Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information for:

Molecular Dynamics Calculations of Molecular Volumes and Volumes of Activation.

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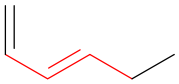
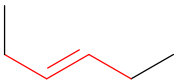
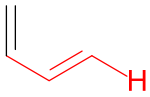
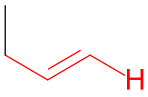
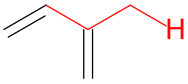
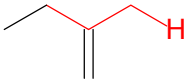
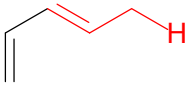
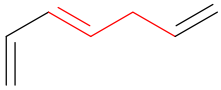
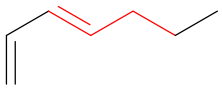
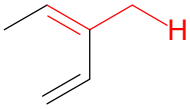
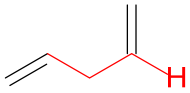
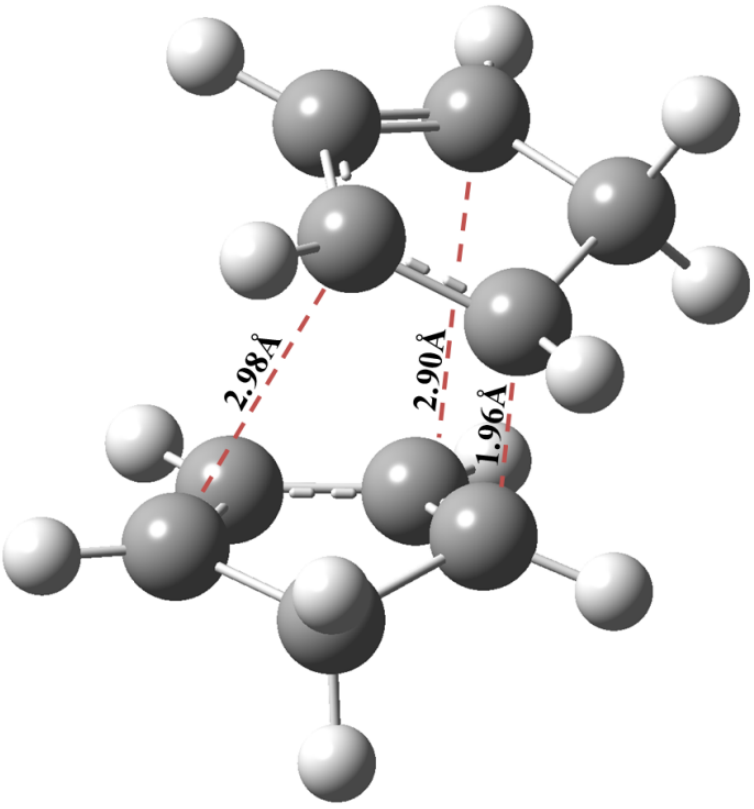
I. OPLS parameters used for missing diene torsions in reactants and solvents.

Dihedral Type		OPLS Parameters					
in diene	in OPLS	C_0	C_1	C_2	C_3	C_4	C_5
		58.576	0.000	-58.576	0.000	0.000	0.000
		58.576	0.000	-58.576	0.000	0.000	0.000
		0.6276	1.8828	0.000	-2.5104	0.000	0.000
		-0.77822	-2.33467	0.000	3.11290	0.000	0.000
		0.52719	-6.39734	-1.69452	7.56467	0.000	0.000
		-0.77822	-2.33467	0.000	3.11290	0.000	0.000
		0.76567	2.29701	0.000	-3.06269	0.000	0.000

