Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Nanostructuring and macroscopic behavior of type V Deep Eutectic Solvents based on monoterpenoids

Lorena Zamora,[a] Cristina Benito, [a] Alberto Gutiérrez,[a] Rafael Alcalde,[a] Noor Alomari, [b] Ahmad Al Bodour,[b] Mert Atilhan,[b*] Santiago Aparicio[a*]

[a] Department of Chemistry, University of Burgos, 09001 Burgos, Spain

[b] Department of Chemical and Paper Engineering, Western Michigan University, Kalamazoo MI 49008-5462, USA

[*]Corresponding authors: mert.atilhan@wmich.edu (M.A.) and sapar@ubu.es (S.A.)

Table S1. Specifications of the considered chemicals.

chemical name	molar mass (g/mol)	purity (mass%)	source	CAS number
cineole (1,3,3-Trimethyl-2-oxabicyclo[2.2.2]octane)	154.25	99.7%	Sigma-Aldrich	470-82-6
carvone (2-Methyl-5-(prop-1-en-2-yl)cyclohex-2-en-1-one)	150.22	99.7%	Acros	6485-40-1
menthol (2-Isopropyl-5-methylcyclohexan-1-ol)	156.27	99.6%	Sigma-Aldrich	2216-51-5
thymol (5-Methyl-2-(propan-2-yl)phenol)	150.22	99.6%	Sigma-Aldrich	89-83-8

Table S2. Thermophysical properties of the studied DES as a function of temperature at atmospheric pressure.

CIN : MEN (1 : 1)				
T / K	ρ / g cm^{-3}	$10^3\alpha_p$ / K_{-1}	n_D	η / $mPa\,s$
293.15	0.91283	0.883	1.46013	9.14
298.15	0.90889	0.887	1.45799	7.04
303.15	0.90494	0.891	1.45585	5.71
308.15	0.90095	0.895	1.45370	4.68
313.15	0.89694	0.899	1.45166	3.87
318.15	0.89289	0.903	1.44966	3.20
323.15	0.88881	0.907	1.44749	2.72
328.15	0.88471	0.911	—	2.35
333.15	0.88062	0.915	—	2.04
338.15	—	—	—	1.75
343.15	—	—	—	1.57
348.15	—	—	—	1.41
353.15	—	—	—	1.27
CIN : THY (1 : 1)				
T / K	ρ / g cm^{-3}	$10^3\alpha_p$ / K_{-1}	n_D	η / $mPa\,s$
293.15	0.95975	0.834	1.49534	25.1
298.15	0.95585	0.837	1.49322	17.7
303.15	0.95189	0.840	1.49111	12.9
308.15	0.94794	0.844	1.48900	9.59
313.15	0.94394	0.848	1.48676	7.31
318.15	0.93993	0.851	1.48470	5.86
323.15	0.93590	0.855	1.48252	4.76
328.15	0.93183	0.859	—	3.19
333.15	0.92774	0.862	—	3.29
338.15	—	—	—	2.80
343.15	—	—	—	2.44
348.15	—	—	—	2.14
353.15	—	—	—	1.90
CAR : MEN (1 : 1)				
T / K	ρ / g cm^{-3}	$10^3\alpha_p$ / K_{-1}	n_D	η / $mPa\,s$
293.15	0.92782	0.827	1.47860	6.24
298.15	0.92404	0.830	1.47641	5.12
303.15	0.92023	0.834	1.47427	4.24
308.15	0.91643	0.837	1.47207	3.56
313.15	0.91261	0.840	1.46988	3.02
318.15	0.90876	0.844	1.46765	2.60
323.15	0.90491	0.848	1.46542	2.26

328.15	0.90101	0.851	—	1.99
333.15	0.89712	0.855	—	1.76
338.15	—	—	—	1.57
343.15	—	—	—	1.42
348.15	—	—	—	1.30
353.15	—	—	—	1.18
CAR : THY (1 : 1)				
T / K	ρ / g cm^{-3}	$10^3\alpha_p$ / K_{-1}	n_D	η / $mPa\,s$
293.15	0.97309	0.804	1.51375	11.6
298.15	0.96920	0.807	1.51178	8.76
303.15	0.96532	0.810	1.50976	6.85
308.15	0.96141	0.813	1.50776	5.55
313.15	0.95752	0.817	1.50560	4.60
318.15	0.95358	0.820	1.50339	3.89
323.15	0.94966	0.824	1.50117	3.30
328.15	0.94573	0.827	—	2.84
333.15	0.94184	0.830	—	2.48
338.15	—	—	—	2.18
343.15	—	—	—	1.95
348.15	—	—	—	1.76
353.15	—	—	—	1.59

- Uncertainty in ρ: ±1 10^{-4} g cm^{-3}
- Uncertainty in η: ±2%
- Uncertainty in n_D: ±1 10^{-5}
- Uncertainty in σ: 5%
- Uncertainty in T: ±0.01 K
- Uncertainty in α_p: ± 0.001 10^{-3} K^{-1}

Table S3. Systems considered for NPT molecular dynamics simulations of for the studied DESs. *L* stands for the dimension of the cubic simulation boxes in the studied temperature range.

HBA	HBD	*N* (HBA)	*N* ([HBD])	*p* / bar	*T* / K	*L* / Å
CIN	MEN	250	250	1	293, 313, 333, 353	54·54·54
CIN	THY	250	250	1	293, 313, 333, 353	54·54·54
CAR	MEN	250	250	1	293, 313, 333, 353	54·54·54
CAR	THY	250	250	1	293, 313, 333, 353	54·54·54

Table S4. Forcefield parameterization for compounds studied in this work.

The general form of the applied force field is:

$$E = \sum_{bonds} k_r (r - r_{eq})^2 + \sum_{angles} k_\theta (\theta - \theta_{eq})^2 + E_{tor}$$

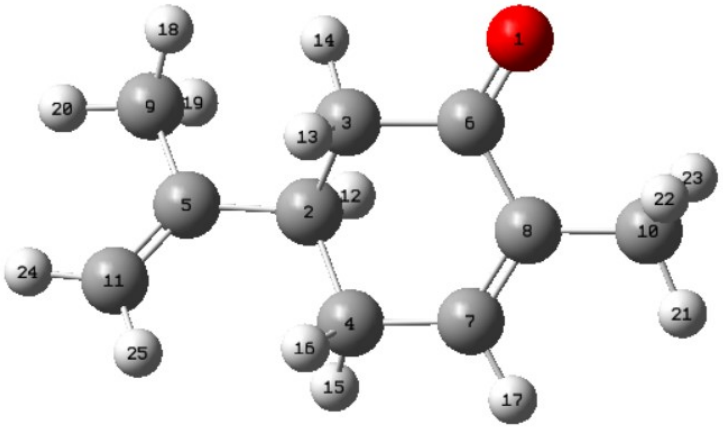
$$+ \sum_i \sum_j \left\{ 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j e^2}{4\pi\varepsilon_0 r_{ij}} \right\}$$

