Electronic Supplementary Information (ESI)

Combining in situ FTIR Spectroscopy, BTEM Analysis, Bulk Density Measurements and DFT for Two Diels-Alder Reactions. A General Approach for Partial Molar Volume and Reaction Volume Analyses.

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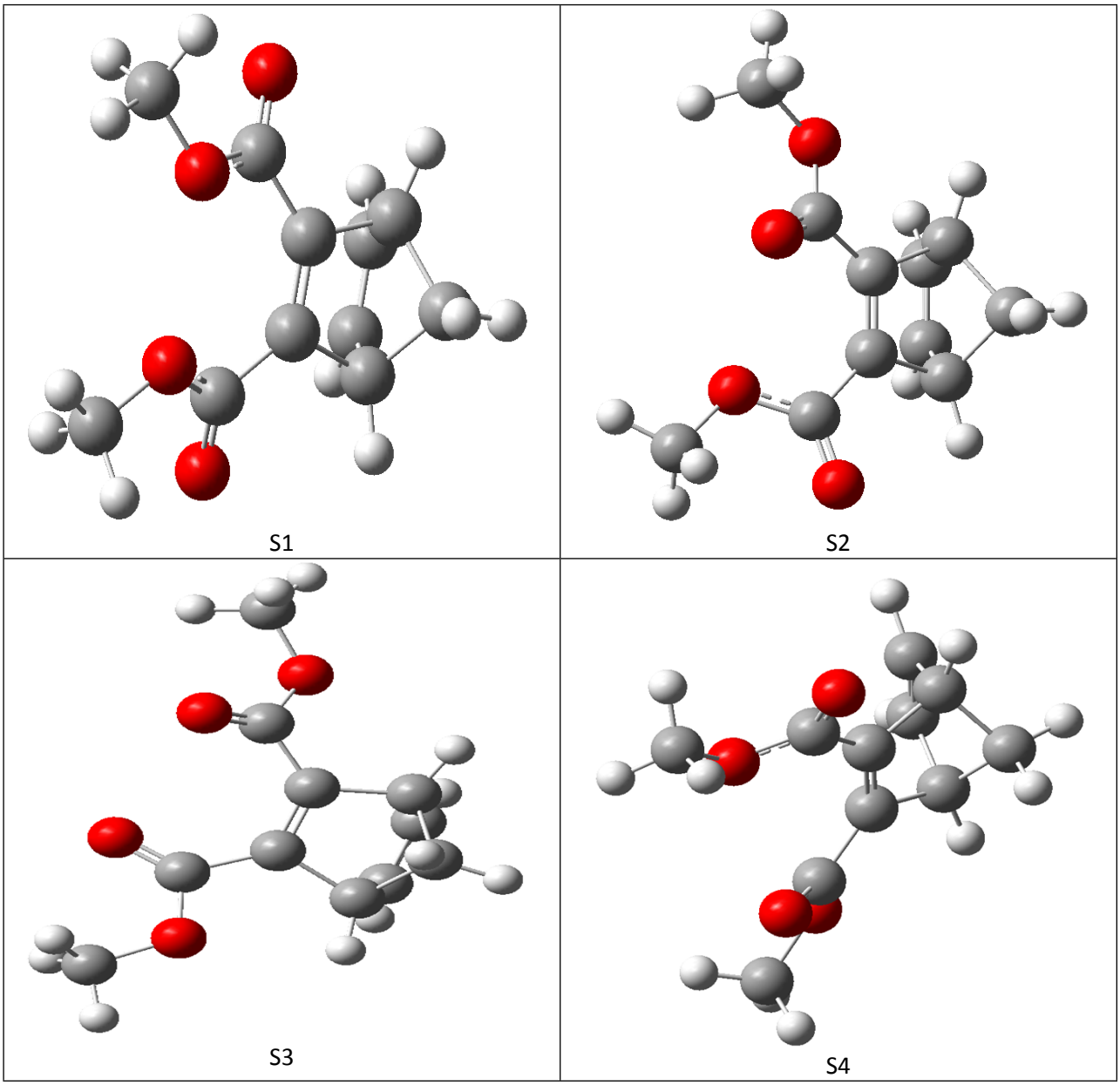

Fig. S1. Optimized geometries of esters with different coordination modes. S4 is the one used in Fig. 12c in the paper.

Table S1 DFT calculated free energies for the four scenarios in Fig S1 Sa,Sb,Sc,Sd.

Structure	Sum of electronic and thermal Free Energies (Hartree/Particle) (298 K,1atm)
S1	-727.107997
S2	-727.111741
S3	-727.110408
S4	-727.111737

Table S2. Comparison of calculated molar volumes of solutes and their corresponding partial molar volumes in toluene at 298.15 K. This is an augmented version of Table 4 in the paper, with the yellow column for SCI-IPCM.

Species	V_{calc}**(cm^3 · mol^{-1})** [a1] IPCM	$V_{m,est}$**(cm^3 · mol^{-1})** [b] **IPCM**	V_{calc}**(cm^3 · mol^{-1})** [a2] SCI-IPCM	$\bar{V}^{\infty}$**(cm^3 · mol^{-1})** [c]
CPD [d]	61.5	82.0 (-1.6%)	69.9 (-16.0%)	83.3
DMAD [d]	95.0	126.7 (1.7%)	115.9 (-7.0%)	124.6
Adduct [d]	144.7	192.9 (14.5%)	166.4 (-2.1%)	170.0
CPD [e]	61.5	82.0 (-0.2%)	69.9 (-15.0%)	82.2
DCPD [e]	111.8	149.1 (11.7%)	121.0 (-9.4%)	133.5
	[a1] from DFT calculations with SCRF=IPCM, [a2] from DFT calculations with SCRF= SCI-IPCM [b] $V_{m,est}=V_{calc}/$ 0.75, deviation to the corresponding PMV is shown in parenthesis [c] PMV obtained from multi-component reaction system [d] from CPD + DMAD reaction [e] from CPD + CPD reaction			

Guassian calculation temperature: 298K