

# Support Information for

**Theoretical Study on the Enthalpies of Formation of C<sub>40</sub>H<sub>56</sub>**

**Carotenes**

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Table s1.  $\Delta H_f$  of polyenes predicted using parametrized additivity method, and AE and GE schemes with semiempirical theories, and theories with minimum basis sets. Values for the test set molecules are in deviations from G3 with atomization scheme.

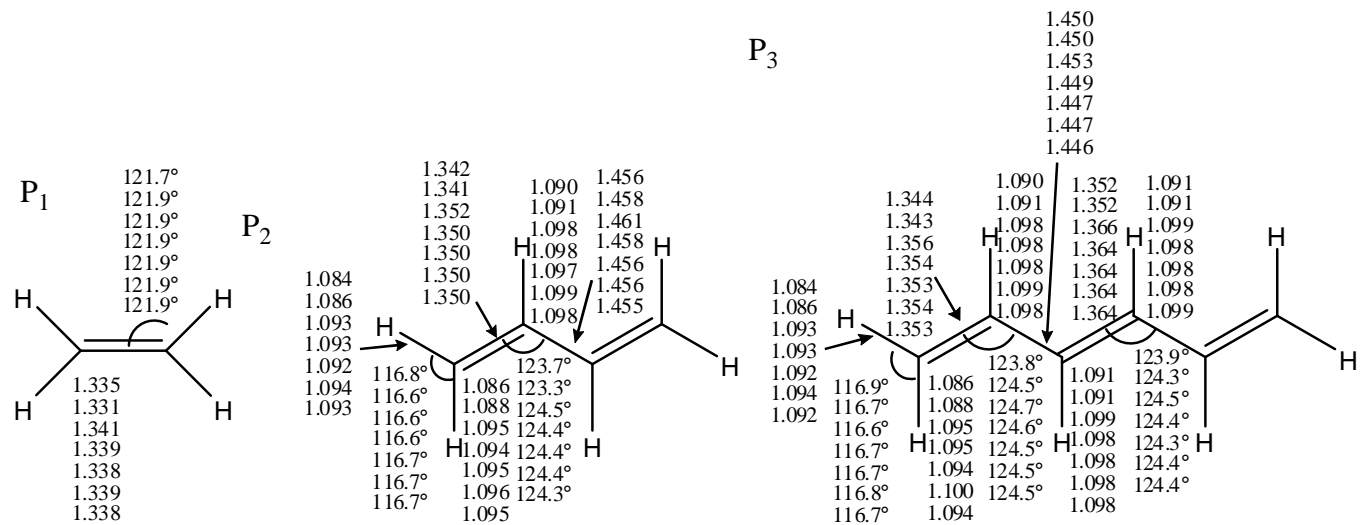
	AE						GE				
	$C_n H_m \rightarrow n C_2 H_4 + m C_2 H_6$						$C_n H_m + l CH_4 \rightarrow \frac{1}{2}(3n - m - l) C_2 H_4 + \frac{1}{2}(m - 2n + 2l) C_2 H_6$				
	Leal <sup>a</sup>	HF <sup>b</sup>	MP2 <sup>b</sup>	B3LYP <sup>b</sup>	AM1	PM3	HF <sup>b</sup>	MP2 <sup>b</sup>	B3LYP <sup>b</sup>	AM1	PM3
P <sub>2</sub>	-0.64	15.55	9.44	12.83	1.90	2.75	0.40	0.15	0.14	0.09	0.17
P <sub>3</sub>	-0.47	12.21	6.63	10.26	0.61	1.35	0.23	0.20	0.37	-0.82	-0.69
P <sub>4</sub>	-0.08	8.94	3.74	7.48	1.50	2.23	0.13	0.18	0.39	0.45	0.74
P <sub>5</sub>	0.48	5.79	0.92	4.70	0.99	1.48	0.16	0.23	0.41	0.32	0.52
P <sub>6</sub>	1.03	2.62	-1.95	1.83	0.62	0.88	0.17	0.23	0.34	0.32	0.46
P <sub>7</sub>	1.50	-0.63	-4.91	-1.16	0.07	0.09	0.10	0.14	0.14	0.16	0.21
P <sub>8</sub>	1.97	-3.88	-7.87	-4.16	-0.61	-0.77	0.03	0.05	-0.06	-0.14	-0.11
P <sub>9</sub>	2.58	-6.99	-10.70	-7.05	-1.12	-1.53	0.09	0.09	-0.15	-0.27	-0.33
C <sub>5</sub> H <sub>8</sub>	-0.55	7.97	3.82	6.81	-0.69	0.35	-1.19	-0.95	-1.10	-1.78	-1.21
C <sub>3</sub> H <sub>10</sub>	0.76	-0.46	-2.13	-0.18	0.46	-0.26	-0.79	-0.74	-1.33	0.42	-0.31
C <sub>6</sub> H <sub>12</sub>	0.61	-3.20	-3.15	-0.94	-0.89	0.91	2.47	2.76	2.69	-0.22	1.88
C <sub>6</sub> H <sub>10</sub>	-1.19	2.68	-0.42	2.54	2.45	0.38	-0.48	-0.68	-0.59	2.08	-0.16
C <sub>10</sub> H <sub>16</sub>	-1.34	-13.38	-13.27	-10.33	-2.12	-3.31	-1.35	-1.63	-1.10	-0.69	-1.26
AAD	0.97	7.38	5.30	5.41	1.07	1.25	0.58	0.62	0.68	0.59	0.61
$\mathcal{E}_C / \mathcal{E}_{CH_4}$ <sup>c</sup>	-37.40164	-37.46600	-37.64021	-4.71122	-4.35643	-39.69763	-39.75137	-40.00415	-6.71680	-6.61369	
$\mathcal{E}_H / \mathcal{E}_{C_2H_4}$ <sup>c</sup>	-0.580174	-0.57553	-0.59636	-0.50213	-0.56537	-77.09477	-77.21474	-77.64120	-11.42749	-10.96936	
$\mathcal{E}_{C_2H_6}$ <sup>c</sup>						-78.26918	-78.37563	-78.84472	-12.43343	-12.10249	
lycopene <sup>d</sup>	87.26	-9.78	4.66	13.44	74.24	65.95	94.04	90.17	98.46	86.62	83.61