Dihedrals (E_{tor}) were described according to:

$$E_{tor} = \sum_{torsions} k_\phi (1 + \cos(m\phi - \delta))$$

Improper dihedrals were described according to:

$$E_{improper} = k_\phi (\phi - \phi_0)^2$$



CAR

label	*q*	σ_{ii} / Å	ε_{ii} / kJ mol^{-1}	#
Ob	-0.54619	3.02905	0.50208	1
Cw	0.21819	3.87541	0.23012	2
C	-0.45801	3.87541	0.23012	3
C	-0.27209	3.87541	0.23012	4
C	0.26515	3.72396	0.28451	5
Cb	0.64635	3.56359	0.46024	6
C	-0.20309	3.72396	0.28451	7
C	0.03985	3.72396	0.28451	8
C	-0.46678	3.87541	0.23012	9
C	-0.52170	3.87541	0.23012	10
C	-0.66532	3.72396	0.28451	11
Hw	0.02436	2.35197	0.09205	12
H	0.13111	2.35197	0.09205	13
H	0.13371	2.35197	0.09205	14
H	0.10059	2.35197	0.09205	15
H	0.12824	2.35197	0.09205	16
H	0.16398	2.35197	0.09205	17

H	0.13509	2.35197	0.09205	18
H	0.11605	2.35197	0.09205	19
H	0.14098	2.35197	0.09205	20
H	0.13838	2.35197	0.09205	21
H	0.16399	2.35197	0.09205	22
H	0.16172	2.35197	0.09205	23
H	0.22992	2.35197	0.09205	24
H	0.19554	2.35197	0.09205	25

Bonds

Atom Numbers		**r_{eq} /Å**	**k_r/ kJ mol^{-1} Å^{-2}**
19	9	1.093	1435.0745
23	10	1.093	1435.0745
12	2	1.093	1435.0745
9	18	1.093	1435.0745
9	20	1.093	1435.0745
9	5	1.482	1366.7245
1	6	1.222	3899.333
14	3	1.093	1435.0745
10	21	1.093	1435.0745
10	8	1.482	1366.7245
10	22	1.093	1435.0745
6	8	1.468	1374.553
6	3	1.492	1261.639
2	5	1.482	1366.7245
2	3	1.508	1282.1115
2	4	1.508	1282.1115
8	7	1.333	2862.019
5	11	1.333	2862.019
3	13	1.093	1435.0745
15	4	1.093	1435.0745
7	17	1.083	1556.724
7	4	1.482	1366.7245
4	16	1.093	1435.0745
11	24	1.083	1556.724
11	25	1.083	1556.724

Angles

Atom Numbers			**θ_{eq} / deg**	**k_θ / kJ mol^{-1} rad^{-2}**
3	2	4	109.608	512.48
3	2	5	109.445	443.23
3	2	12	110.549	383
4	2	5	109.445	443.23
4	2	12	110.549	383
5	2	12	110.292	380.59
2	3	6	107.517	467.91
2	3	13	110.549	383
2	3	14	110.549	383
6	3	13	108.385	391.44
6	3	14	108.385	391.44
13	3	14	108.836	310.74
2	4	7	109.445	443.23
2	4	15	110.549	383
2	4	16	110.549	383
7	4	15	110.292	380.59
7	4	16	110.292	380.59
15	4	16	108.836	310.74
2	5	9	118.043	452.86
2	5	11	122.141	404.68
9	5	11	122.141	404.68
1	6	3	124.41	564.87
1	6	8	122.623	563.67
3	6	8	116.853	666.04
4	7	8	122.141	404.68
4	7	17	120.108	268.59
8	7	17	121.004	322.18
6	8	7	111.297	328.2
6	8	10	116.104	420.34
7	8	10	122.141	404.68
5	9	18	110.292	380.59
5	9	19	110.292	380.59
5	9	20	110.292	380.59
18	9	19	108.836	310.74
18	9	20	108.836	310.74
19	9	20	108.836	310.74
8	10	21	110.292	380.59
8	10	22	110.292	380.59

8	10	23	110.292	380.59	
21	10	22	108.836	310.74	
21	10	23	108.836	310.74	
22	10	23	108.836	310.74	
5	11	24	121.004	322.18	
5	11	25	121.004	322.18	
24	11	25	119.523	219.8	

Dihedrals

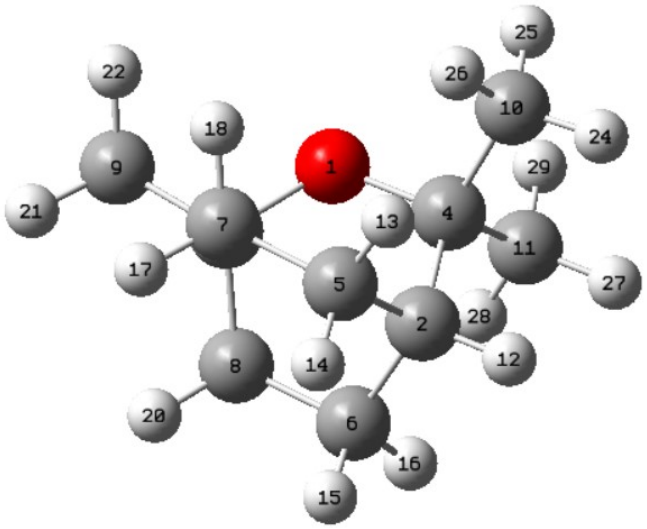
Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	6	3	2	0	1.7238	1
1	6	3	2	180	0.2929	2
1	6	3	2	0	0.682	3
1	6	3	13	0	1.3807	1
1	6	3	13	180	-2.9455	2
1	6	3	13	0	0.6443	3
1	6	3	14	0	1.3807	1
1	6	3	14	180	-2.9455	2
1	6	3	14	0	0.6443	3
1	6	8	7	0	0.7573	1
1	6	8	7	180	4.138	2
1	6	8	10	0	-0.841	1
1	6	8	10	180	4.2426	2
1	6	8	10	0	-0.6653	3
2	3	6	8	180	0.8368	2
2	3	6	8	0	0.6276	3
2	4	7	8	0	-1.0334	1
2	4	7	8	180	0.5732	2
2	4	7	8	0	-1.318	3
2	4	7	17	0	0.1548	1
2	4	7	17	0	0.7489	3
2	5	9	18	180	-0.3849	2
2	5	9	18	0	0.4602	3
2	5	9	19	180	-0.3849	2
2	5	9	19	0	0.4602	3
2	5	9	20	180	-0.3849	2
2	5	9	20	0	0.4602	3
2	5	11	24	180	25.104	2
2	5	11	25	180	25.104	2
3	2	4	7	0	-0.615	1
3	2	4	7	180	0.9163	2
3	2	4	7	0	1.2217	3
3	2	4	15	0	1.3389	1
3	2	4	15	180	-1.318	2
3	2	4	15	0	0.5523	3
3	2	4	16	0	1.3389	1
3	2	4	16	180	-1.318	2
3	2	4	16	0	0.5523	3
3	2	5	9	0	0.8745	1
3	2	5	9	180	0.6192	2
3	2	5	9	0	0.5899	3
3	2	5	11	0	-1.0334	1
3	2	5	11	180	0.5732	2
3	2	5	11	0	-1.318	3
3	6	8	7	0	-0.682	1
3	6	8	7	180	3.2468	2
3	6	8	7	0	-1.0167	3
3	6	8	10	0	0.2845	1
3	6	8	10	180	3.7614	2
3	6	8	10	0	1.318	3
4	2	3	6	0	0.1381	1
4	2	3	6	180	-0.3264	2
4	2	3	6	0	0.2971	3
4	2	3	13	0	1.3389	1
4	2	3	13	180	-1.318	2
4	2	3	13	0	0.5523	3
4	2	3	14	0	1.3389	1
4	2	3	14	180	-1.318	2
4	2	3	14	0	0.5523	3
4	2	5	9	0	0.8745	1
4	2	5	9	180	0.6192	2
4	2	5	9	0	0.5899	3
4	2	5	11	0	-1.0334	1
4	2	5	11	180	0.5732	2
4	2	5	11	0	-1.318	3
4	7	8	6	180	25.104	2

