	-1.82	-0.49	1.66	3.00	-1.68	-0.35	1.77	3.10	-1.31	0.02	-3.24	-1.91	-2.43	-1.10
Reaction2	9.94	0.94	8.00	-1.00	8.09	-0.91	14.63	5.64	8.17	-0.83	14.88	5.89	9.18	0.19	5.57	-3.43	7.04	-1.96
Reaction3	3.52	0.09	2.59	-0.85	2.63	-0.81	4.48	1.04	2.43	-1.00	4.40	0.96	2.38	-1.06	2.00	-1.43	2.31	-1.12
Reaction4	1.97	1.64	-1.92	-2.25	-1.19	-1.52	5.80	5.47	-2.27	-2.60	5.97	5.64	-2.91	-3.23	-3.80	-4.13	-2.41	-2.74
Reaction5	-0.62	2.32	-6.31	-3.38	-5.29	-2.35	5.02	7.96	-6.71	-3.77	5.21	8.15	-7.81	-4.87	-8.99	-6.05	-6.95	-4.02
MAD		1.07		1.62		1.21		4.62		1.71		4.75		1.87		3.39		2.19

Functional	M06L		TPSSh		B3LYP		PBE0		M06		CAM-B3LYP		wB97XD		B3LYP-D3	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
Reaction1	-1.34	0.00	5.36	6.69	6.50	7.83	3.87	5.20	-3.53	-2.20	3.67	5.01	-0.50	0.84	0.84	2.17
Reaction2	7.58	-1.42	20.06	11.06	23.42	14.42	18.48	9.48	6.23	-2.76	18.59	9.59	9.92	0.92	12.86	3.86
Reaction3	1.31	-2.13	5.77	2.33	6.20	2.77	5.21	1.78	1.62	-1.82	5.22	1.79	1.52	-1.92	2.42	-1.02
Reaction4	-6.65	-6.98	12.74	12.41	13.51	13.18	9.13	8.80	-5.60	-5.93	8.53	8.20	-6.88	-7.20	-3.12	-3.45
Reaction5	-12.63	-9.69	15.40	18.34	16.29	19.23	9.98	12.92	-11.29	-8.35	9.04	11.98	-13.35	-10.41	-8.07	-5.13
MAD		4.04		10.17		11.49		7.64		4.21		7.31		4.26		3.13

Table S8. Reaction energies (ΔE, kcal/mol) and errors (Er, kcal/mol) for the IDHC5 set obtained with the Def2-TZVPP basis set.

Functional	PBEQIDH		PBEQIDHD3(0)		PBEQIDHD3(BJ)		PBE0DH		PBE0DHD3(BJ)		B2PLYP		B2PLYPD3(0)		DSDPBEP86		revDSDPBEP86D3BJ	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
Reaction1	0.16	1.50	-0.82	0.51	-0.69	0.64	2.69	4.02	-0.65	0.68	3.20	4.53	0.26	1.59	-1.87	-0.54	-1.01	0.32
Reaction2	11.86	2.86	9.92	0.92	10.01	1.02	16.41	7.41	9.94	0.95	17.40	8.40	11.91	2.91	7.91	-1.08	9.48	0.48
Reaction3	4.59	1.16	3.66	0.22	3.70	0.27	5.48	2.05	3.43	0.00	5.60	2.17	3.58	0.14	3.20	-0.23	3.54	0.11
Reaction4	5.51	5.18	1.62	1.29	2.34	2.02	9.18	8.85	1.11	0.78	9.90	9.57	1.22	0.89	0.21	-0.12	1.72	1.39
Reaction5	4.62	7.56	-1.08	1.86	-0.05	2.89	9.96	12.90	-1.77	1.17	11.00	13.94	-1.75	1.19	-3.03	-0.09	-0.82	2.12
MAD		3.65		0.96		1.37		7.05		0.72		7.72		1.34		0.41		0.88

Functional	M06L		TPSSh		B3LYP		PBE0		M06		CAM-B3LYP		wB97XD		B3LYP-D3	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
Reaction1	-0.12	1.21	6.23	7.56	8.39	9.72	4.95	6.28	-2.37	-1.04	5.39	6.73	0.91	2.24	2.73	4.06
Reaction2	9.65	0.66	21.46	12.46	26.74	17.74	20.34	11.35	8.47	-0.53	21.67	12.67	12.35	3.35	16.18	7.18
Reaction3	2.54	-0.90	6.64	3.21	7.40	3.96	6.19	2.76	2.54	-0.89	6.41	2.97	2.51	-0.92	3.61	0.18
Reaction4	-2.62	-2.94	15.84	15.51	17.80	17.47	12.48	12.15	-2.68	-3.01	12.70	12.37	-3.37	-3.70	1.16	0.84
Reaction5	-6.75	-3.81	19.90	22.84	22.48	25.41	14.81	17.75	-7.16	-4.22	15.05	17.99	-8.30	-5.36	-1.89	1.05
MAD		1.90		12.32		14.86		10.06		1.94		10.55		3.11		2.66

Table S9. Reaction energies (ΔE, kcal/mol) and errors (Er, kcal/mol) for the PAH5 set obtained with the DH-SVPD basis set.

Functional	PBEQIDH		PBEQIDHD3(0)		PBEQIDHD3(BJ)		PBE0DH		PBE0DHD3(BJ)		B2PLYP		B2PLYPD3(0)		DSDPBEP86		revDSDPBEP86D3(BJ)	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
	6.41	0.41	6.46	0.46	6.50	0.51	6.17	0.17	6.42	0.42	5.59	0.41	5.71	0.29	6.01	0.01	5.84	0.16
	0.53	0.02	0.60	0.10	0.67	0.17	0.27	0.23	0.59	0.09	-0.04	0.54	0.08	0.42	0.43	0.08	0.28	0.22
	3.61	0.24	3.73	0.36	3.84	0.47	3.11	0.26	3.69	0.32	2.51	0.86	2.73	0.64	3.35	0.02	3.06	0.31
	6.11	0.14	6.06	0.08	6.11	0.13	6.23	0.25	6.22	0.25	5.69	0.29	5.50	0.48	5.61	0.36	5.55	0.43
	13.56	0.89	13.75	1.08	13.90	1.24	12.80	0.13	13.65	0.99	11.30	1.37	11.65	1.02	12.66	0.01	12.19	0.48
MAD		0.34		0.42		0.50		0.21		0.41		0.69		0.57		0.09		0.32

Functional	M06L		TPSSh		B3LYP		PBE0		M06		CAM-B3LYP		wB97XD		B3LYP-D3	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
Reaction1	5.44	0.56	5.20	0.80	5.10	0.90	5.63	0.37	5.75	0.25	6.29	-0.29	6.68	-0.68	5.33	0.67
Reaction2	0.01	0.49	-0.26	0.77	-0.56	1.07	-0.11	0.61	0.12	0.38	0.35	0.15	0.89	-0.39	-0.30	0.80
Reaction3	2.63	0.74	2.02	1.35	1.51	1.86	2.36	1.01	2.62	0.75	3.06	0.31	3.92	-0.55	1.98	1.39
Reaction4	6.05	-0.08	5.82	0.15	5.79	0.19	6.00	-0.02	5.89	0.09	6.83	-0.85	6.64	-0.66	5.47	0.51
Reaction5	10.97	1.70	10.25	2.42	9.75	2.92	11.27	1.40	11.69	0.98	13.08	-0.41	14.35	-1.69	10.48	2.18
MAD	0.71		1.10		1.38		0.68		0.49		0.40		0.79		1.11	

Table S10. Reaction energies (ΔE, kcal/mol) and errors (Er, kcal/mol) for the PAH5 set obtained with the cc-pVQZ basis set.

Functional	PBEQIDH		PBEQIDHD3(0)		PBEQIDHD3(BJ)		PBE0DH		PBE0DHD3(BJ)		revDSDPBEP86D3(BJ)	
	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er	ΔE	Er
	6.39	-0.39	6.44	-0.44	6.49	-0.49	6.15	-0.15	6.40	-0.40	5.83	0.17
	0.43	0.07	0.51	-0.01	0.57	-0.07	0.17	0.33	6.20	-5.70	0.18	0.32
	3.48	-0.11	3.61	-0.24	3.72	-0.35	2.96	0.41	3.54	-0.17	2.95	0.42
	6.23	-0.26	6.18	-0.20	6.22	-0.25	6.21	-0.24	6.20	-0.23	5.72	0.25
	13.39	-0.72	13.58	-0.91	13.74	-1.07	12.61	0.05	13.47	-0.80	12.03	0.64
MAD		0.31		0.36		0.45		0.24		1.46		0.36

Table S11. Reaction energies (ΔE, kcal/mol) and errors (Er, kcal/mol) for the Cope set obtained with the DH-SVPD basis set.