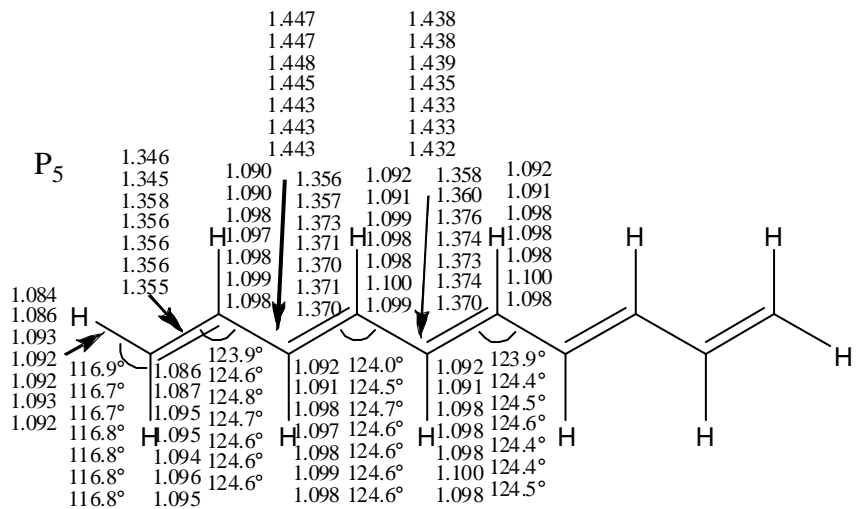
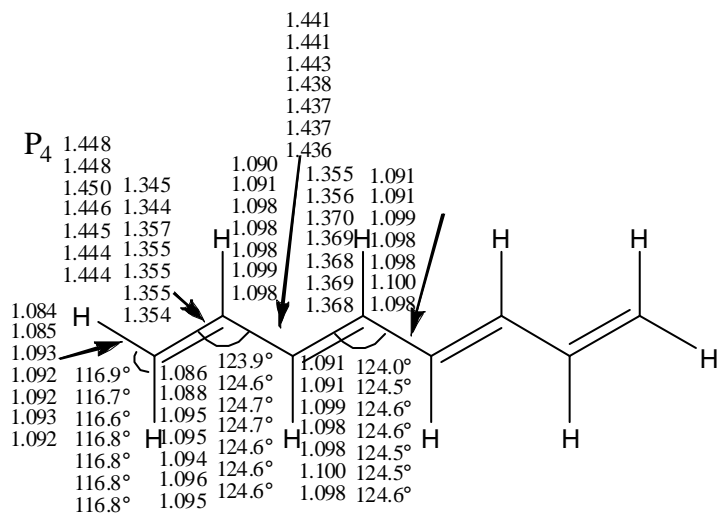
<sup>a</sup> Empirical parameters from ref. 36. <sup>b</sup> Using the STO-3G basis set. <sup>c</sup> In hartrees. <sup>d</sup> In kcal/mol.