4	7	8	10	0	-0.8452	1
4	7	8	10	180	25.104	2
5	2	3	6	0	0.6276	3
5	2	3	13	0	0.6736	1
5	2	3	13	180	-0.8577	2
5	2	3	13	0	0.3012	3
5	2	3	14	0	0.6736	1
5	2	3	14	180	-0.8577	2
5	2	3	14	0	0.3012	3
5	2	4	7	0	0.6276	3
5	2	4	15	0	0.6736	1
5	2	4	15	180	-0.8577	2
5	2	4	15	0	0.3012	3
5	2	4	16	0	0.6736	1
5	2	4	16	180	-0.8577	2
5	2	4	16	0	0.3012	3
6	3	2	12	0	-0.5356	1
6	3	2	12	180	0.1213	2
6	8	7	17	180	3.7656	2
6	8	10	21	0	-0.2259	3
6	8	10	22	0	-0.2259	3
6	8	10	23	0	-0.2259	3
7	4	2	12	0	0.6736	1
7	4	2	12	180	-0.8577	2
7	4	2	12	0	0.3012	3
7	8	10	21	0	1.0502	1
7	8	10	21	180	-0.8577	2
7	8	10	21	0	-1.1213	3
7	8	10	22	0	1.0502	1
7	8	10	22	180	-0.8577	2
7	8	10	22	0	-1.1213	3
7	8	10	23	0	1.0502	1
7	8	10	23	180	-0.8577	2
7	8	10	23	0	-1.1213	3
8	6	3	13	0	0.2427	3
8	6	3	14	0	0.2427	3
8	7	4	15	0	1.0502	1
8	7	4	15	180	-0.8577	2
8	7	4	15	0	-1.1213	3
8	7	4	16	0	1.0502	1
8	7	4	16	180	-0.8577	2
8	7	4	16	0	-1.1213	3
9	5	2	12	180	-0.3849	2
9	5	2	12	0	0.4602	3
9	5	11	24	180	25.104	2
9	5	11	25	180	25.104	2
10	8	7	17	180	25.104	2
11	5	2	12	0	1.0502	1
11	5	2	12	180	-0.8577	2
11	5	2	12	0	-1.1213	3
11	5	9	18	0	1.0502	1
11	5	9	18	180	-0.8577	2
11	5	9	18	0	-1.1213	3
11	5	9	19	0	1.0502	1
11	5	9	19	180	-0.8577	2
11	5	9	19	0	-1.1213	3
11	5	9	20	0	1.0502	1
11	5	9	20	180	-0.8577	2
11	5	9	20	0	-1.1213	3
12	2	3	13	0	0.5941	1
12	2	3	13	180	-2.8995	2
12	2	3	13	0	0.6569	3
12	2	3	14	0	0.5941	1
12	2	3	14	180	-2.8995	2
12	2	3	14	0	0.6569	3
12	2	4	15	0	0.5941	1
12	2	4	15	180	-2.8995	2
12	2	4	15	0	0.6569	3
12	2	4	16	0	0.5941	1
12	2	4	16	180	-2.8995	2
12	2	4	16	0	0.6569	3
15	4	7	17	0	-1.0962	1
15	4	7	17	180	-0.477	2
15	4	7	17	0	0.4351	3
16	4	7	17	0	-1.0962	1
16	4	7	17	180	-0.477	2

16	4	7	17	0	0.4351	3

Improper

Atom Numbers				ϕ_0 / deg	k_ϕ / kJ mol^{-1}
6	3	1	8	0	83.1026
3	2	6	14	0	0
3	14	6	13	0	0
2	5	3	4	0	0
2	5	3	12	0	0
8	10	6	7	0	15.6565
5	9	2	11	0	18.0665
4	7	2	15	0	0
4	15	2	16	0	0
7	4	8	17	0	7.8324
9	19	5	18	0	0
9	19	5	20	0	0
10	23	8	21	0	0
10	23	8	22	0	0
11	24	5	25	0	3.615



CIN

label	q	σ_{ii} / Å	ϵ_{ii} / kJ mol^{-1}	#
Ot	-0.72761	3.15378	0.63639	1
C	-0.08927	3.87541	0.23012	2
Ct	0.75687	3.87541	0.23012	3
Ct	1.04073	3.87541	0.23012	4
C	-0.08549	3.87541	0.23012	5
C	-0.08738	3.87541	0.23012	6
C	-0.18232	3.87541	0.23012	7
C	-0.18023	3.87541	0.23012	8
C	-0.63026	3.87541	0.23012	9
C	-0.70350	3.87541	0.23012	10
C	-0.70845	3.87541	0.23012	11
H	-0.00540	2.35197	0.09205	12
H	0.01879	2.35197	0.09205	13
H	0.04321	2.35197	0.09205	14
H	0.04397	2.35197	0.09205	15
H	0.01897	2.35197	0.09205	16
H	0.03083	2.35197	0.09205	17
H	0.03650	2.35197	0.09205	18
H	0.03537	2.35197	0.09205	19
H	0.03065	2.35197	0.09205	20
H	0.11376	2.35197	0.09205	21
H	0.15723	2.35197	0.09205	22
H	0.15731	2.35197	0.09205	23
H	0.12854	2.35197	0.09205	24
H	0.16015	2.35197	0.09205	25
H	0.16709	2.35197	0.09205	26
H	0.12962	2.35197	0.09205	27
H	0.16886	2.35197	0.09205	28
H	0.16145	2.35197	0.09205	29