	Functionals	PBEQIDH					PBEQIDHD3(0)						PBEQIDHD3(BJ)					
		Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
		ΔE	Er		ΔEr	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
H	**TS**	16.32	-1.21				TS	16.26	-1.15				TS	16.24	-1.12			
CH3	**TS_{1-2}**	15.64	1.12	**2**	-0.28	-0.28	TS_{1-2}	15.59	1.07	**2**	-0.27	-0.26	TS_{1-2}	15.57	1.05	**2**	-0.26	-0.26
	TS_{2-3}	15.96	-0.59	**3**	-1.55	-0.68	TS_{2-3}	15.93	-0.56	**3**	-1.47	-0.61	TS_{2-3}	15.91	-0.54	**3**	-1.50	-0.63
	TS_{3-4}	14.53	-0.53	**4**	-1.26	-0.59	TS_{3-4}	14.56	-0.56	**4**	-1.16	-0.49	TS_{3-4}	14.51	-0.50	**4**	-1.19	-0.52
NH3	**TS_{1-2}**	14.87	0.85	**2**	-1.08	0.62	TS_{1-2}	14.81	0.78	**2**	-1.09	0.64	TS_{1-2}	14.81	0.78	**2**	-1.06	0.61
	TS_{2-3}	11.40	0.11	**3**	-5.37	1.56	TS_{2-3}	11.37	0.14	**3**	-5.31	1.50	TS_{2-3}	11.39	0.12	**3**	-5.34	1.53
	TS_{3-4}	10.54	0.26	**4**	-4.58	1.22	TS_{3-4}	10.56	0.24	**4**	-4.49	1.13	TS_{3-4}	10.50	0.30	**4**	-4.53	1.17
CN	**TS_{1-2}**	16.45	-1.08	**2**	-2.88	0.56	TS_{1-2}	16.39	-1.02	**2**	-2.87	0.55	TS_{1-2}	16.38	-1.01	**2**	-2.86	0.54
	TS_{2-3}	10.09	-0.25	**3**	-6.19	1.09	TS_{2-3}	10.07	-0.22	**3**	-6.13	1.03	TS_{2-3}	10.05	-0.21	**3**	-6.14	1.04
	TS_{3-4}	11.33	-0.36	**4**	-5.05	0.88	TS_{3-4}	11.34	-0.36	**4**	-4.99	0.81	TS_{3-4}	11.31	-0.33	**4**	-4.98	0.81
OH	**TS_{1-2}**	17.30	1.47	**2**	0.86	0.50	TS_{1-2}	17.26	1.42	**2**	0.85	0.52	TS_{1-2}	17.23	1.40	**2**	0.87	0.50
	TS_{2-3}	15.25	0.22	**3**	-1.92	1.11	TS_{2-3}	15.20	0.17	**3**	-1.89	1.08	TS_{2-3}	15.22	0.19	**3**	-1.91	1.10
	TS_{3-4}	14.09	0.12	**4**	-3.94	1.08	TS_{3-4}	14.08	0.11	**4**	-3.87	1.01	TS_{3-4}	14.03	0.07	**4**	-3.91	1.05
MAD			0.63			0.85			0.60			0.80			0.59			0.81

	PBE0DH						PBE0DHD3(BJ)						B2PLYP				
	Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
	ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
TS	17.49	-2.38				TS	17.13	-2.02				TS	12.68	2.43			
TS1-2	16.85	2.33	2	-0.43	-0.42	TS1-2	16.56	2.04	2	-0.29	-0.28	TS1-2	11.99	-2.53	2	-0.38	-0.37
TS2-3	16.82	-1.45	3	-2.01	-1.14	TS2-3	16.68	-1.31	3	-1.71	-0.84	TS2-3	12.21	3.16	3	-1.70	-0.84
TS3-4	15.22	-1.21	4	-1.73	-1.06	TS3-4	15.20	-1.20	4	-1.34	-0.68	TS3-4	10.68	3.33	4	-1.47	-0.80
TS1-2	16.05	2.02	2	-1.21	0.75	TS1-2	15.78	1.75	2	-1.10	0.65	TS1-2	11.32	2.70	2	-1.03	0.57
TS2-3	11.81	0.29	3	-5.94	2.13	TS2-3	11.86	0.35	3	-5.72	1.91	TS2-3	8.17	3.34	3	-5.38	1.57
TS3-4	11.11	0.31	4	-5.13	1.77	TS3-4	11.03	0.24	4	-4.84	1.48	TS3-4	6.87	3.93	4	-4.65	1.29
TS1-2	17.65	-2.28	2	-3.05	0.73	TS1-2	17.37	-2.00	2	-2.94	0.62	TS1-2	12.80	2.57	2	-2.98	0.66
TS2-3	10.67	-0.83	3	-6.67	1.56	TS2-3	10.59	-0.75	3	-6.41	1.30	TS2-3	6.25	3.60	3	-6.60	1.49
TS3-4	12.01	-1.04	4	-5.51	1.34	TS3-4	11.95	-0.97	4	-5.18	1.01	TS3-4	7.20	3.78	4	-5.41	1.23
TS1-2	18.43	2.59	2	0.74	0.62	TS1-2	18.15	2.31	2	0.81	0.56	TS1-2	13.60	2.23	2	0.96	0.40
TS2-3	15.83	0.80	3	-2.39	1.58	TS2-3	15.78	0.75	3	-2.28	1.47	TS2-3	12.14	2.89	3	-1.65	0.84
TS3-4	14.76	0.80	4	-4.34	1.48	TS3-4	14.57	0.60	4	-4.17	1.31	TS3-4	10.75	3.21	4	-3.63	0.77
MAD		1.41			1.22			1.25			1.01			3.05			0.90

	B2PLYPD3(0)					DSDPBEP86					revDSDPBEP86-D3(BJ)					
	Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
	ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
TS	12.39	2.72				TS	14.12	0.99				TS	14.97	0.15			
TS1-2	11.78	-2.74	2	-0.19	-0.18	TS1-2	13.49	-1.03	2	-0.13	-0.12	TS1-2	14.33	-0.19	2	-0.18	-0.17
TS2-3	12.23	3.14	3	-1.30	-0.43	TS2-3	14.08	1.29	3	-1.09	-0.22	TS2-3	14.87	0.50	3	-1.14	-0.28
TS3-4	10.83	3.18	4	-1.01	-0.34	TS3-4	12.80	1.21	4	-0.80	-0.13	TS3-4	13.58	0.43	4	-0.87	-0.21
TS1-2	11.08	-2.95	2	-0.92	-0.46	TS1-2	12.80	-1.23	2	-0.85	-0.39	TS1-2	13.64	-0.39	2	-0.86	-0.40
TS2-3	8.19	-3.33	3	-5.06	-1.25	TS2-3	10.09	-1.43	3	-4.68	-0.87	TS2-3	10.73	-0.78	3	-4.60	-0.79
TS3-4	6.95	-3.85	4	-4.27	-0.91	TS3-4	9.05	-1.75	4	-3.95	-0.59	TS3-4	9.94	-0.85	4	-3.91	-0.56
TS1-2	12.55	2.82	2	-2.90	0.58	TS1-2	14.30	1.07	2	-2.65	0.33	TS1-2	15.14	0.23	2	-2.62	0.30
TS2-3	6.12	3.72	3	-6.44	1.33	TS2-3	8.40	1.44	3	-5.74	0.63	TS2-3	9.18	0.66	3	-5.65	0.54
TS3-4	7.10	3.88	4	-5.20	1.02	TS3-4	9.51	1.47	4	-4.61	0.44	TS3-4	10.39	0.59	4	-4.58	0.41
TS1-2	13.38	-2.45	2	1.00	0.37	TS1-2	15.10	-0.74	2	1.01	0.36	TS1-2	15.88	0.04	2	0.98	0.38
TS2-3	12.11	-2.93	3	-1.38	0.57	TS2-3	13.75	-1.28	3	-1.37	0.56	TS2-3	14.46	-0.57	3	-1.31	0.50
TS3-4	10.79	-3.18	4	-3.29	0.44	TS3-4	12.49	-1.48	4	-3.35	0.50	TS3-4	13.37	-0.60	4	-3.30	0.44
		3.14			0.66			1.26			0.43			0.46			0.41