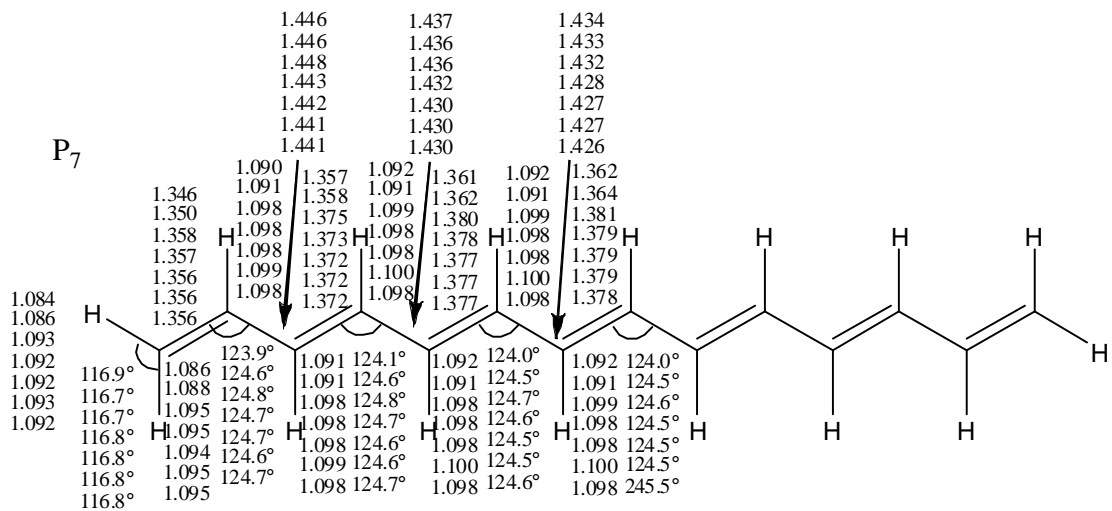
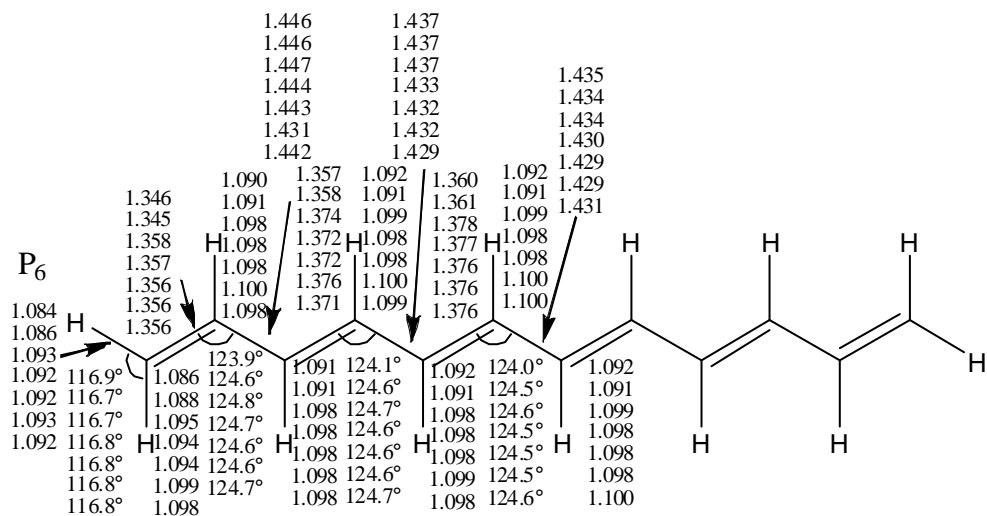
Table s2.  $\Delta H_f$  of small molecules predicted using atomization scheme, the results in parentheses are the deviations from experimental values.