Bonds

Atom Numbers		r_{eq} /Å	k_r/ kJ mol^{-1} Å^{-2}
28	11	1.093	1435.0745
16	6	1.093	1435.0745
19	8	1.093	1435.0745
27	11	1.093	1435.0745
20	8	1.093	1435.0745
8	6	1.508	1282.1115
8	3	1.508	1282.1115
11	29	1.093	1435.0745
11	4	1.508	1282.1115
6	15	1.093	1435.0745
6	2	1.508	1282.1115
23	9	1.093	1435.0745
9	21	1.093	1435.0745
9	3	1.508	1282.1115
9	22	1.093	1435.0745
1	4	1.418	1519.6875
1	3	1.418	1519.6875
4	2	1.508	1282.1115
4	10	1.508	1282.1115
3	7	1.508	1282.1115
2	12	1.093	1435.0745
2	5	1.508	1282.1115
14	5	1.093	1435.0745
25	10	1.093	1435.0745
5	7	1.508	1282.1115
5	13	1.093	1435.0745
10	24	1.093	1435.0745
10	26	1.093	1435.0745
7	17	1.093	1435.0745
7	18	1.093	1435.0745

Angles

Atom Numbers			θ_{eq} / deg	k_θ / kJ mol^{-1} rad^{-2}
3	1	4	106.926	720.84
4	2	5	109.608	512.48
4	2	6	109.608	512.48
4	2	12	110.549	383
5	2	6	109.608	512.48
5	2	12	110.549	383
6	2	12	110.549	383
1	3	7	108.133	597.39
1	3	8	108.133	597.39
1	3	9	108.133	597.39
7	3	8	109.608	512.48
7	3	9	109.608	512.48
8	3	9	109.608	512.48
1	4	2	108.133	597.39
1	4	10	108.133	597.39
1	4	11	108.133	597.39
2	4	10	109.608	512.48
2	4	11	109.608	512.48
10	4	11	109.608	512.48
2	5	7	109.608	512.48
2	5	13	110.549	383
2	5	14	110.549	383
7	5	13	110.549	383
7	5	14	110.549	383
13	5	14	108.836	310.74
2	6	8	109.608	512.48
2	6	15	110.549	383
2	6	16	110.549	383
8	6	15	110.549	383
8	6	16	110.549	383
15	6	16	108.836	310.74
3	7	5	109.608	512.48
3	7	17	110.549	383
3	7	18	110.549	383
5	7	17	110.549	383
5	7	18	110.549	383
17	7	18	108.836	310.74
3	8	6	109.608	512.48
3	8	19	110.549	383
3	8	20	110.549	383
6	8	19	110.549	383
6	8	20	110.549	383

19	8	20	108.836	310.74
3	9	21	110.549	383
3	9	22	110.549	383
3	9	23	110.549	383
21	9	22	108.836	310.74
21	9	23	108.836	310.74
22	9	23	108.836	310.74
4	10	24	110.549	383
4	10	25	110.549	383
4	10	26	110.549	383
24	10	25	108.836	310.74
24	10	26	108.836	310.74
25	10	26	108.836	310.74
4	11	27	110.549	383
4	11	28	110.549	383
4	11	29	110.549	383
27	11	28	108.836	310.74
27	11	29	108.836	310.74
28	11	29	108.836	310.74

Dihedrals

Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	3	7	5	0	-1.4393	1
1	3	7	5	180	3.6777	2
1	3	7	5	0	0.9958	3
1	3	7	17	0	-1.3682	1
1	3	7	17	180	2.2426	2
1	3	7	17	0	0.5858	3
1	3	7	18	0	-1.3682	1
1	3	7	18	180	2.2426	2
1	3	7	18	0	0.5858	3
1	3	8	6	0	-1.4393	1
1	3	8	6	180	3.6777	2
1	3	8	6	0	0.9958	3
1	3	8	19	0	-1.3682	1
1	3	8	19	180	2.2426	2
1	3	8	19	0	0.5858	3
1	3	8	20	0	-1.3682	1
1	3	8	20	180	2.2426	2
1	3	8	20	0	0.5858	3
1	3	9	21	0	-1.3682	1
1	3	9	21	180	2.2426	2
1	3	9	21	0	0.5858	3
1	3	9	22	0	-1.3682	1
1	3	9	22	180	2.2426	2
1	3	9	22	0	0.5858	3
1	3	9	23	0	-1.3682	1
1	3	9	23	180	2.2426	2
1	3	9	23	0	0.5858	3
1	4	2	5	0	-1.4393	1
1	4	2	5	180	3.6777	2
1	4	2	5	0	0.9958	3
1	4	2	6	0	-1.4393	1
1	4	2	6	180	3.6777	2
1	4	2	6	0	0.9958	3
1	4	2	12	0	-1.3682	1
1	4	2	12	180	2.2426	2
1	4	2	12	0	0.5858	3
1	4	10	24	0	-1.3682	1
1	4	10	24	180	2.2426	2
1	4	10	24	0	0.5858	3
1	4	10	25	0	-1.3682	1
1	4	10	25	180	2.2426	2
1	4	10	25	0	0.5858	3
1	4	10	26	0	-1.3682	1
1	4	10	26	180	2.2426	2
1	4	10	26	0	0.5858	3
1	4	11	27	0	-1.3682	1
1	4	11	27	180	2.2426	2
1	4	11	27	0	0.5858	3
1	4	11	28	0	-1.3682	1
1	4	11	28	180	2.2426	2
1	4	11	28	0	0.5858	3
1	4	11	29	0	-1.3682	1
1	4	11	29	180	2.2426	2
1	4	11	29	0	0.5858	3