	Functional	M06L					TPSSh						B3LYP					
		Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
		ΔE	Er		ΔEr	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
H	TS	16.70	-1.59				TS	13.90	1.21				TS	13.58	1.53			
CH3	TS1-2	16.16	1.64	2	-0.52	-0.52	TS1-2	13.28	-1.24	2	-0.76	-0.75	TS1-2	12.92	-1.60	2	-0.64	-0.63
	TS2-3	15.31	0.06	3	-2.57	-1.70	TS2-3	12.67	2.70	3	-2.68	-1.81	TS2-3	12.56	2.81	3	-2.51	-1.64
	TS3-4	13.91	0.10	4	-2.12	-1.46	TS3-4	10.95	3.05	4	-2.39	-1.73	TS3-4	10.73	3.28	4	-2.29	-1.62
NH3	TS1-2	15.60	1.57	2	-0.76	0.31	TS1-2	12.61	1.42	2	-1.28	0.82	TS1-2	12.22	1.81	2	-1.29	0.83
	TS2-3	9.88	1.63	3	-7.04	3.23	TS2-3	8.20	3.32	3	-6.62	2.81	TS2-3	7.96	3.56	3	-6.40	2.59
	TS3-4	9.34	1.46	4	-6.02	2.66	TS3-4	6.88	3.91	4	-5.78	2.43	TS3-4	6.72	4.08	4	-5.63	2.27
CN	TS1-2	16.81	-1.44	2	-3.72	1.40	TS1-2	14.00	1.37	2	-3.56	1.24	TS1-2	13.72	1.65	2	-3.34	1.02
	TS2-3	8.17	1.67	3	-8.43	3.32	TS2-3	6.12	3.72	3	-8.01	2.90	TS2-3	6.13	3.71	3	-7.55	2.44
	TS3-4	9.64	1.34	4	-6.86	2.69	TS3-4	7.17	3.81	4	-6.57	2.39	TS3-4	7.13	3.85	4	-6.28	2.11
OH	TS1-2	17.64	1.81	2	1.02	0.35	TS1-2	14.86	0.98	2	0.70	0.66	TS1-2	14.42	1.41	2	0.77	0.60
	TS2-3	13.82	1.21	3	-3.40	2.59	TS2-3	12.09	2.94	3	-3.06	2.25	TS2-3	12.27	2.76	3	-2.38	1.57
	TS3-4	13.07	0.89	4	-5.22	2.36	TS3-4	10.58	3.38	4	-4.81	1.95	TS3-4	10.89	3.08	4	-4.22	1.36
MAD			1.26			1.88			2.54			1.81			2.70			1.56

	PBE0						M06						CAM-B3LYP				
	Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
	ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
TS	16.28	-1.17				TS	18.26	-3.15				TS	18.57	-3.45			
TS1-2	15.66	1.15	2	-0.57	-0.56	TS1-2	17.74	3.23	2	-0.06	-0.05	TS1-2	17.92	3.41	2	-0.43	-0.43
TS2-3	15.28	0.09	3	-2.45	-1.58	TS2-3	17.69	-2.32	3	-1.59	-0.72	TS2-3	17.93	-2.56	3	-2.02	-1.16
TS3-4	13.55	0.46	4	-2.16	-1.50	TS3-4	16.44	-2.43	4	-1.29	-0.63	TS3-4	16.21	-2.21	4	-1.82	-1.15
TS1-2	14.88	0.85	2	-1.34	0.88	TS1-2	17.01	2.98	2	-0.71	0.25	TS1-2	17.16	3.13	2	-1.14	0.68
TS2-3	10.16	1.35	3	-6.61	2.80	TS2-3	12.19	0.68	3	-5.58	1.77	TS2-3	12.66	1.14	3	-5.75	1.94
TS3-4	9.23	1.56	4	-5.76	2.40	TS3-4	12.27	1.47	4	-4.79	1.44	TS3-4	12.29	1.49	4	-5.04	1.68
TS1-2	16.42	-1.05	2	-3.26	0.94	TS1-2	18.47	-3.10	2	-3.03	0.71	TS1-2	18.76	-3.39	2	-2.77	0.45
TS2-3	8.96	0.88	3	-7.35	2.24	TS2-3	10.97	-1.13	3	-6.72	1.62	TS2-3	11.93	-2.09	3	-6.24	1.14
TS3-4	10.13	0.85	4	-6.08	1.90	TS3-4	12.73	-1.75	4	-5.53	1.35	TS3-4	13.31	-2.33	4	-5.26	1.08
TS1-2	17.19	1.36	2	0.62	0.75	TS1-2	19.19	3.36	2	1.21	0.16	TS1-2	19.42	3.58	2	0.96	0.40
TS2-3	14.19	0.84	3	-3.00	2.19	TS2-3	16.27	1.24	3	-1.98	1.17	TS2-3	17.22	2.19	3	-1.82	1.01
TS3-4	12.97	1.00	4	-4.80	1.94	TS3-4	15.95	1.98	4	-3.96	1.10	TS3-4	16.34	2.37	4	-3.71	0.85
MAD		0.97			1.64			2.22			0.91			2.57			1.00

	wB97XD						B3LYP-D3				
	Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
	ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
TS	18.26	-3.15				TS	13.06	2.05			
TS1-2	17.67	3.15	2	-0.40	-0.39	TS1-2	12.52	-2.00	2	-0.33	-0.33
TS2-3	17.61	-2.24	3	-1.90	-1.03	TS2-3	12.56	2.81	3	-1.83	-0.96
TS3-4	16.13	-2.13	4	-1.56	-0.89	TS3-4	10.96	3.04	4	-1.47	-0.80
TS1-2	16.87	2.84	2	-1.16	0.70	TS1-2	11.77	2.26	2	-1.12	0.66
TS2-3	12.27	0.76	3	-5.73	1.92	TS2-3	7.96	3.56	3	-5.85	2.04
TS3-4	12.07	1.27	4	-4.93	1.57	TS3-4	6.85	3.95	4	-4.95	1.59
TS1-2	18.42	-3.05	2	-2.87	0.55	TS1-2	13.26	2.11	2	-3.23	0.91
TS2-3	11.59	-1.75	3	-6.29	1.19	TS2-3	5.87	3.97	3	-7.27	2.17
TS3-4	13.05	-2.08	4	-5.22	1.05	TS3-4	6.94	4.03	4	-5.91	1.74
TS1-2	19.08	3.25	2	0.68	0.68	TS1-2	14.03	1.80	2	0.82	0.55
TS2-3	16.19	1.16	3	-2.47	1.66	TS2-3	12.17	2.86	3	-1.93	1.12
TS3-4	15.42	1.45	4	-4.28	1.42	TS3-4	10.92	3.05	4	-3.62	0.76
MAD		2.18			1.09			2.88			1.13

Table S12. Reaction energies (ΔE, kcal/mol) and errors (Er, kcal/mol) for the Cope set obtained with the Def2-TZVPP basis set.

	Functionals	PBEQIDH					PBEQIDHD3(0)						PBEQIDHD3(BJ)					
		Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
		ΔE	Er		ΔEr	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
H	TS	15.70	-0.58				TS	15.63	-0.52				TS	15.61	-0.50			
CH3	TS1-2	15.06	0.54	2	-0.10	-0.10	TS1-2	15.01	0.49	2	-0.09	-0.08	TS1-2	14.99	0.47	2	-0.08	-0.07
	TS2-3	15.50	-0.13	3	-1.44	-0.57	TS2-3	15.47	-0.10	3	-1.37	-0.50	TS2-3	15.45	-0.08	3	-1.39	-0.53
	TS3-4	14.01	-0.01	4	-1.19	-0.52	TS3-4	14.04	-0.04	4	-1.08	-0.41	TS3-4	13.99	0.02	4	-1.12	-0.45
NH3	TS1-2	14.43	0.40	2	-0.76	0.31	TS1-2	14.36	0.34	2	-0.78	0.32	TS1-2	14.36	0.34	2	-0.75	0.29
	TS2-3	11.19	0.32	3	-5.14	1.33	TS2-3	11.17	0.35	3	-5.08	1.27	TS2-3	11.19	0.33	3	-5.11	1.30
	TS3-4	10.10	0.70	4	-4.46	1.10	TS3-4	10.12	0.68	4	-4.37	1.01	TS3-4	10.06	0.74	4	-4.41	1.05
CN	TS1-2	15.89	-0.52	2	-2.66	0.34	TS1-2	15.84	-0.47	2	-2.65	0.33	TS1-2	15.83	-0.46	2	-2.65	0.32
	TS2-3	9.72	0.12	3	-6.02	0.91	TS2-3	9.69	0.15	3	-5.96	0.85	TS2-3	9.68	0.16	3	-5.97	0.86
	TS3-4	10.87	0.10	4	-4.87	0.70	TS3-4	10.88	0.10	4	-4.81	0.63	TS3-4	10.85	0.13	4	-4.80	0.63
OH	TS1-2	16.64	0.81	2	1.21	0.15	TS1-2	16.60	0.76	2	1.20	0.17	TS1-2	16.57	0.74	2	1.22	0.15
	TS2-3	14.85	0.19	3	-1.86	1.05	TS2-3	14.80	0.23	3	-1.83	1.02	TS2-3	14.82	0.21	3	-1.85	1.04
	TS3-4	13.53	0.44	4	-3.93	1.08	TS3-4	13.52	0.45	4	-3.86	1.01	TS3-4	13.47	0.49	4	-3.91	1.05
MAD			0.37			0.68			0.36			0.63			0.36			0.65