	Expt.	G3	G2	G3MP2B3
CH <sub>4</sub>	-17.9 ± 0.1	-18.13 (-0.2)	-18.60 (-0.7)	-17.59 (0.3)
C <sub>2</sub> H <sub>4</sub>	12.5 ± 0.1	12.33 (-0.2)	12.77 (0.3)	11.80 (-0.7)
C <sub>2</sub> H <sub>6</sub>	-20.08 ± 0.04	-20.39 (-0.31)	-20.58 (-0.50)	-19.47 (0.61)
C <sub>4</sub> H <sub>6</sub>	26.3 ± 0.2	26.65 (0.4)	28.03 (1.7)	25.30 (-1.0)

Figure s1. Geometrical parameters of  $P_n$  ( $n=1\sim 9$ ) optimized at MP2(Full) and DFT using 6-31G(d). The first to seventh entries are results obtained from MP2, B3LYP, BLYP, BPW91, MPWPW91, PBEPBE, and BB95 methods, respectively.







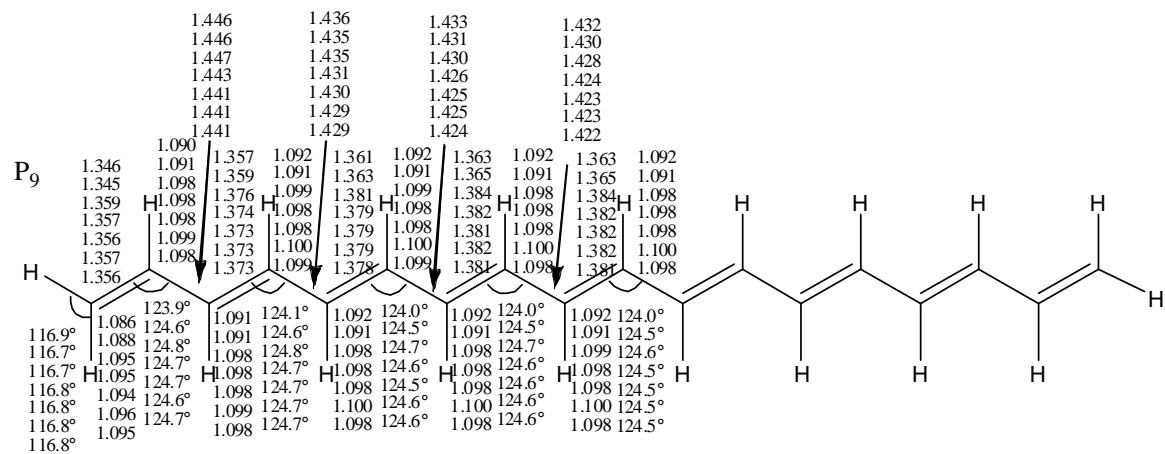
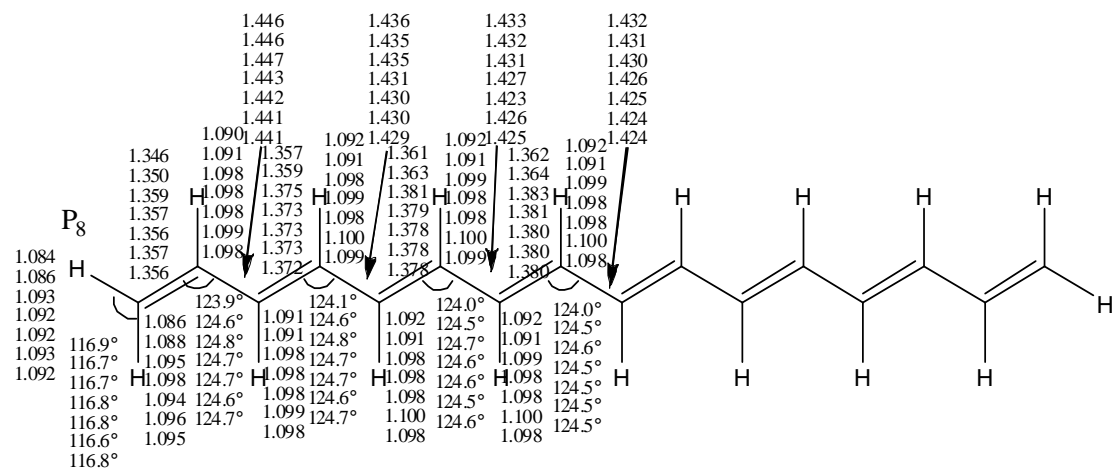
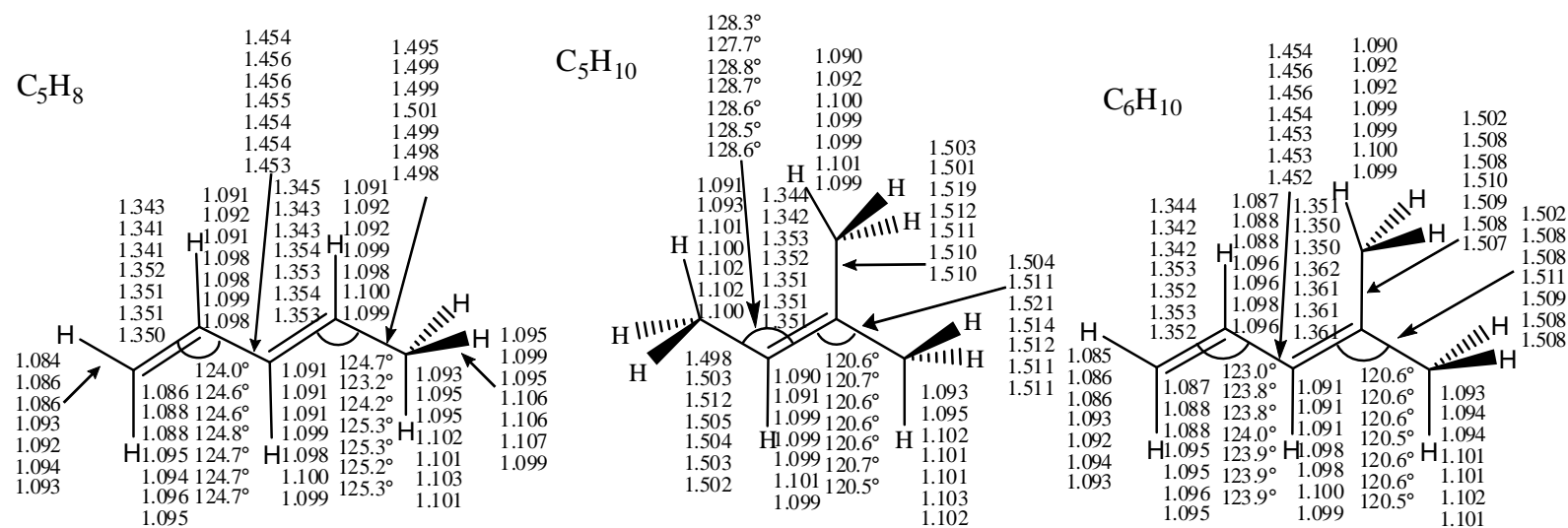