II. Optimized geometries of TS's for reactions (6)-(8)

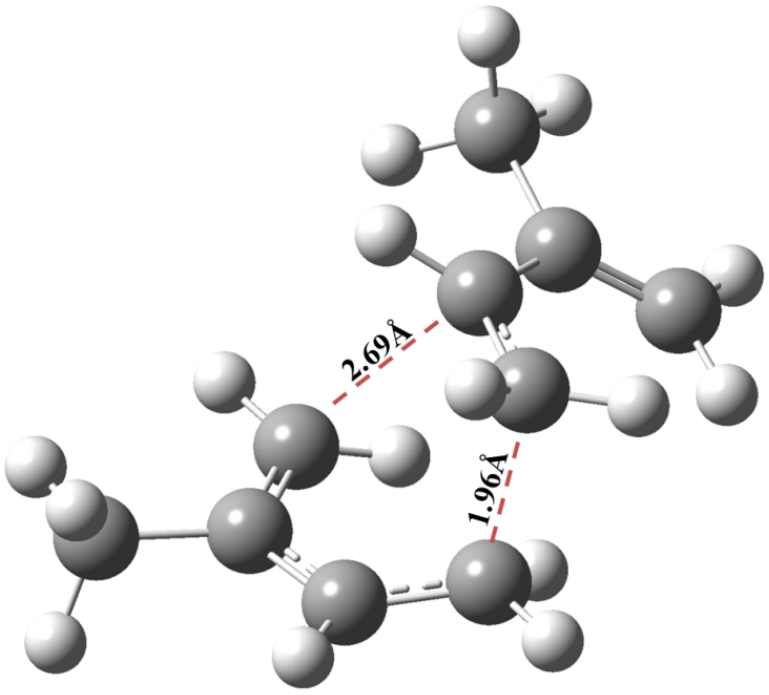
Reaction (6): Cyclopentadiene dimerization (B3LYP/6-31++G)

C	-0.00927800	0.03123800	0.00259700
H	-0.00585000	0.00910500	1.08419000
C	1.14194000	0.01317400	-0.83775500
H	2.10973000	0.34692800	-0.47014400
C	0.66285300	0.44882200	-2.22953500
H	0.80303600	1.54051000	-2.32488400
H	1.19143100	-0.01931300	-3.06462500
C	-0.81366800	0.13105900	-2.14808100
H	-1.48453400	0.13561300	-2.99869500
C	-1.17550100	0.03273300	-0.82182300
H	-2.18798800	-0.08738500	-0.45403800
C	1.58884100	-1.86554100	-1.17602200
H	2.52854900	-1.70557400	-1.69989700
C	0.47214800	-2.45350000	-1.83880300
H	0.30286000	-2.46983300	-2.90690800
C	1.60318200	-2.44807600	0.24434500
H	2.28497300	-3.31706200	0.26281000
H	1.94293900	-1.75550900	1.01980900
C	0.17327000	-2.91852900	0.39414900
H	-0.26581100	-3.23915400	1.33118400
C	-0.39761300	-3.02096400	-0.85329500
H	-1.38328600	-3.42055400	-1.06247400



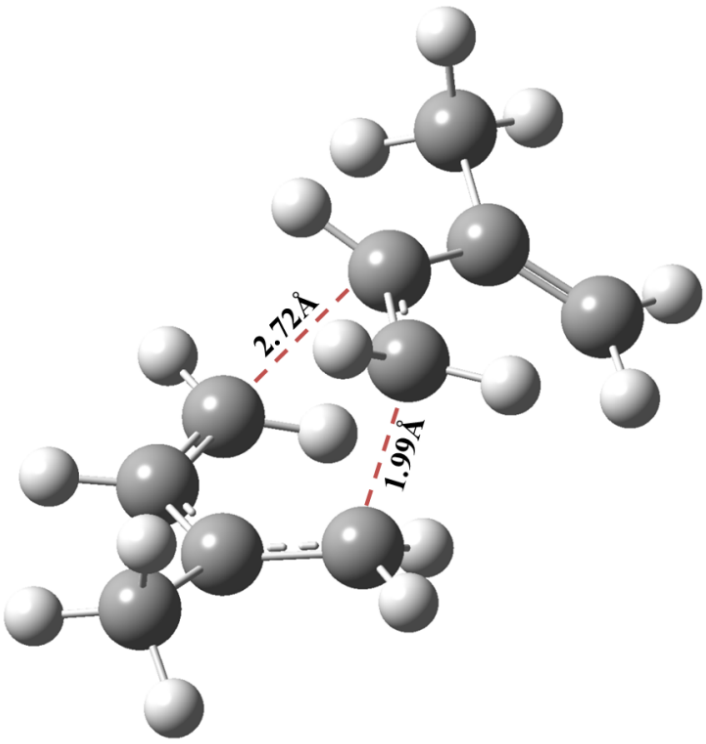
Reaction (7): Isoprene dimerization – 1,3 TS (B3LYP/6-31++G)