	PBE0DH						PBE0DHD3(BJ)						B2PLYP				
	Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
	ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
TS	16.75	-1.63				TS	16.38	-1.27				TS	12.05	3.07			
TS1-2	16.13	1.62	2	-0.26	-0.25	TS1-2	15.84	1.33	2	-0.12	-0.12	TS1-2	11.39	-3.13	2	-0.24	-0.23
TS2-3	16.25	-0.88	3	-1.88	-1.01	TS2-3	16.12	-0.75	3	-1.58	-0.71	TS2-3	11.69	3.68	3	-1.64	-0.78
TS3-4	14.60	-0.60	4	-1.62	-0.95	TS3-4	14.59	-0.58	4	-1.24	-0.57	TS3-4	10.13	3.88	4	-1.41	-0.74
TS1-2	15.47	1.44	2	-0.94	0.48	TS1-2	15.19	1.16	2	-0.83	0.37	TS1-2	10.87	3.16	2	-0.71	0.25
TS2-3	11.46	0.05	3	-5.70	1.89	TS2-3	11.52	0.01	3	-5.48	1.67	TS2-3	7.97	3.54	3	-5.06	1.25
TS3-4	10.57	0.23	4	-4.98	1.63	TS3-4	10.49	0.31	4	-4.69	1.34	TS3-4	6.54	4.26	4	-4.40	1.05
TS1-2	16.96	-1.59	2	-2.86	0.53	TS1-2	16.69	-1.32	2	-2.74	0.42	TS1-2	12.22	3.15	2	-2.86	0.54
TS2-3	10.18	-0.33	3	-6.50	1.39	TS2-3	10.09	-0.25	3	-6.23	1.13	TS2-3	5.76	4.08	3	-6.51	1.40
TS3-4	11.43	-0.46	4	-5.32	1.14	TS3-4	11.37	-0.39	4	-4.99	0.81	TS3-4	6.67	4.31	4	-5.27	1.10
TS1-2	17.64	1.80	2	1.05	0.31	TS1-2	17.36	1.52	2	1.12	0.25	TS1-2	12.93	2.90	2	1.26	0.11
TS2-3	15.33	0.30	3	-2.27	1.46	TS2-3	15.28	0.25	3	-2.16	1.35	TS2-3	11.69	3.34	3	-1.54	0.73
TS3-4	14.16	0.19	4	-4.26	1.40	TS3-4	13.96	0.01	4	-4.09	1.23	TS3-4	10.24	3.73	4	-3.57	0.71
MAD		0.86			1.04			0.70			0.83			3.56			0.74

B2PLYPD3(0)						DSDPBEP86						revDSDPBEP86-D3(BJ)					
Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies		
ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er	
11.76	3.35				TS	13.59	1.52				TS	14.45	0.67				
11.18	-3.34	2	-0.05	-0.04	TS1-2	13.01	-1.51	2	0.05	0.05	TS1-2	13.86	-0.66	2	0.00	0.01	
11.72	3.65	3	-1.24	-0.37	TS2-3	13.70	1.67	3	-1.01	-0.14	TS2-3	14.51	0.86	3	-1.06	-0.19	
10.27	3.73	4	-0.95	-0.28	TS3-4	12.36	1.65	4	-0.73	-0.07	TS3-4	13.15	0.85	4	-0.80	-0.14	
10.63	-3.40	2	-0.60	-0.14	TS1-2	12.46	-1.57	2	-0.49	-0.04	TS1-2	13.32	-0.71	2	-0.50	-0.05	
7.99	-3.52	3	-4.74	-0.93	TS2-3	10.02	-1.50	3	-4.37	-0.56	TS2-3	10.67	-0.84	3	-4.29	-0.48	
6.62	-4.18	4	-4.02	-0.67	TS3-4	8.78	-2.02	4	-3.75	-0.39	TS3-4	9.70	-1.10	4	-3.71	-0.35	
11.97	3.40	2	-2.79	0.47	TS1-2	13.83	1.54	2	-2.47	0.15	TS1-2	14.69	0.68	2	-2.45	0.13	
5.63	4.21	3	-6.35	1.25	TS2-3	8.07	1.77	3	-5.60	0.50	TS2-3	8.86	0.98	3	-5.51	0.41	
6.57	4.41	4	-5.06	0.89	TS3-4	9.12	1.86	4	-4.45	0.28	TS3-4	10.01	0.97	4	-4.42	0.25	
12.72	-3.12	2	1.29	0.07	TS1-2	14.54	-1.30	2	1.36	0.00	TS1-2	15.33	-0.51	2	1.34	0.03	
11.65	-3.38	3	-1.27	0.46	TS2-3	13.43	-1.60	3	-1.29	0.48	TS2-3	14.16	-0.87	3	-1.22	0.41	
10.27	-3.70	4	-3.23	0.37	TS3-4	12.03	-1.93	4	-3.34	0.49	TS3-4	12.93	-1.04	4	-3.28	0.42	
MAD	3.65			0.50			1.65			0.26			0.83			0.24	

	Functionals	M06L					TPSSh						B3LYP					
		Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
		ΔE	Er		ΔEr	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
H	TS	16.31	-1.19				TS	13.06	2.05				TS	12.83	2.29			
CH3	TS1-2	15.79	1.28	2	-0.46	-0.46	TS1-2	12.44	-2.07	2	-0.64	-0.63	TS1-2	12.18	-2.34	2	-0.56	-0.55
	TS2-3	14.92	0.45	3	-2.60	-1.74	TS2-3	11.98	3.39	3	-2.57	-1.70	TS2-3	11.90	3.47	3	-2.47	-1.60
	TS3-4	13.50	0.50	4	-2.18	-1.51	TS3-4	10.23	3.77	4	-2.30	-1.63	TS3-4	10.04	3.97	4	-2.23	-1.56
NH3	TS1-2	15.37	1.34	2	-0.59	0.13	TS1-2	11.90	2.13	2	-1.06	0.60	TS1-2	11.62	2.41	2	-1.02	0.57
	TS2-3	9.55	1.97	3	-6.97	3.16	TS2-3	7.75	3.77	3	-6.33	2.52	TS2-3	7.60	3.92	3	-6.05	2.24
	TS3-4	9.00	1.80	4	-6.01	2.65	TS3-4	6.29	4.50	4	-5.58	2.23	TS3-4	6.29	4.50	4	-5.34	1.99
CN	TS1-2	16.42	-1.05	2	-3.61	1.28	TS1-2	13.22	2.15	2	-3.42	1.10	TS1-2	13.00	2.37	2	-3.29	0.97
	TS2-3	7.85	2.00	3	-8.41	3.30	TS2-3	5.49	4.35	3	-7.86	2.75	TS2-3	5.47	4.37	3	-7.50	2.40
	TS3-4	9.17	1.81	4	-6.83	2.66	TS3-4	6.48	4.50	4	-6.38	2.21	TS3-4	6.44	4.54	4	-6.16	1.99
OH	TS1-2	17.15	1.32	2	1.27	0.10	TS1-2	13.97	1.87	2	0.93	0.43	TS1-2	13.63	2.21	2	0.99	0.38
	TS2-3	13.45	1.58	3	-3.44	2.63	TS2-3	11.47	3.56	3	-2.89	2.08	TS2-3	11.69	3.34	3	-2.20	1.39
	TS3-4	12.67	1.30	4	-5.17	2.31	TS3-4	9.93	4.04	4	-4.67	1.81	TS3-4	10.34	3.62	4	-4.05	1.20
MAD			1.35			1.83			3.24			1.64			3.33			1.40

	PBE0						M06						CAM-B3LYP				
	Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
	ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
TS	15.48	-0.36				TS	17.98	-2.87				TS	17.79	-2.67			
TS1-2	14.88	0.36	2	-0.42	-0.41	TS1-2	17.53	3.01	2	0.07	0.08	TS1-2	17.16	2.64	2	-0.33	-0.33
TS2-3	14.65	0.72	3	-2.30	-1.44	TS2-3	17.56	-2.19	3	-1.46	-0.59	TS2-3	17.28	-1.91	3	-1.96	-1.09
TS3-4	12.89	1.11	4	-2.04	-1.37	TS3-4	16.31	-2.31	4	-1.16	-0.49	TS3-4	15.52	-1.52	4	-1.74	-1.07
TS1-2	14.22	0.19	2	-1.08	0.63	TS1-2	16.94	2.91	2	-0.43	0.03	TS1-2	16.55	2.52	2	-0.86	0.40
TS2-3	9.77	1.74	3	-6.32	2.51	TS2-3	11.92	0.41	3	-5.64	1.83	TS2-3	12.28	0.76	3	-5.43	1.62
TS3-4	8.69	2.10	4	-5.55	2.19	TS3-4	11.92	1.12	4	-4.86	1.50	TS3-4	11.82	1.02	4	-4.78	1.42
TS1-2	15.66	-0.29	2	-3.11	0.79	TS1-2	18.19	-2.82	2	-2.93	0.61	TS1-2	18.02	-2.65	2	-2.72	0.40
TS2-3	8.37	1.47	3	-7.19	2.09	TS2-3	10.81	-0.96	3	-6.64	1.54	TS2-3	11.26	-1.41	3	-6.20	1.09
TS3-4	9.48	1.50	4	-5.88	1.71	TS3-4	12.47	-1.50	4	-5.41	1.23	TS3-4	12.60	-1.62	4	-5.13	0.96
TS1-2	16.34	0.51	2	0.88	0.48	TS1-2	18.82	2.99	2	1.47	-0.10	TS1-2	18.58	2.75	2	1.20	0.17
TS2-3	13.63	1.41	3	-2.82	2.01	TS2-3	15.86	0.83	3	-2.24	1.43	TS2-3	16.63	1.60	3	-1.64	0.83
TS3-4	12.36	1.60	4	-4.64	1.79	TS3-4	15.45	1.48	4	-4.10	1.24	TS3-4	15.76	1.80	4	-3.57	0.71
MAD		1.03			1.45			1.95			0.89			1.91			0.84