Figure s2. Geometrical parameters of alkenes optimized at MP2(Full) and DFT using 6-31G(*d*). The first to seventh entries are results obtained from MP2, B3LYP, BLYP, BPW91, MPWPW91, PBEPBPE, and BB95 methods, respectively.



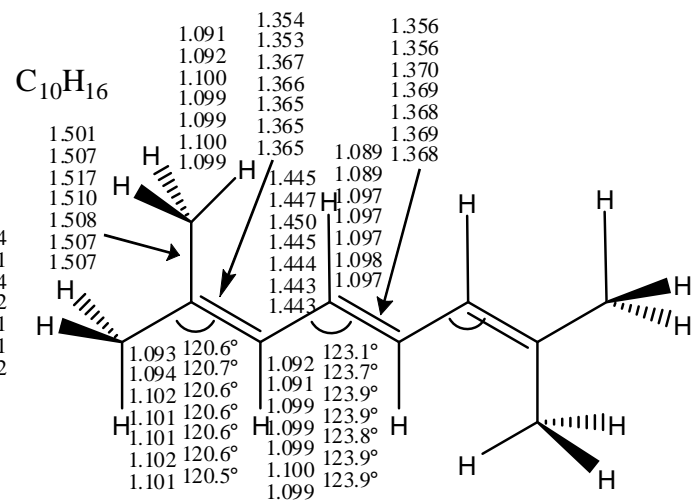
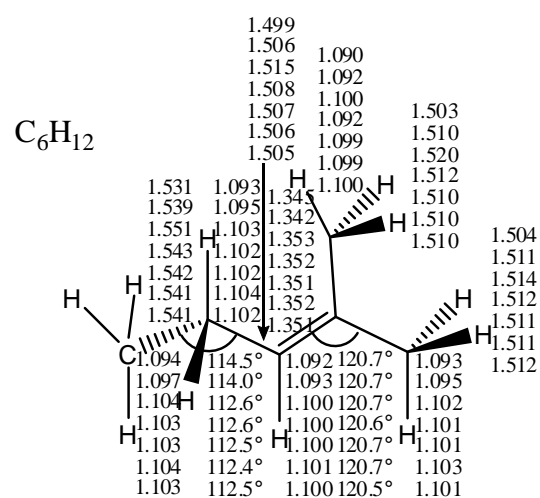
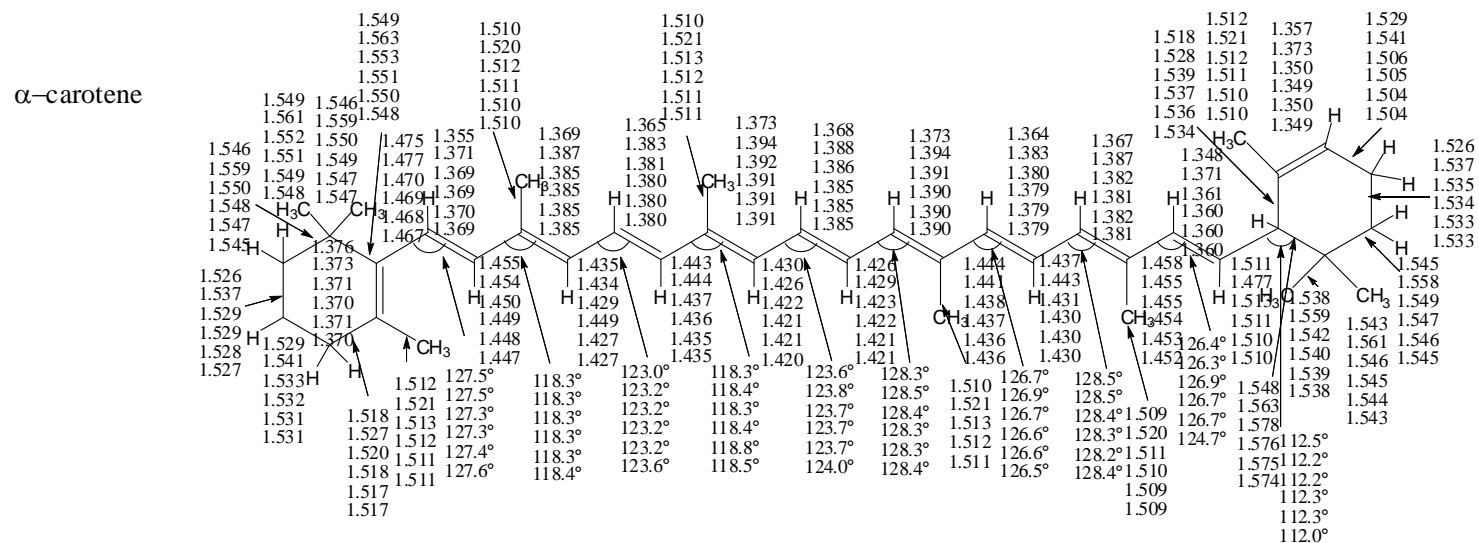
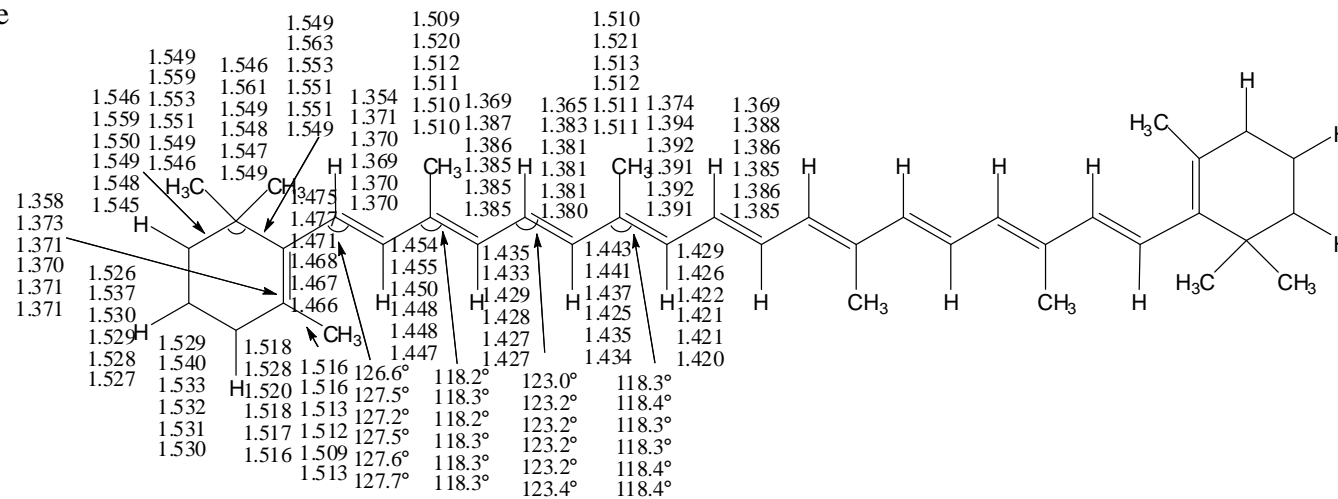


