Supporting Information: Accurate Treatment of Energetics and Geometry of Carbon and Hydrocarbon Compounds within Tight-Binding Model

Autor: Alexander A. Voityuk

Table SI1. Experimental and calculated heats of formation of hydrocarbons, in kcal/mol

MOLECULE	EXP.	PNTB[a]	TB[b]
HYDROGEN	0.0	-5.3	-7.5
CH	142.4	131.8	135.2
CH3 RADICAL	34.8	39.6	19.5
METHANE	-17.8	-10.7	-43.2
C2H5 RADICAL	28.0	32.6	-3.3
ETHANE	-20.0	-16.6	-61.6
CH2=CH RADICAL	63.4	69.2	31.4
ETHYLENE	12.5	12.6	-29.5
HCC RADICAL	123.0	114.7	75.8
ACETYLENE	54.5	46.1	-3.6
N-C3H7 RADICAL	24.0	27.0	-19.2
I-C3H7 RADICAL	22.3	25.7	-23.2
PROPANE	-25.0	-22.7	-77.8
PROPENE	4.8	6.0	-46.6
PROPYNE	44.2	39.1	-24.7
C3H5 RADICAL	39.0	38.9	-4.2
ALLENE	45.5	40.7	-15.0
N-C4H9 RADICAL	18.0	20.5	-36.0
S-C4H9 RADICAL	17.0	19.7	-38.8

T-C4H9 RADICAL	11.0	19.2	-40.2
N-BUTANE	-30.0	-28.9	-93.9
ISOBUTANE	-32.1	-28.9	-91.7
1-BUTENE	0.0	0.5	-61.8
TRANS-2-BUTENE	-2.7	-0.3	-63.2
CIS-2-BUTENE	-1.7	0.4	-62.4
ISOBUTENE	-4.0	-0.6	-61.3
1,2-BUTADIENE	38.8	34.6	-31.7
1,3-TRANS-BUTADIENE	26.3	24.5	-34.0
1-BUTYNE	39.5	33.1	-40.4
2-BUTYNE	34.8	32.7	-45.1
N-PENTANE	-35.1	-35.0	-110.0
NEOPENTANE	-40.2	-35.1	-103.4
TRANS-1,3-PENTADIENE	18.2	18.0	-51.0
CIS-1,3-PENTADIENE	19.5	18.7	-51.0
1,4-PENTADIENE	25.2	23.6	-46.1
N-HEXANE	-39.9	-41.2	-126.1
2,2,3,3-TETRAMETHYLBUTANE	-56.2	-50.6	-142.7
2,2,3,3-TETRAMETHYLPENTANE	-56.7	-55.7	-158.1
N-DECANE	-59.6	-65.7	-190.5
TRI-T-BUTHYLMETHANE	-56.2	-63.3	-197.5
CYCLOPROPYL RADICAL	66.9	76.3	51.0
CYCLOPROPANE	12.7	18.1	-16.1
CIS-DIMETHYLCYCLOPROPANE	1.3	6.2	-47.7

CYCLOPROPENE	66.2	70.3	39.6
1-METHYLCYCLOPROPENE	58.2	64.4	21.2
METHYLENECYCLOPROPANE	47.9	48.5	5.0
CYCLOBUTANE	6.8	1.2	-34.2
CYCLOBUTENE	37.5	37.6	8.9
1,2-DIMETHYLCYCLOBUTENE	19.8	26.8	-23.3
METHYLENECYCLOBUTANE	29.0	25.2	-17.9
CYCLOPENTANE	-18.3	-24.2	-74.8
CYCLOPENTENE	8.1	5.0	-41.7
C-C5H5 RADICAL	58.0	59.0	28.3
CYCLOPENTADIENE	32.1	33.5	-7.3
3,4-DIMETHYLENECYCLOBUTENE	80.4	82.9	39.7
FULVENE	53.5	49.5	4.4
CYCLOHEXANE, CHAIR	-29.5	-35.8	-97.4
CYCLOHEXENE, HALF CHAIR	-1.2	-6.3	-66.4
1,3-CYCLOHEXADIENE	25.4	20.9	-36.8
C6H5 RADICAL	79.0	80.6	36.5
BENZENE	19.7	19.8	-30.7
C6H5CH2 RADICAL	49.0	47.5	-4.1
TOLUENE	12.0	13.8	-44.9
ETHYLBENZENE	7.1	7.9	-61.0
STYRENE	35.3	33.2	-32.5
INDENE	39.1	40.7	-7.6
MESITELENE	-3.8	1.9	-73.2
NAPHTHALENE	35.9	35.5	-20.4

ANTHRACENE	55.2	53.6	-7.5
PHENANTRENE	49.0	49.3	-12.2
AZULENE	73.5	62.0	9.0
BIPHENYLENE	100.5	102.4	59.9
CYCLOHEPTATRIENE	43.2	38.0	-26.0
BICYCLOBUTANE	51.9	66.0	46.4
TRANS-BICYCLOPROPYL	30.9	40.7	-1.8
BICYCLO[2.1.0]PENTANE	37.8	38.3	14.9
SPIROCYCLOPENTANE	44.3	53.9	21.2
NORBORNANE	-13.1	-23.2	-62.2
NORBORNADIENE	58.8	46.2	17.0
CYCLO[2,2,2]-OCTANE	-23.6	-37.6	-91.9
ADAMANTANE	-32.2	-48.9	-95.0
CUBANE	148.7	124.6	171.5
C60	634.8	630.5	975.3
Mean error (83 comparisons)		-0.632	-47.671
Mean absolute error		4.588	56.426

[a] Suggested model
[b] TB method developed by Zhao and Lu (Zhao J.; Lu, J.P. *Phys. Lett. A* **2003**, *319*, 523)