	wB97XD						B3LYP-D3				
	Barrier Heights			Reaction Energies			Barrier Heights			Reaction Energies	
	ΔE	Er		ΔE	Er		ΔE	Er		ΔE	Er
TS	17.49	-2.38				TS	12.31	2.81			
TS1-2	16.93	2.41	2	-0.26	-0.25	TS1-2	11.78	-2.74	2	-0.25	-0.24
TS2-3	17.01	-1.64	3	-1.78	-0.91	TS2-3	11.90	3.47	3	-1.79	-0.92
TS3-4	15.49	-1.48	4	-1.46	-0.79	TS3-4	10.27	3.73	4	-1.41	-0.74
TS1-2	16.26	2.23	2	-0.90	0.44	TS1-2	11.17	2.86	2	-0.86	0.40
TS2-3	11.79	0.27	3	-5.52	1.71	TS2-3	7.60	3.92	3	-5.50	1.69
TS3-4	11.48	0.68	4	-4.79	1.43	TS3-4	6.43	4.37	4	-4.66	1.31
TS1-2	17.70	-2.33	2	-2.75	0.43	TS1-2	12.55	2.83	2	-3.18	0.86
TS2-3	11.00	-1.15	3	-6.18	1.07	TS2-3	5.22	4.62	3	-7.23	2.12
TS3-4	12.38	-1.41	4	-5.07	0.89	TS3-4	6.25	4.72	4	-5.79	1.62
TS1-2	18.24	2.41	2	0.94	0.43	TS1-2	13.24	2.60	2	1.04	0.33
TS2-3	15.58	0.55	3	-2.35	1.54	TS2-3	11.59	3.44	3	-1.75	0.94
TS3-4	14.79	0.82	4	-4.17	1.31	TS3-4	10.37	3.60	4	-3.45	0.60
MAD		1.52			0.93			3.52			0.98

Table S13. DLPNO-CCSD(T) reaction energies (kcal/mol) computed with the aug-cc-pVTZ and aug-cc-pVQZ basis sets and extrapolated at complete basis set limit according to a two point extrapolation scheme (alpha = 5.79 and beta = 3.05).

	aug-cc-pVTZ	aug-cc-pVQZ	CBS
n-octane→tetramethylbutane	-2.491	-1.807	-1.331
n-undecane→hexamethylbutane	6.419	7.951	8.996
$C_{14}H_{30}$ (linear)→$C_{28}H_{20}$ (folded)	1.951	2.836	3.434
$C_{22}H_{46}$ (linear)→$C_{22}H_{46}$ (folded)	-2.407	-0.776	0.328
$C_{30}H_{62}$ (linear)→$C_{30}H_{62}$ (folded)	-6.871	-4.527	-2.939

n_oktane
26

C	-0.1614620000	4.4569880000	0.0000000000
C	-0.8313160000	3.0940090000	0.0000000000
C	0.1614620000	1.9436090000	0.0000000000
C	-0.4965940000	0.5746890000	0.0000000000
C	0.4965940000	-0.5746890000	0.0000000000
C	-0.1614620000	-1.9436090000	0.0000000000
C	0.8313160000	-3.0940090000	0.0000000000
C	0.1614620000	-4.4569880000	0.0000000000
H	-0.8934560000	5.2668790000	0.0000000000
H	0.4730940000	4.5827170000	0.8810000000
H	0.4730940000	4.5827170000	-0.8810000000
H	-1.4849260000	3.0045060000	-0.8745100000
H	-1.4849260000	3.0045060000	0.8745100000
H	0.8165870000	2.0315690000	-0.8750300000
H	0.8165870000	2.0315690000	0.8750300000
H	-1.1515520000	0.4875230000	-0.8750580000
H	-1.1515520000	0.4875230000	0.8750580000
H	1.1515520000	-0.4875230000	-0.8750580000
H	1.1515520000	-0.4875230000	0.8750580000
H	-0.8165870000	-2.0315690000	-0.8750300000
H	-0.8165870000	-2.0315690000	0.8750300000
H	1.4849260000	-3.0045060000	-0.8745100000
H	1.4849260000	-3.0045060000	0.8745100000
H	-0.4730940000	-4.5827170000	-0.8810000000
H	0.8934560000	-5.2668790000	0.0000000000
H	-0.4730940000	-4.5827170000	0.8810000000

branched_oktane
26

C	0.0000000000	0.0000000000	0.7850770000
C	0.0000000000	0.0000000000	-0.7850770000
C	-0.8372550000	1.1548960000	1.3384700000
C	1.4187970000	0.1476360000	1.3384700000
C	-0.5815420000	-1.3025320000	1.3384700000
C	0.8372550000	1.1548960000	-1.3384700000
C	-1.4187970000	0.1476360000	-1.3384700000
C	0.5815420000	-1.3025320000	-1.3384700000
H	-0.5274160000	2.1199500000	0.9330490000
H	-1.8997390000	1.0242590000	1.1286450000
H	-0.7219640000	1.2048940000	2.4237940000
H	1.8369030000	1.1330930000	1.1286450000
H	1.4044510000	0.0227930000	2.4237940000
H	2.0996380000	-0.6032190000	0.9330490000
H	-1.5722220000	-1.5167300000	0.9330490000
H	0.0628360000	-2.1573510000	1.1286450000
H	-0.6824860000	-1.2276860000	2.4237940000
H	0.5274160000	2.1199500000	-0.9330490000
H	1.8997390000	1.0242590000	-1.1286450000
H	0.7219640000	1.2048940000	-2.4237940000
H	-1.8369030000	1.1330930000	-1.1286450000
H	-1.4044510000	0.0227930000	-2.4237940000
H	-2.0996380000	-0.6032190000	-0.9330490000
H	1.5722220000	-1.5167300000	-0.9330490000
H	-0.0628360000	-2.1573510000	-1.1286450000
H	0.6824860000	-1.2276860000	-2.4237940000

n_undecane
35

C	-0.0000000000	6.3450380000	-0.3789880000
C	-0.0000000000	5.0823900000	0.4649910000
C	-0.0000000000	3.8110060000	-0.3672980000
C	-0.0000000000	2.5407330000	0.4654110000
C	-0.0000000000	1.2703640000	-0.3675820000
C	-0.0000000000	0.0000000000	0.4653030000
C	-0.0000000000	-1.2703640000	-0.3675820000
C	-0.0000000000	-2.5407330000	0.4654110000
C	-0.0000000000	-3.8110060000	-0.3672980000
C	-0.0000000000	-5.0823900000	0.4649910000
C	-0.0000000000	-6.3450380000	-0.3789880000
H	-0.0000000000	7.2446090000	0.2395850000
H	0.8810110000	6.3857710000	-1.0246220000
H	-0.8810110000	6.3857710000	-1.0246220000
H	-0.8745170000	5.0800660000	1.1246890000
H	0.8745170000	5.0800660000	1.1246890000
H	-0.8750400000	3.8119030000	-1.0282810000
H	0.8750400000	3.8119030000	-1.0282810000
H	-0.8750510000	2.5406430000	1.1261520000
H	0.8750510000	2.5406430000	1.1261520000
H	-0.8750110000	1.2704030000	-1.0283270000
H	0.8750110000	1.2704030000	-1.0283270000
H	-0.8750100000	0.0000000000	1.1260810000
H	0.8750100000	-0.0000000000	1.1260810000
H	-0.8750110000	-1.2704030000	-1.0283270000
H	0.8750110000	-1.2704030000	-1.0283270000
H	-0.8750510000	-2.5406430000	1.1261520000
H	0.8750510000	-2.5406430000	1.1261520000
H	-0.8750400000	-3.8119030000	-1.0282810000
H	0.8750400000	-3.8119030000	-1.0282810000
H	-0.8745170000	-5.0800660000	1.1246890000
H	0.8745170000	-5.0800660000	1.1246890000
H	-0.8810110000	-6.3857710000	-1.0246220000
H	-0.0000000000	-7.2446090000	0.2395850000
H	0.8810110000	-6.3857710000	-1.0246220000

```
branched_undecane
35

 C       -0.0000000000        2.5638690000        0.6644410000
 C       -0.2071220000        1.3398980000       -0.2435140000
 C       -0.0000000000        0.0000000000        0.5880770000
 C        0.2071220000       -1.3398980000       -0.2435140000
 C       -0.0000000000       -2.5638690000        0.6644410000
 C        0.7816050000        1.5199830000       -1.3971640000
 C       -1.6246990000        1.4857480000       -0.8123520000
 C        1.2167240000        0.1798430000        1.5061700000
 C       -1.2167240000       -0.1798430000        1.5061700000
 C        1.6246990000       -1.4857480000       -0.8123520000
 C       -0.7816050000       -1.5199830000       -1.3971640000
 H        1.0411250000        2.6846400000        0.9638090000
 H       -0.2862660000        3.4630940000        0.1144810000
 H       -0.6111230000        2.5298680000        1.5675510000
 H        0.6111230000       -2.5298680000        1.5675510000
 H       -1.0411250000       -2.6846400000        0.9638090000
 H        0.2862660000       -3.4630940000        0.1144810000
 H        1.8178070000        1.4414110000       -1.0645050000
 H        0.6256670000        0.8074210000       -2.2054780000
 H        0.6535500000        2.5196740000       -1.8201820000
 H       -2.3746350000        1.5352220000       -0.0221800000
 H       -1.6854640000        2.4227190000       -1.3714940000
 H       -1.9034100000        0.6847960000       -1.4914620000
 H        2.0954080000        0.5417480000        0.9708590000
 H        0.9982850000        0.8880030000        2.3049680000
 H        1.4887590000       -0.7614270000        1.9839180000
 H       -2.0954080000       -0.5417480000        0.9708590000
 H       -0.9982850000       -0.8880030000        2.3049680000
 H       -1.4887590000        0.7614270000        1.9839180000
 H        2.3746350000       -1.5352220000       -0.0221800000
 H        1.6854640000       -2.4227190000       -1.3714940000
 H        1.9034100000       -0.6847960000       -1.4914620000
 H       -1.8178070000       -1.4414110000       -1.0645050000
 H       -0.6256670000       -0.8074210000       -2.2054780000
 H       -0.6535500000       -2.5196740000       -1.8201820000
```