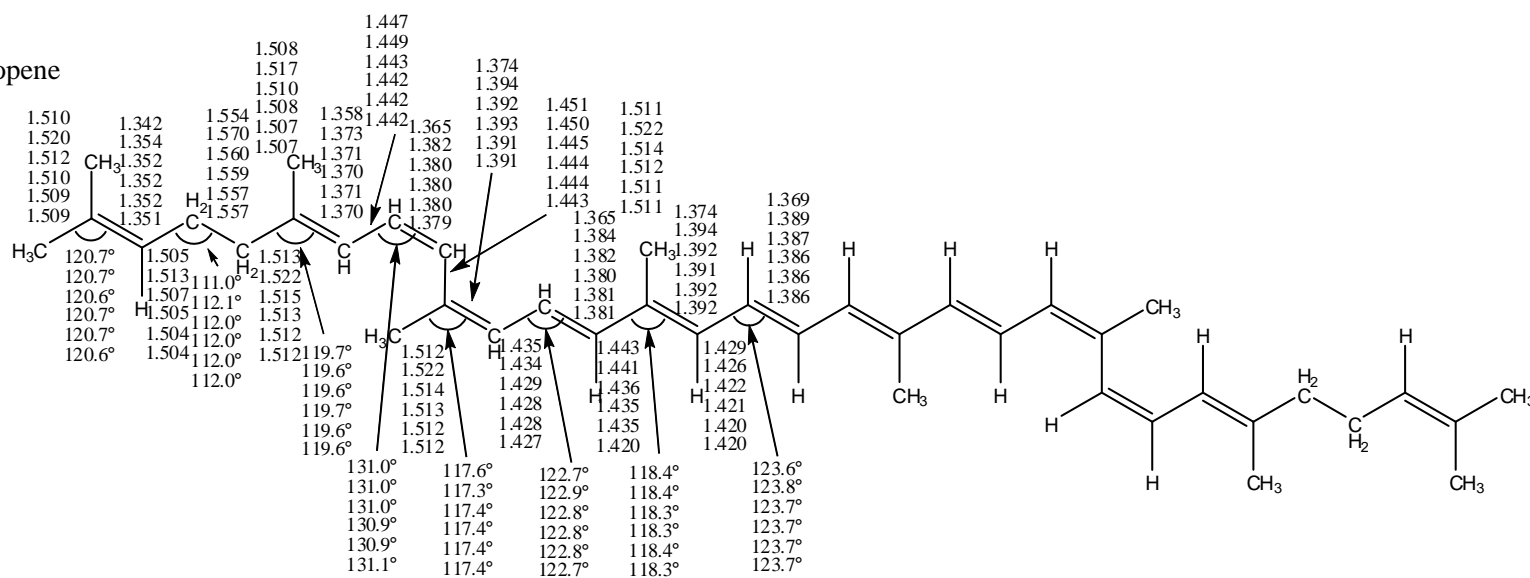
Figure s3. Geometrical parameters of carotenes optimized at DFT using 6-31G(*d*). The first to sixth entries are results obtained from MP2, B3LYP, BLYP, BPW91, MPWPW91, PBE/PBE, and BB95 methods, respectively.



$\beta$ -carotene



prolycopene



lycopene