2	4	1	3	0	-1.4267	1
2	4	1	3	180	1.5816	2
2	4	1	3	0	1.5816	3
2	4	10	24	0	1.3389	1
2	4	10	24	180	-1.318	2
2	4	10	24	0	0.5523	3
2	4	10	25	0	1.3389	1
2	4	10	25	180	-1.318	2
2	4	10	25	0	0.5523	3
2	4	10	26	0	1.3389	1
2	4	10	26	180	-1.318	2
2	4	10	26	0	0.5523	3
2	4	11	27	0	1.3389	1
2	4	11	27	180	-1.318	2
2	4	11	27	0	0.5523	3
2	4	11	28	0	1.3389	1
2	4	11	28	180	-1.318	2
2	4	11	28	0	0.5523	3
2	4	11	29	0	1.3389	1
2	4	11	29	180	-1.318	2
2	4	11	29	0	0.5523	3
2	5	7	3	0	0.2134	1
2	5	7	3	180	1.4267	2
2	5	7	3	0	0.6945	3
2	5	7	17	0	1.3389	1
2	5	7	17	180	-1.318	2
2	5	7	17	0	0.5523	3
2	5	7	18	0	1.3389	1
2	5	7	18	180	-1.318	2
2	5	7	18	0	0.5523	3
2	6	8	3	0	0.2134	1
2	6	8	3	180	1.4267	2
2	6	8	3	0	0.6945	3
2	6	8	19	0	1.3389	1
2	6	8	19	180	-1.318	2
2	6	8	19	0	0.5523	3
2	6	8	20	0	1.3389	1
2	6	8	20	180	-1.318	2
2	6	8	20	0	0.5523	3
3	1	4	10	0	-1.4267	1
3	1	4	10	180	1.5816	2
3	1	4	10	0	1.5816	3
3	1	4	11	0	-1.4267	1
3	1	4	11	180	1.5816	2
3	1	4	11	0	1.5816	3
3	7	5	13	0	1.3389	1
3	7	5	13	180	-1.318	2
3	7	5	13	0	0.5523	3
3	7	5	14	0	1.3389	1
3	7	5	14	180	-1.318	2
3	7	5	14	0	0.5523	3
3	8	6	15	0	1.3389	1
3	8	6	15	180	-1.318	2
3	8	6	15	0	0.5523	3
3	8	6	16	0	1.3389	1
3	8	6	16	180	-1.318	2
3	8	6	16	0	0.5523	3
4	1	3	7	0	-1.4267	1
4	1	3	7	180	1.5816	2
4	1	3	7	0	1.5816	3
4	1	3	8	0	-1.4267	1
4	1	3	8	180	1.5816	2
4	1	3	8	0	1.5816	3
4	1	3	9	0	-1.4267	1
4	1	3	9	180	1.5816	2
4	1	3	9	0	1.5816	3
4	2	5	7	0	0.2134	1
4	2	5	7	180	1.4267	2
4	2	5	7	0	0.6945	3
4	2	5	13	0	1.3389	1
4	2	5	13	180	-1.318	2
4	2	5	13	0	0.5523	3
4	2	5	14	0	1.3389	1
4	2	5	14	180	-1.318	2
4	2	5	14	0	0.5523	3
4	2	6	8	0	0.2134	1

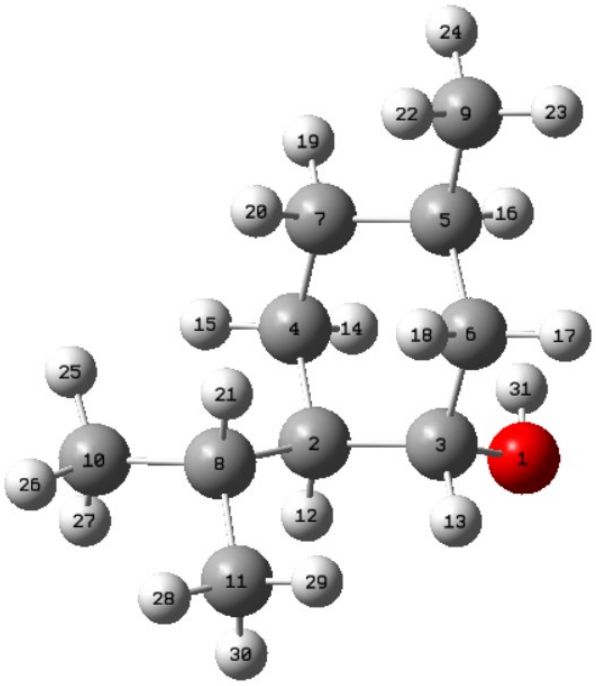
4	2	6	8	180	1.4267	2
4	2	6	8	0	0.6945	3
4	2	6	15	0	1.3389	1
4	2	6	15	180	-1.318	2
4	2	6	15	0	0.5523	3
4	2	6	16	0	1.3389	1
4	2	6	16	180	-1.318	2
4	2	6	16	0	0.5523	3
5	2	4	10	0	0.2134	1
5	2	4	10	180	1.4267	2
5	2	4	10	0	0.6945	3
5	2	4	11	0	0.2134	1
5	2	4	11	180	1.4267	2
5	2	4	11	0	0.6945	3
5	2	6	8	0	0.2134	1
5	2	6	8	180	1.4267	2
5	2	6	8	0	0.6945	3
5	2	6	15	0	1.3389	1
5	2	6	15	180	-1.318	2
5	2	6	15	0	0.5523	3
5	2	6	16	0	1.3389	1
5	2	6	16	180	-1.318	2
5	2	6	16	0	0.5523	3
5	7	3	8	0	0.2134	1
5	7	3	8	180	1.4267	2
5	7	3	8	0	0.6945	3
5	7	3	9	0	0.2134	1
5	7	3	9	180	1.4267	2
5	7	3	9	0	0.6945	3
6	2	4	10	0	0.2134	1
6	2	4	10	180	1.4267	2
6	2	4	10	0	0.6945	3
6	2	4	11	0	0.2134	1
6	2	4	11	180	1.4267	2
6	2	4	11	0	0.6945	3
6	2	5	7	0	0.2134	1
6	2	5	7	180	1.4267	2
6	2	5	7	0	0.6945	3
6	2	5	13	0	1.3389	1
6	2	5	13	180	-1.318	2
6	2	5	13	0	0.5523	3
6	2	5	14	0	1.3389	1
6	2	5	14	180	-1.318	2
6	2	5	14	0	0.5523	3
6	8	3	7	0	0.2134	1
6	8	3	7	180	1.4267	2
6	8	3	7	0	0.6945	3
6	8	3	9	0	0.2134	1
6	8	3	9	180	1.4267	2
6	8	3	9	0	0.6945	3
7	3	8	19	0	1.3389	1
7	3	8	19	180	-1.318	2
7	3	8	19	0	0.5523	3
7	3	8	20	0	1.3389	1
7	3	8	20	180	-1.318	2
7	3	8	20	0	0.5523	3
7	3	9	21	0	1.3389	1
7	3	9	21	180	-1.318	2
7	3	9	21	0	0.5523	3
7	3	9	22	0	1.3389	1
7	3	9	22	180	-1.318	2
7	3	9	22	0	0.5523	3
7	3	9	23	0	1.3389	1
7	3	9	23	180	-1.318	2
7	3	9	23	0	0.5523	3
7	5	2	12	0	1.3389	1
7	5	2	12	180	-1.318	2
7	5	2	12	0	0.5523	3
8	3	7	17	0	1.3389	1
8	3	7	17	180	-1.318	2
8	3	7	17	0	0.5523	3
8	3	7	18	0	1.3389	1
8	3	7	18	180	-1.318	2
8	3	7	18	0	0.5523	3
8	3	9	21	0	1.3389	1
8	3	9	21	180	-1.318	2