C14H30_linear
44

C	-4.1655020000	7.1345060000	0.0000000000
C	-4.1790630000	5.6157540000	0.0000000000
C	-2.7859090000	5.0088000000	0.0000000000
C	-2.7859090000	3.4898780000	0.0000000000
C	-1.3928220000	2.8841740000	0.0000000000
C	-1.3929890000	1.3651560000	0.0000000000
C	0.0000690000	0.7595050000	0.0000000000
C	-0.0000690000	-0.7595050000	0.0000000000
C	1.3929890000	-1.3651560000	0.0000000000
C	1.3928220000	-2.8841740000	0.0000000000
C	2.7859090000	-3.4898780000	0.0000000000
C	2.7859090000	-5.0088000000	0.0000000000
C	4.1790630000	-5.6157540000	0.0000000000
C	4.1655020000	-7.1345060000	0.0000000000
H	-5.1759490000	7.5475530000	0.0000000000
H	-3.6479830000	7.5225080000	0.8809950000
H	-3.6479830000	7.5225080000	-0.8809950000
H	-4.7293630000	5.2520020000	-0.8744830000
H	-4.7293630000	5.2520020000	0.8744830000
H	-2.2335810000	5.3718430000	-0.8750070000
H	-2.2335810000	5.3718430000	0.8750070000
H	-3.3383860000	3.1275520000	-0.8750440000
H	-3.3383860000	3.1275520000	0.8750440000
H	-0.8402780000	3.2464100000	-0.8750080000
H	-0.8402780000	3.2464100000	0.8750080000
H	-1.9455250000	1.0028930000	-0.8750120000
H	-1.9455250000	1.0028930000	0.8750120000
H	0.5526110000	1.1217640000	-0.8750100000
H	0.5526110000	1.1217640000	0.8750100000
H	-0.5526110000	-1.1217640000	-0.8750100000
H	-0.5526110000	-1.1217640000	0.8750100000
H	1.9455250000	-1.0028930000	-0.8750120000
H	1.9455250000	-1.0028930000	0.8750120000
H	0.8402780000	-3.2464100000	-0.8750080000
H	0.8402780000	-3.2464100000	0.8750080000
H	3.3383860000	-3.1275520000	-0.8750440000
H	3.3383860000	-3.1275520000	0.8750440000
H	2.2335810000	-5.3718430000	-0.8750070000
H	2.2335810000	-5.3718430000	0.8750070000
H	4.7293630000	-5.2520020000	-0.8744830000
H	4.7293630000	-5.2520020000	0.8744830000
H	3.6479830000	-7.5225080000	-0.8809950000
H	5.1759490000	-7.5475530000	0.0000000000
H	3.6479830000	-7.5225080000	0.8809950000

C14H30_folded
44

C	0.9575780000	1.8254380000	0.0880150000
C	1.3004120000	1.0453580000	1.3455020000
C	0.5508850000	1.5226670000	2.5846200000
C	0.5508850000	0.5309240000	3.7484530000
C	-0.5508850000	-0.5309240000	3.7484530000
C	-0.5508850000	-1.5226670000	2.5846200000
C	-1.3004120000	-1.0453580000	1.3455020000
C	-0.9575780000	-1.8254380000	0.0880150000
C	-1.5753230000	-1.2382870000	-1.1693490000
C	-1.1329020000	-1.9320330000	-2.4464650000
C	-1.7058690000	-1.2907070000	-3.6979900000
C	1.5753230000	1.2382870000	-1.1693490000
C	1.1329020000	1.9320330000	-2.4464650000
C	1.7058690000	1.2907070000	-3.6979900000
H	1.2604860000	2.8730180000	0.1996200000
H	-0.1330880000	1.8417530000	-0.0298230000
H	1.0871630000	-0.0102520000	1.1641000000
H	2.3785130000	1.0971020000	1.5342070000
H	-0.4848690000	1.7622670000	2.3182170000
H	0.9927570000	2.4684360000	2.9137730000
H	1.5265720000	0.0320620000	3.7922990000
H	0.4607660000	1.0882110000	4.6856930000
H	-1.5265720000	-0.0320620000	3.7922990000
H	-0.4607660000	-1.0882110000	4.6856930000
H	0.4848690000	-1.7622670000	2.3182170000
H	-0.9927570000	-2.4684360000	2.9137730000
H	-1.0871630000	0.0102520000	1.1641000000
H	-2.3785130000	-1.0971020000	1.5342070000
H	0.1330880000	-1.8417530000	-0.0298230000
H	-1.2604860000	-2.8730180000	0.1996200000
H	-1.3095280000	-0.1760550000	-1.2318510000
H	-2.6686660000	-1.2696540000	-1.0950780000
H	-0.0382720000	-1.9198300000	-2.4966440000
H	-1.4201870000	-2.9881590000	-2.4051290000
H	-1.3970330000	-0.2451030000	-3.7775600000
H	-1.3748900000	-1.8036260000	-4.6030180000
H	-2.7985520000	-1.3099260000	-3.6855250000
H	1.3095280000	0.1760550000	-1.2318510000
H	2.6686660000	1.2696540000	-1.0950780000
H	0.0382720000	1.9198300000	-2.4966440000
H	1.4201870000	2.9881590000	-2.4051290000
H	1.3970330000	0.2451030000	-3.7775600000
H	1.3748900000	1.8036260000	-4.6030180000
H	2.7985520000	1.3099260000	-3.6855250000