Table SI2. Bond lengths (Å) and bond angles (degrees)

MOLECULE	VARIABLE	EXP.	PNTB
HYDROGEN	H-H	0.741	0.760
METHANE	C-H	1.087	1.091
ETHANE	C-C	1.535	1.499
	C-H	1.094	1.093
	HCC	111.2	110.3
ETHYLENE	C=C	1.339	1.319
	C-H	1.087	1.082
	HCC	121.3	122.3
ACETYLENE	C-H	1.063	1.052
	C#C	1.202	1.206
PROPANE	C-C	1.526	1.500
	C1-H4	1.089	1.093
	C1-H5	1.094	1.093
	C2-H7	1.096	1.095
	CCC	112.4	110.7
	H7C2H8	106.1	107.8
	H4C1C2	111.8	111.1
	H5C1H6	107.3	108.5
PROPENE	C=C	1.336	1.321
	C-C	1.501	1.478
	C1-H4	1.081	1.082
	C1-H5	1.091	1.083
	C2-H6	1.090	1.084
	C3-H7	1.085	1.093
	C3-H8	1.098	1.097
	CCC	124.3	123.4
	H4C1C2	121.5	123.1
	H5C1C2	120.5	121.5
	H6C2C1	119.0	121.1
	H7C3C2	111.2	110.1
	H8C3H9	106.2	107.4
PROPYNE	C#C	1.206	1.207
	C-C	1.459	1.434
	C1-H	1.056	1.053
	C3-H	1.105	1.099
	C2C3H	110.2	111.2

ALLENE	C=C	1.308	1.300
	C-H	1.087	1.087
	HCH	118.2	114.2
n-BUTANE	C1-C2	1.531	1.499
	C2-C3	1.531	1.502
	CCC	113.8	111.4
ISOBUTANE	C-C	1.525	1.502
	CCC	111.2	110.0
TRANS-2-BUTENE	C-C	1.508	1.478
	C=C	1.347	1.323
	CCC	123.8	124.0
ISOBUTENE	C=C	1.342	1.323
	C-C	1.508	1.479
	CCC	122.2	122.4
1,3-TRANS-BUTADIENE	C=C	1.348	1.331
	C-C	1.468	1.436
	CCC	124.3	124.3
2-BUTYNE	C-C	1.468	1.437
	C#C	1.214	1.207
	C-H	1.116	1.099
	HCC	110.7	111.3
VINYLACETYLENE	C#C	1.215	1.212
	C-C	1.434	1.403
	C=C	1.344	1.332
	C2C3C4	123.1	124.8
DIACETYLENE	C#C	1.218	1.217
	C-C	1.384	1.353
	C-H	1.046	1.051
BUTATRIENE	C1=C2	1.318	1.313
	C2=C3	1.283	1.265
	C1-H	1.083	1.086
NEOPENTANE	C-C	1.539	1.504
	C-H	1.120	1.093
	HCC	110.0	110.1
CYCLOPROPANE	C-C	1.510	1.506
	C-H	1.074	1.076
	HCH	115.9	116.3

CYCLOPROPENE	C=C	1.296	1.302
	C-C	1.509	1.526
	C1-H	1.072	1.058
	C3-H	1.088	1.081
	HC1C2	149.9	153.1
	HC3H	114.6	116.3
CYCLOBUTANE	C-C	1.554	1.529
	C-H	1.109	1.088
	HCH	106.4	109.9
CYCLOBUTENE	C=C	1.342	1.333
	C-C	1.517	1.512
	C-C	1.566	1.552
	C1-H	1.083	1.074
	C3-H	1.094	1.088
	HC1C2	133.5	135.4
	HC3H	109.2	110.6
CYCLOPENTANE	C-C	1.546	1.518
	C-H	1.114	1.093
	HCC	111.7	110.1
CYCLOPENTADIENE	C=C	1.345	1.339
	C2-C3	1.468	1.462
	C1-C5	1.506	1.498
FULVENE	C1-C2	1.470	1.459
	C2=C3	1.355	1.354
	C3-C4	1.476	1.456
	C1=C6	1.349	1.334
CYCLOHEXANE, CHAIR	C-C	1.536	1.503
	C-H	1.121	1.094
	HCH	107.5	108.1
CYCLOHEXENE, HALF CHAIR	C=C	1.335	1.323
	C2-C3	1.504	1.483
	C3-C4	1.515	1.504
	C4-C5	1.550	1.501
BENZENE	C-C	1.397	1.385
	C-H	1.083	1.083
NAPHTHALENE	C1-C2	1.381	1.368
	C2-C3	1.417	1.403
	C1-C9	1.422	1.407
	C9-C10	1.412	1.419

BICYCLOBUTANE	C1-C2	1.498	1.495
	C1-C3	1.497	1.557
	C1-H	1.071	1.059
	C2-Heq	1.093	1.082
	C2-Hax	1.093	1.085
BICYCLO[2.1.0]PENTANE	C1-C2	1.528	1.506
	C2-C3	1.565	1.538
	C1-C4	1.536	1.549
	C1-C5	1.507	1.498
SPIROCYCLOPENTANE	C1-C2	1.469	1.472
	C2-C3	1.519	1.537
	C2-H	1.091	1.078
	HC2H	118.4	116.1
NORBORNANE	C1-C2	1.536	1.515
	C2-C3	1.573	1.516
	C1-C7	1.546	1.523
NORBORNADIENE	C1-C2	1.535	1.520
	C2=C3	1.343	1.327
	C1-C7	1.573	1.531

Mean error (100 bond lengths)	-0.012
Mean Absolute error	0.015
Mean error (31 bond angles)	0.31
Mean absolute error	1.39