8	3	9	21	0	0.5523	3
8	3	9	22	0	1.3389	1
8	3	9	22	180	-1.318	2
8	3	9	22	0	0.5523	3
8	3	9	23	0	1.3389	1
8	3	9	23	180	-1.318	2
8	3	9	23	0	0.5523	3
8	6	2	12	0	1.3389	1
8	6	2	12	180	-1.318	2
8	6	2	12	0	0.5523	3
9	3	7	17	0	1.3389	1
9	3	7	17	180	-1.318	2
9	3	7	17	0	0.5523	3
9	3	7	18	0	1.3389	1
9	3	7	18	180	-1.318	2
9	3	7	18	0	0.5523	3
9	3	8	19	0	1.3389	1
9	3	8	19	180	-1.318	2
9	3	8	19	0	0.5523	3
9	3	8	20	0	1.3389	1
9	3	8	20	180	-1.318	2
9	3	8	20	0	0.5523	3
10	4	2	12	0	1.3389	1
10	4	2	12	180	-1.318	2
10	4	2	12	0	0.5523	3
10	4	11	27	0	1.3389	1
10	4	11	27	180	-1.318	2
10	4	11	27	0	0.5523	3
10	4	11	28	0	1.3389	1
10	4	11	28	180	-1.318	2
10	4	11	28	0	0.5523	3
10	4	11	29	0	1.3389	1
10	4	11	29	180	-1.318	2
10	4	11	29	0	0.5523	3
11	4	2	12	0	1.3389	1
11	4	2	12	180	-1.318	2
11	4	2	12	0	0.5523	3
11	4	10	24	0	1.3389	1
11	4	10	24	180	-1.318	2
11	4	10	24	0	0.5523	3
11	4	10	25	0	1.3389	1
11	4	10	25	180	-1.318	2
11	4	10	25	0	0.5523	3
11	4	10	26	0	1.3389	1
11	4	10	26	180	-1.318	2
11	4	10	26	0	0.5523	3
12	2	5	13	0	0.5941	1
12	2	5	13	180	-2.8995	2
12	2	5	13	0	0.6569	3
12	2	5	14	0	0.5941	1
12	2	5	14	180	-2.8995	2
12	2	5	14	0	0.6569	3
12	2	6	15	0	0.5941	1
12	2	6	15	180	-2.8995	2
12	2	6	15	0	0.6569	3
12	2	6	16	0	0.5941	1
12	2	6	16	180	-2.8995	2
12	2	6	16	0	0.6569	3
13	5	7	17	0	0.5941	1
13	5	7	17	180	-2.8995	2
13	5	7	17	0	0.6569	3
13	5	7	18	0	0.5941	1
13	5	7	18	180	-2.8995	2
13	5	7	18	0	0.6569	3
14	5	7	17	0	0.5941	1
14	5	7	17	180	-2.8995	2
14	5	7	17	0	0.6569	3
14	5	7	18	0	0.5941	1
14	5	7	18	180	-2.8995	2
14	5	7	18	0	0.6569	3
15	6	8	19	0	0.5941	1
15	6	8	19	180	-2.8995	2
15	6	8	19	0	0.6569	3
15	6	8	20	0	0.5941	1
15	6	8	20	180	-2.8995	2
15	6	8	20	0	0.6569	3

16	6	8	19	0	0.5941	1
16	6	8	19	180	-2.8995	2
16	6	8	19	0	0.6569	3
16	6	8	20	0	0.5941	1
16	6	8	20	180	-2.8995	2
16	6	8	20	0	0.6569	3

Improper

	Atom Numbers			**ϕ_0 / deg**	**k_ϕ / kJ mol^{-1}**
4	2	1	11	0	0
4	11	1	10	0	0
2	6	4	5	0	0
2	6	4	12	0	0
3	9	1	8	0	0
3	8	1	7	0	0
5	7	2	14	0	0
5	14	2	13	0	0
6	8	2	16	0	0
6	16	2	15	0	0
7	5	3	17	0	0
7	5	3	18	0	0
8	6	3	19	0	0
8	19	3	20	0	0
9	23	3	21	0	0
9	23	3	22	0	0
10	25	4	24	0	0
10	25	4	26	0	0
11	28	4	27	0	0
11	28	4	29	0	0



MEN

label	***q***	**σ_{ii} / Å**	**ϵ_{ii} / kJ mol^{-1}**	**#**
O2	-0.76638	3.12000	0.70788	1
C	-0.22659	3.50000	0.27610	2
C2	0.51479	3.50000	0.27610	3
C	-0.04496	3.50000	0.27610	4
C	0.62366	3.50000	0.27610	5
C	-0.57888	3.50000	0.27610	6
C	-0.25652	3.50000	0.27610	7
C	0.56109	3.50000	0.27610	8
C	-0.56219	3.50000	0.27610	9
C	-0.55873	3.50000	0.27610	10
C	-0.58099	3.50000	0.27610	11
H	0.04793	2.50000	0.12552	12
H	0.05556	2.50000	0.12552	13
H	0.00327	2.50000	0.12552	14

H	0.05121	2.50000	0.12552	15
H	-0.09023	2.50000	0.12552	16
H	0.12304	2.50000	0.12552	17
H	0.10552	2.50000	0.12552	18
H	0.04575	2.50000	0.12552	19
H	0.05679	2.50000	0.12552	20
H	-0.05547	2.50000	0.12552	21
H	0.12361	2.50000	0.12552	22
H	0.12775	2.50000	0.12552	23
H	0.10872	2.50000	0.12552	24
H	0.12442	2.50000	0.12552	25
H	0.11805	2.50000	0.12552	26
H	0.12875	2.50000	0.12552	27
H	0.13773	2.50000	0.12552	28
H	0.09569	2.50000	0.12552	29
H	0.13184	2.50000	0.12552	30
H2	0.43578	0.40001	0.19246	31

Bonds

Atom Numbers		**r_{eq} /Å**	**k_r/ kJ mol^{-1} Å^{-2}**
1	3	1.418	1519.6875
1	31	0.972	2346.8265
2	3	1.508	1282.1115
2	4	1.508	1282.1115
2	8	1.508	1282.1115
2	12	1.093	1435.0745
3	6	1.508	1282.1115
3	13	1.093	1435.0745
4	7	1.508	1282.1115
4	14	1.093	1435.0745
4	15	1.093	1435.0745
5	6	1.508	1282.1115
5	7	1.508	1282.1115
5	9	1.508	1282.1115
5	16	1.093	1435.0745
6	17	1.093	1435.0745
6	18	1.093	1435.0745
7	19	1.093	1435.0745
7	20	1.093	1435.0745
8	10	1.508	1282.1115
8	11	1.508	1282.1115
8	21	1.093	1435.0745
9	22	1.093	1435.0745
9	23	1.093	1435.0745
9	24	1.093	1435.0745
10	25	1.093	1435.0745
10	26	1.093	1435.0745
10	27	1.093	1435.0745
11	28	1.093	1435.0745
11	29	1.093	1435.0745
11	30	1.093	1435.0745