C	0.90747100	1.77450000	-0.43225600
H	0.20642600	1.51522700	-1.22640800
H	1.05666400	2.84905300	-0.33596500
C	2.03138600	0.95294900	-0.21922700
H	2.91826100	1.39884700	0.22994600
C	1.97105700	-0.46227900	-0.29495500
C	3.15297700	-1.26837900	0.22145300
H	4.03209100	-1.12392200	-0.42032700
H	3.43921200	-0.96635300	1.23713300
H	2.92809500	-2.33960500	0.23735600
C	0.81608800	-1.09752900	-0.71363800
H	0.72985800	-2.17948000	-0.65785400
H	0.05284700	-0.59186300	-1.28802900
C	-0.37626400	1.40624500	1.00848400
H	-1.00675800	2.26283900	0.77288300
H	0.26168900	1.57879200	1.87056400
C	-0.95713300	0.12397600	0.89168900
H	-0.61606100	-0.66201000	1.55812600
C	-2.12024100	-0.18886600	0.06288900
C	-2.69257100	-1.58577500	0.22698400
H	-3.02699600	-1.75093400	1.25999200
H	-1.93619800	-2.35057900	0.00752200
H	-3.54717100	-1.74959200	-0.43623800
C	-2.67471400	0.68116300	-0.82223400
H	-3.53121100	0.39893300	-1.42650700
H	-2.30908900	1.69461900	-0.95733800



Reaction (7): Isoprene dimerization – 1,4 TS (B3LYP/6-31++G)

C	-1.31397800	-1.01945400	-0.63824800
H	-0.55180500	-0.87542400	-1.40254200
H	-1.77437100	-2.00636600	-0.67532500
C	-2.13995400	0.06596100	-0.28165200
C	-3.50542100	-0.19740300	0.31810400
H	-4.10658200	-0.86099900	-0.31495300
H	-3.42312700	-0.68241000	1.30445900
H	-4.06562100	0.73311900	0.45874900
C	-1.59297700	1.37565100	-0.22342800
H	-2.20597400	2.14871300	0.24041600
C	-0.29925200	1.69253500	-0.57237300
H	0.09106400	2.68951200	-0.38825900
H	0.31337600	1.05178900	-1.19219300
C	0.00111000	-1.25347400	0.83302100
H	0.32387600	-2.23112800	0.47739800
H	-0.69165600	-1.31375500	1.66873900
C	0.96622800	-0.22679500	0.87257600
H	0.86761200	0.54903400	1.62546600
C	2.19398400	-0.20874000	0.07946900
C	3.18409900	0.89063200	0.42184000
H	3.51559600	0.80603900	1.46547200
H	2.72617300	1.88236700	0.30948100
H	4.06928400	0.84819900	-0.21984300
C	2.46279000	-1.08816800	-0.92198500
H	3.38535600	-1.02850500	-1.49090300
H	1.78702700	-1.89464700	-1.19010300



Reaction (8): Methyl-methane hydrogen transfer (B3LYP/6-31++G)**

C	-0.26079600	0.00000000	0.09220400
H	-0.17925100	0.00000100	1.17875300
H	1.00880500	-0.00000100	-0.35666900
H	-0.70505500	-0.91069900	-0.30841500
H	-0.70505400	0.91069900	-0.30841700
C	2.27840600	-0.00000200	-0.80554100
H	2.72266700	-0.91069500	-0.40491100
H	2.19686100	-0.00001500	-1.89209000
H	2.72266100	0.91070300	-0.40493100