C22H46_linear
68

C	-0.4164410000	6.9865440000	0.0000000000
C	0.4164510000	5.7162420000	0.0000000000
C	-0.4165310000	4.4459840000	0.0000000000
C	0.4163850000	3.1756970000	0.0000000000
C	-0.4165290000	1.9054110000	0.0000000000
C	0.4164410000	0.6351540000	0.0000000000
C	-0.4164410000	-0.6351540000	0.0000000000
C	0.4165290000	-1.9054110000	0.0000000000
C	-0.4163850000	-3.1756970000	0.0000000000
C	0.4165310000	-4.4459840000	0.0000000000
C	-0.4164510000	-5.7162420000	0.0000000000
C	0.4164410000	-6.9865440000	0.0000000000
C	-0.4165630000	-8.2567950000	0.0000000000
C	0.4163840000	-9.5271230000	0.0000000000
C	-0.4163480000	-10.7974370000	0.0000000000
C	0.4160650000	-12.0687900000	0.0000000000
C	-0.4278440000	-13.3315570000	0.0000000000
C	0.4165630000	8.2567950000	0.0000000000
C	-0.4163840000	9.5271230000	0.0000000000
C	0.4163480000	10.7974370000	0.0000000000
C	-0.4160650000	12.0687900000	0.0000000000
C	0.4278440000	13.3315570000	0.0000000000
H	-1.0771300000	6.9865670000	0.8750110000
H	-1.0771300000	6.9865670000	-0.8750110000
H	1.0771420000	5.7162020000	-0.8750090000
H	1.0771420000	5.7162020000	0.8750090000
H	-1.0772230000	4.4460040000	-0.8750080000
H	-1.0772230000	4.4460040000	0.8750080000
H	1.0770840000	3.1756980000	-0.8750060000
H	1.0770840000	3.1756980000	0.8750060000
H	-1.0772270000	1.9053890000	-0.8750060000
H	-1.0772270000	1.9053890000	0.8750060000
H	1.0771370000	0.6351820000	-0.8750070000
H	1.0771370000	0.6351820000	0.8750070000
H	-1.0771370000	-0.6351820000	-0.8750070000
H	-1.0771370000	-0.6351820000	0.8750070000
H	1.0772270000	-1.9053890000	-0.8750060000
H	1.0772270000	-1.9053890000	0.8750060000
H	-1.0770840000	-3.1756980000	-0.8750060000
H	-1.0770840000	-3.1756980000	0.8750060000
H	1.0772230000	-4.4460040000	-0.8750080000
H	1.0772230000	-4.4460040000	0.8750080000
H	-1.0771420000	-5.7162020000	-0.8750090000
H	-1.0771420000	-5.7162020000	0.8750090000
H	1.0771300000	-6.9865670000	-0.8750110000
H	1.0771300000	-6.9865670000	0.8750110000
H	-1.0772410000	-8.2567590000	-0.8750060000
H	-1.0772410000	-8.2567590000	0.8750060000
H	1.0770530000	-9.5270240000	-0.8750460000
H	1.0770530000	-9.5270240000	0.8750460000
H	-1.0772830000	-10.7982500000	-0.8750080000
H	-1.0772830000	-10.7982500000	0.8750080000
H	1.0757040000	-12.0662500000	-0.8744820000
H	1.0757040000	-12.0662500000	0.8744820000
H	-1.0733680000	-13.3723510000	-0.8809860000
H	0.1908000000	-14.2309290000	0.0000000000
H	-1.0733680000	-13.3723510000	0.8809860000
H	1.0772410000	8.2567590000	-0.8750060000
H	1.0772410000	8.2567590000	0.8750060000
H	-1.0770530000	9.5270240000	-0.8750460000
H	-1.0770530000	9.5270240000	0.8750460000
H	1.0772830000	10.7982500000	-0.8750080000
H	1.0772830000	10.7982500000	0.8750080000
H	-1.0757040000	12.0662500000	-0.8744820000
H	-1.0757040000	12.0662500000	0.8744820000
H	1.0733680000	13.3723510000	-0.8809860000
H	-0.1908000000	14.2309290000	0.0000000000
H	1.0733680000	13.3723510000	0.8809860000

C22H46_folded
68

C	2.0355120000	-0.1842100000	-2.6212890000
C	1.5813410000	0.5295710000	-3.8830700000
C	1.5813410000	-0.3572600000	-5.1237030000
C	0.7441120000	0.1782270000	-6.2859980000
C	-0.7441120000	-0.1782270000	-6.2859980000
C	-1.5813410000	0.3572600000	-5.1237030000
C	-1.5813410000	-0.5295710000	-3.8830700000
C	-2.0355120000	0.1842100000	-2.6212890000
C	-1.8563620000	-0.6499700000	-1.3641690000
C	-2.1384730000	0.1124070000	-0.0813800000
C	-1.8660870000	-0.6988970000	1.1733500000
C	-2.1021050000	0.0747470000	2.4586300000
C	-1.8226240000	-0.7354670000	3.7122570000
C	-2.0528240000	0.0394040000	4.9986320000
C	-1.7825040000	-0.7836220000	6.2456980000
C	1.8563620000	0.6499700000	-1.3641690000
C	2.1384730000	-0.1124070000	-0.0813800000
C	1.8660870000	0.6988970000	1.1733500000
C	2.1021050000	-0.0747470000	2.4586300000
C	1.8226240000	0.7354670000	3.7122570000
C	2.0528240000	-0.0394040000	4.9986320000
C	1.7825040000	0.7836220000	6.2456980000
H	3.0813190000	-0.4976020000	-2.7186950000
H	1.4563060000	-1.1097410000	-2.5140210000
H	0.5785880000	0.9259870000	-3.7099300000
H	2.2137600000	1.4055240000	-4.0654400000
H	1.2265050000	-1.3597990000	-4.8588200000
H	2.6159800000	-0.4928640000	-5.4540330000
H	0.8492180000	1.2690520000	-6.3285930000
H	1.1643260000	-0.1966140000	-7.2241120000
H	-0.8492180000	-1.2690520000	-6.3285930000
H	-1.1643260000	0.1966140000	-7.2241120000
H	-1.2265050000	1.3597990000	-4.8588200000
H	-2.6159800000	0.4928640000	-5.4540330000
H	-0.5785880000	-0.9259870000	-3.7099300000
H	-2.2137600000	-1.4055240000	-4.0654400000
H	-1.4563060000	1.1097410000	-2.5140210000
H	-3.0813190000	0.4976020000	-2.7186950000
H	-0.8257520000	-1.0229960000	-1.3336440000
H	-2.4955150000	-1.5390350000	-1.4135060000
H	-1.5221570000	1.0195200000	-0.0626850000
H	-3.1791730000	0.4568870000	-0.0769950000
H	-0.8291520000	-1.0546050000	1.1523380000
H	-2.4924720000	-1.5986270000	1.1696560000
H	-1.4727450000	0.9728710000	2.4599810000
H	-3.1375540000	0.4344940000	2.4821170000
H	-0.7873600000	-1.0955520000	3.6878270000
H	-2.4525690000	-1.6329680000	3.7127410000
H	-1.4158690000	0.9307410000	4.9988830000
H	-3.0841230000	0.4081620000	5.0165830000
H	-0.7502860000	-1.1414520000	6.2646860000
H	-1.9479570000	-0.2040630000	7.1559160000
H	-2.4345040000	-1.6598090000	6.2859980000
H	0.8257520000	1.0229960000	-1.3336440000
H	2.4955150000	1.5390350000	-1.4135060000
H	1.5221570000	-1.0195200000	-0.0626850000
H	3.1791730000	-0.4568870000	-0.0769950000
H	0.8291520000	1.0546050000	1.1523380000
H	2.4924720000	1.5986270000	1.1696560000
H	1.4727450000	-0.9728710000	2.4599810000
H	3.1375540000	-0.4344940000	2.4821170000
H	0.7873600000	1.0955520000	3.6878270000
H	2.4525690000	1.6329680000	3.7127410000
H	1.4158690000	-0.9307410000	4.9988830000
H	3.0841230000	-0.4081620000	5.0165830000
H	0.7502860000	1.1414520000	6.2646860000
H	1.9479570000	0.2040630000	7.1559160000
H	2.4345040000	1.6598090000	6.2859980000