Angles

Atom Numbers			**θ_{eq} / deg**	**k_θ / kJ mol^{-1} rad^{-2}**
3	1	31	106.503	477.55
3	2	4	109.608	512.48
3	2	8	109.608	512.48
3	2	12	110.549	383
4	2	8	109.608	512.48
4	2	12	110.549	383
8	2	12	110.549	383
1	3	2	108.133	597.39
1	3	6	108.133	597.39
1	3	13	108.577	470.32
2	3	6	109.608	512.48
2	3	13	110.549	383
6	3	13	110.549	383
2	4	7	109.608	512.48
2	4	14	110.549	383
2	4	15	110.549	383
7	4	14	110.549	383
7	4	15	110.549	383
14	4	15	108.836	310.74
6	5	7	109.608	512.48
6	5	9	109.608	512.48
6	5	16	110.549	383

7	5	9	109.608	512.48
7	5	16	110.549	383
9	5	16	110.549	383
3	6	5	109.608	512.48
3	6	17	110.549	383
3	6	18	110.549	383
5	6	17	110.549	383
5	6	18	110.549	383
17	6	18	108.836	310.74
4	7	5	109.608	512.48
4	7	19	110.549	383
4	7	20	110.549	383
5	7	19	110.549	383
5	7	20	110.549	383
19	7	20	108.836	310.74
2	8	10	109.608	512.48
2	8	11	109.608	512.48
2	8	21	110.549	383
10	8	11	109.608	512.48
10	8	21	110.549	383
11	8	21	110.549	383
5	9	22	110.549	383
5	9	23	110.549	383
5	9	24	110.549	383
22	9	23	108.836	310.74
22	9	24	108.836	310.74
23	9	24	108.836	310.74
8	10	25	110.549	383
8	10	26	110.549	383
8	10	27	110.549	383
25	10	26	108.836	310.74
25	10	27	108.836	310.74
26	10	27	108.836	310.74
8	11	28	110.549	383
8	11	29	110.549	383
8	11	30	110.549	383
28	11	29	108.836	310.74
28	11	30	108.836	310.74
29	11	30	108.836	310.74

Dihedrals

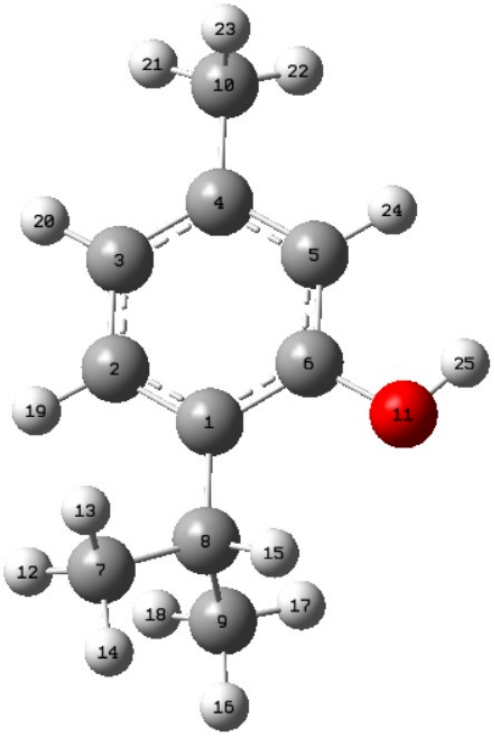
Atom Numbers				**δ / deg**	**k_ϕ / kJ mol^{-1}**	**m**
1	3	2	4	0	-1.4393	1
1	3	2	4	180	3.6777	2
1	3	2	4	0	0.9958	3
1	3	2	8	0	-1.4393	1
1	3	2	8	180	3.6777	2
1	3	2	8	0	0.9958	3
1	3	2	12	0	-1.3682	1
1	3	2	12	180	2.2426	2
1	3	2	12	0	0.5858	3
1	3	6	5	0	-1.4393	1
1	3	6	5	180	3.6777	2
1	3	6	5	0	0.9958	3
1	3	6	17	0	-1.3682	1
1	3	6	17	180	2.2426	2
1	3	6	17	0	0.5858	3
1	3	6	18	0	-1.3682	1
1	3	6	18	180	2.2426	2
1	3	6	18	0	0.5858	3
2	3	1	31	180	0.5648	2
2	3	1	31	0	0.4937	3
2	3	6	5	0	0.2134	1
2	3	6	5	180	1.4267	2
2	3	6	5	0	0.6945	3
2	3	6	17	0	1.3389	1
2	3	6	17	180	-1.318	2
2	3	6	17	0	0.5523	3
2	3	6	18	0	1.3389	1
2	3	6	18	180	-1.318	2
2	3	6	18	0	0.5523	3
2	4	7	5	0	0.2134	1
2	4	7	5	180	1.4267	2
2	4	7	5	0	0.6945	3
2	4	7	19	0	1.3389	1
2	4	7	19	180	-1.318	2

2	4	7	19	0	0.5523	3
2	4	7	20	0	1.3389	1
2	4	7	20	180	-1.318	2
2	4	7	20	0	0.5523	3
2	8	10	25	0	1.3389	1
2	8	10	25	180	-1.318	2
2	8	10	25	0	0.5523	3
2	8	10	26	0	1.3389	1
2	8	10	26	180	-1.318	2
2	8	10	26	0	0.5523	3
2	8	10	27	0	1.3389	1
2	8	10	27	180	-1.318	2
2	8	10	27	0	0.5523	3
2	8	11	28	0	1.3389	1
2	8	11	28	180	-1.318	2
2	8	11	28	0	0.5523	3
2	8	11	29	0	1.3389	1
2	8	11	29	180	-1.318	2
2	8	11	29	0	0.5523	3
2	8	11	30	0	1.3389	1
2	8	11	30	180	-1.318	2
2	8	11	30	0	0.5523	3
3	2	4	7	0	0.2134	1
3	2	4	7	180	1.4267	2
3	2	4	7	0	0.6945	3
3	2	4	14	0	1.3389	1
3	2	4	14	180	-1.318	2
3	2	4	14	0	0.5523	3
3	2	4	15	0	1.3389	1
3	2	4	15	180	-1.318	2
3	2	4	15	0	0.5523	3
3	2	8	10	0	0.2134	1
3	2	8	10	180	1.4267	2
3	2	8	10	0	0.6945	3
3	2	8	11	0	0.2134	1
3	2	8	11	180	1.4267	2
3	2	8	11	0	0.6945	3
3	2	8	21	0	1.3389	1
3	2	8	21	180	-1.318	2
3	2	8	21	0	0.5523	3
3	6	5	7	0	0.2134	1
3	6	5	7	180	1.4267	2
3	6	5	7	0	0.6945	3
3	6	5	9	0	0.2134	1
3	6	5	9	180	1.4267	2
3	6	5	9	0	0.6945	3
3	6	5	16	0	1.3389	1
3	6	5	16	180	-1.318	2
3	6	5	16	0	0.5523	3
4	2	3	6	0	0.2134	1
4	2	3	6	180	1.4267	2
4	2	3	6	0	0.6945	3
4	2	3	13	0	1.3389	1
4	2	3	13	180	-1.318	2
4	2	3	13	0	0.5523	3
4	2	8	10	0	0.2134	1
4	2	8	10	180	1.4267	2
4	2	8	10	0	0.6945	3
4	2	8	11	0	0.2134	1
4	2	8	11	180	1.4267	2
4	2	8	11	0	0.6945	3
4	2	8	21	0	1.3389	1
4	2	8	21	180	-1.318	2
4	2	8	21	0	0.5523	3
4	7	5	6	0	0.2134	1
4	7	5	6	180	1.4267	2
4	7	5	6	0	0.6945	3
4	7	5	9	0	0.2134	1
4	7	5	9	180	1.4267	2
4	7	5	9	0	0.6945	3
4	7	5	16	0	1.3389	1
4	7	5	16	180	-1.318	2
4	7	5	16	0	0.5523	3
5	6	3	13	0	1.3389	1
5	6	3	13	180	-1.318	2
5	6	3	13	0	0.5523	3