C30H62_linear
92

C	-0.4281720000	-18.4125220000	0.0000000000
C	0.4158710000	-17.1498560000	0.0000000000
C	-0.4164180000	-15.8784370000	0.0000000000
C	0.4163810000	-14.6081840000	0.0000000000
C	-0.4165170000	-13.3378360000	0.0000000000
C	0.4164800000	-12.0675980000	0.0000000000
C	-0.4164220000	-10.7973080000	0.0000000000
C	0.4165270000	-9.5270520000	0.0000000000
C	-0.4163830000	-8.2567730000	0.0000000000
C	0.4165420000	-6.9865040000	0.0000000000
C	-0.4163800000	-5.7162330000	0.0000000000
C	0.4165270000	-4.4459540000	0.0000000000
C	-0.4164060000	-3.1756900000	0.0000000000
C	0.4164910000	-1.9054040000	0.0000000000
C	-0.4164470000	-0.6351440000	0.0000000000
C	0.4164470000	0.6351440000	0.0000000000
C	-0.4164910000	1.9054040000	0.0000000000
C	0.4164060000	3.1756900000	0.0000000000
C	-0.4165270000	4.4459540000	0.0000000000
C	0.4163800000	5.7162330000	0.0000000000
C	-0.4165420000	6.9865040000	0.0000000000
C	0.4163830000	8.2567730000	0.0000000000
C	-0.4165270000	9.5270520000	0.0000000000
C	0.4164220000	10.7973080000	0.0000000000
C	-0.4164800000	12.0675980000	0.0000000000
C	0.4165170000	13.3378360000	0.0000000000
C	-0.4163810000	14.6081840000	0.0000000000
C	0.4164180000	15.8784370000	0.0000000000
C	-0.4158710000	17.1498560000	0.0000000000
C	0.4281720000	18.4125220000	0.0000000000
H	0.1903530000	-19.3119650000	0.0000000000
H	-1.0736950000	-18.4532300000	0.8809800000
H	-1.0736950000	-18.4532300000	-0.8809800000
H	1.0755020000	-17.1473850000	-0.8744750000
H	1.0755020000	-17.1473850000	0.8744750000
H	-1.0773490000	-15.8792000000	-0.8750010000
H	-1.0773490000	-15.8792000000	0.8750010000
H	1.0770430000	-14.6081120000	-0.8750390000
H	1.0770430000	-14.6081120000	0.8750390000
H	-1.0771880000	-13.3377900000	-0.8750010000
H	-1.0771880000	-13.3377900000	0.8750010000
H	1.0771590000	-12.0676100000	-0.8750060000
H	1.0771590000	-12.0676100000	0.8750060000
H	-1.0771080000	-10.7972900000	-0.8750020000
H	-1.0771080000	-10.7972900000	0.8750020000
H	1.0772140000	-9.5270590000	-0.8750020000
H	1.0772140000	-9.5270590000	0.8750020000
H	-1.0770730000	-8.2567680000	-0.8750000000
H	-1.0770730000	-8.2567680000	0.8750000000
H	1.0772320000	-6.9865030000	-0.8750010000
H	1.0772320000	-6.9865030000	0.8750010000
H	-1.0770720000	-5.7162370000	-0.8750000000
H	-1.0770720000	-5.7162370000	0.8750000000
H	1.0772180000	-4.4459460000	-0.8750000000
H	1.0772180000	-4.4459460000	0.8750000000
H	-1.0770980000	-3.1757000000	-0.8750000000
H	-1.0770980000	-3.1757000000	0.8750000000
H	1.0771830000	-1.9053930000	-0.8750000000
H	1.0771830000	-1.9053930000	0.8750000000
H	-1.0771390000	-0.6351560000	-0.8750000000
H	-1.0771390000	-0.6351560000	0.8750000000
H	1.0771390000	0.6351560000	-0.8750000000
H	1.0771390000	0.6351560000	0.8750000000
H	-1.0771830000	1.9053930000	-0.8750000000
H	-1.0771830000	1.9053930000	0.8750000000
H	1.0770980000	3.1757000000	-0.8750000000
H	1.0770980000	3.1757000000	0.8750000000
H	-1.0772180000	4.4459460000	-0.8750000000
H	-1.0772180000	4.4459460000	0.8750000000
H	1.0770720000	5.7162370000	-0.8750000000
H	1.0770720000	5.7162370000	0.8750000000
H	-1.0772320000	6.9865030000	-0.8750010000
H	-1.0772320000	6.9865030000	0.8750010000
H	1.0770730000	8.2567680000	-0.8750000000
H	1.0770730000	8.2567680000	0.8750000000
H	-1.0772140000	9.5270590000	-0.8750020000
H	-1.0772140000	9.5270590000	0.8750020000
H	1.0771080000	10.7972900000	-0.8750020000

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H        1.0771080000       10.7972900000        0.8750020000
H       -1.0771590000       12.0676100000       -0.8750060000
H       -1.0771590000       12.0676100000        0.8750060000
H        1.0771880000       13.3377900000       -0.8750010000
H        1.0771880000       13.3377900000        0.8750010000
H       -1.0770430000       14.6081120000       -0.8750390000
H       -1.0770430000       14.6081120000        0.8750390000
H        1.0773490000       15.8792000000       -0.8750010000
H        1.0773490000       15.8792000000        0.8750010000
H       -1.0755020000       17.1473850000       -0.8744750000
H       -1.0755020000       17.1473850000        0.8744750000
H        1.0736950000       18.4532300000       -0.8809800000
H       -0.1903530000       19.3119650000        0.0000000000
H        1.0736950000       18.4532300000        0.8809800000
```

C30H62_folded
92

C	2.0005820000	-0.4217150000	-5.1586380000
C	1.6325990000	0.3400300000	-6.4204530000
C	1.5275770000	-0.5413390000	-7.6605250000
C	0.7599670000	0.0889650000	-8.8233420000
C	-0.7599670000	-0.0889650000	-8.8233420000
C	-1.5275770000	0.5413390000	-7.6605250000
C	-1.6325990000	-0.3400300000	-6.4204530000
C	-2.0005820000	0.4217150000	-5.1586380000
C	-1.9179500000	-0.4266210000	-3.9009180000
C	-2.1130280000	0.3643820000	-2.6192990000
C	-1.9289450000	-0.4683610000	-1.3625820000
C	-2.0835260000	0.3297610000	-0.0799790000
C	-1.8868370000	-0.4993400000	1.1770580000
C	-2.0506040000	0.2987710000	2.4586040000
C	-1.8627820000	-0.5300730000	3.7171180000
C	1.9179500000	0.4266210000	-3.9009180000
C	2.1130280000	-0.3643820000	-2.6192990000
C	1.9289450000	0.4683610000	-1.3625820000
C	2.0835260000	-0.3297610000	-0.0799790000
C	1.8868370000	0.4993400000	1.1770580000
C	2.0506040000	-0.2987710000	2.4586040000
C	1.8627820000	0.5300730000	3.7171180000
C	2.0389310000	-0.2670600000	4.9976940000
C	1.8580810000	0.5619880000	6.2570120000
C	-2.0389310000	0.2670600000	4.9976940000
C	-1.8580810000	-0.5619880000	6.2570120000
C	-2.0344020000	0.2353470000	7.5381520000
C	2.0344020000	-0.2353470000	7.5381520000
C	1.8580810000	0.6044690000	8.7908300000
C	-1.8580810000	-0.6044690000	8.7908300000
H	3.0032970000	-0.8536840000	-5.2555180000
H	1.3184040000	-1.2742760000	-5.0520780000
H	0.6835160000	0.8516790000	-6.2469780000
H	2.3634560000	1.1354880000	-6.6037860000
H	1.0561040000	-1.4944750000	-7.3951110000
H	2.5388810000	-0.7990180000	-7.9904610000
H	0.9933180000	1.1596960000	-8.8662740000
H	1.1330780000	-0.3333140000	-9.7612130000
H	-0.9933180000	-1.1596960000	-8.8662740000
H	-1.1330780000	0.3333140000	-9.7612130000
H	-1.0561040000	1.4944750000	-7.3951110000
H	-2.5388810000	0.7990180000	-7.9904610000
H	-0.6835160000	-0.8516790000	-6.2469780000
H	-2.3634560000	-1.1354880000	-6.6037860000
H	-1.3184040000	1.2742760000	-5.0520780000
H	-3.0032970000	0.8536840000	-5.2555180000
H	-0.9361970000	-0.9138230000	-3.8692860000
H	-2.6535790000	-1.2376700000	-3.9500800000
H	-1.4014140000	1.1989340000	-2.6034340000
H	-3.1098490000	0.8205540000	-2.6144440000
H	-0.9354220000	-0.9317280000	-1.3815170000
H	-2.6469390000	-1.2968550000	-1.3645980000
H	-1.3664430000	1.1595740000	-0.0822890000
H	-3.0770680000	0.7928870000	-0.0573660000
H	-0.8899490000	-0.9548250000	1.1582250000
H	-2.5983590000	-1.3334780000	1.1763710000
H	-1.3357380000	1.1303640000	2.4617060000
H	-3.0454000000	0.7595900000	2.4735460000
H	-0.8651030000	-0.9837850000	3.7068870000
H	-2.5727550000	-1.3654970000	3.7099110000
H	2.6535790000	1.2376700000	-3.9500800000
H	0.9361970000	0.9138230000	-3.8692860000
H	3.1098490000	-0.8205540000	-2.6144440000
H	1.4014140000	-1.1989340000	-2.6034340000
H	2.6469390000	1.2968550000	-1.3645980000
H	0.9354220000	0.9317280000	-1.3815170000
H	3.0770680000	-0.7928870000	-0.0573660000
H	1.3664430000	-1.1595740000	-0.0822890000
H	2.5983590000	1.3334780000	1.1763710000
H	0.8899490000	0.9548250000	1.1582250000
H	3.0454000000	-0.7595900000	2.4735460000
H	1.3357380000	-1.1303640000	2.4617060000
H	2.5727550000	1.3654970000	3.7099110000
H	0.8651030000	0.9837850000	3.7068870000
H	3.0350660000	-0.7251840000	5.0051940000
H	1.3263640000	-1.1005390000	5.0066070000
H	2.5707010000	1.3953360000	6.2485270000
H	0.8618580000	1.0192970000	6.2504360000

H	-3.0350660000	0.7251840000	5.0051940000
H	-1.3263640000	1.1005390000	5.0066070000
H	-2.5707010000	-1.3953360000	6.2485270000
H	-0.8618580000	-1.0192970000	6.2504360000
H	-3.0276770000	0.6971710000	7.5403930000
H	-1.3185300000	1.0646140000	7.5457190000
H	1.3185300000	-1.0646140000	7.5457190000
H	3.0276770000	-0.6971710000	7.5403930000
H	0.8629040000	1.0542710000	8.8258290000
H	1.9835860000	0.0091390000	9.6972530000
H	2.5872850000	1.4178850000	8.8234430000
H	-2.5872850000	-1.4178850000	8.8234430000
H	-0.8629040000	-1.0542710000	8.8258290000
H	-1.9835860000	-0.0091390000	9.6972530000