5	7	4	14	0	1.3389	1
5	7	4	14	180	-1.318	2
5	7	4	14	0	0.5523	3
5	7	4	15	0	1.3389	1
5	7	4	15	180	-1.318	2
5	7	4	15	0	0.5523	3
6	3	1	31	180	0.5648	2
6	3	1	31	0	0.4937	3
6	3	2	8	0	0.2134	1
6	3	2	8	180	1.4267	2
6	3	2	8	0	0.6945	3
6	3	2	12	0	1.3389	1
6	3	2	12	180	-1.318	2
6	3	2	12	0	0.5523	3
6	5	7	19	0	1.3389	1
6	5	7	19	180	-1.318	2
6	5	7	19	0	0.5523	3
6	5	7	20	0	1.3389	1
6	5	7	20	180	-1.318	2
6	5	7	20	0	0.5523	3
6	5	9	22	0	1.3389	1
6	5	9	22	180	-1.318	2
6	5	9	22	0	0.5523	3
6	5	9	23	0	1.3389	1
6	5	9	23	180	-1.318	2
6	5	9	23	0	0.5523	3
6	5	9	24	0	1.3389	1
6	5	9	24	180	-1.318	2
6	5	9	24	0	0.5523	3
7	4	2	8	0	0.2134	1
7	4	2	8	180	1.4267	2
7	4	2	8	0	0.6945	3
7	4	2	12	0	1.3389	1
7	4	2	12	180	-1.318	2
7	4	2	12	0	0.5523	3
7	5	6	17	0	1.3389	1
7	5	6	17	180	-1.318	2
7	5	6	17	0	0.5523	3
7	5	6	18	0	1.3389	1
7	5	6	18	180	-1.318	2
7	5	6	18	0	0.5523	3
7	5	9	22	0	1.3389	1
7	5	9	22	180	-1.318	2
7	5	9	22	0	0.5523	3
7	5	9	23	0	1.3389	1
7	5	9	23	180	-1.318	2
7	5	9	23	0	0.5523	3
7	5	9	24	0	1.3389	1
7	5	9	24	180	-1.318	2
7	5	9	24	0	0.5523	3
8	2	3	13	0	1.3389	1
8	2	3	13	180	-1.318	2
8	2	3	13	0	0.5523	3
8	2	4	14	0	1.3389	1
8	2	4	14	180	-1.318	2
8	2	4	14	0	0.5523	3
8	2	4	15	0	1.3389	1
8	2	4	15	180	-1.318	2
8	2	4	15	0	0.5523	3
9	5	6	17	0	1.3389	1
9	5	6	17	180	-1.318	2
9	5	6	17	0	0.5523	3
9	5	6	18	0	1.3389	1
9	5	6	18	180	-1.318	2
9	5	6	18	0	0.5523	3
9	5	7	19	0	1.3389	1
9	5	7	19	180	-1.318	2
9	5	7	19	0	0.5523	3
9	5	7	20	0	1.3389	1
9	5	7	20	180	-1.318	2
9	5	7	20	0	0.5523	3
10	8	2	12	0	1.3389	1
10	8	2	12	180	-1.318	2
10	8	2	12	0	0.5523	3
10	8	11	28	0	1.3389	1
10	8	11	28	180	-1.318	2

10	8	11	28	0	0.5523	3
10	8	11	29	0	1.3389	1
10	8	11	29	180	-1.318	2
10	8	11	29	0	0.5523	3
10	8	11	30	0	1.3389	1
10	8	11	30	180	-1.318	2
10	8	11	30	0	0.5523	3
11	8	2	12	0	1.3389	1
11	8	2	12	180	-1.318	2
11	8	2	12	0	0.5523	3
11	8	10	25	0	1.3389	1
11	8	10	25	180	-1.318	2
11	8	10	25	0	0.5523	3
11	8	10	26	0	1.3389	1
11	8	10	26	180	-1.318	2
11	8	10	26	0	0.5523	3
11	8	10	27	0	1.3389	1
11	8	10	27	180	-1.318	2
11	8	10	27	0	0.5523	3
12	2	3	13	0	0.5941	1
12	2	3	13	180	-2.8995	2
12	2	3	13	0	0.6569	3
12	2	4	14	0	0.5941	1
12	2	4	14	180	-2.8995	2
12	2	4	14	0	0.6569	3
12	2	4	15	0	0.5941	1
12	2	4	15	180	-2.8995	2
12	2	4	15	0	0.6569	3
12	2	8	21	0	0.5941	1
12	2	8	21	180	-2.8995	2
12	2	8	21	0	0.6569	3
13	3	1	31	0	1.2468	1
13	3	1	31	180	-0.5774	2
13	3	1	31	0	0.7238	3
13	3	6	17	0	0.5941	1
13	3	6	17	180	-2.8995	2
13	3	6	17	0	0.6569	3
13	3	6	18	0	0.5941	1
13	3	6	18	180	-2.8995	2
13	3	6	18	0	0.6569	3
14	4	7	19	0	0.5941	1
14	4	7	19	180	-2.8995	2
14	4	7	19	0	0.6569	3
14	4	7	20	0	0.5941	1
14	4	7	20	180	-2.8995	2
14	4	7	20	0	0.6569	3
15	4	7	19	0	0.5941	1
15	4	7	19	180	-2.8995	2
15	4	7	19	0	0.6569	3
15	4	7	20	0	0.5941	1
15	4	7	20	180	-2.8995	2
15	4	7	20	0	0.6569	3
16	5	6	17	0	0.5941	1
16	5	6	17	180	-2.8995	2
16	5	6	17	0	0.6569	3
16	5	6	18	0	0.5941	1
16	5	6	18	180	-2.8995	2
16	5	6	18	0	0.6569	3
16	5	7	19	0	0.5941	1
16	5	7	19	180	-2.8995	2
16	5	7	19	0	0.6569	3
16	5	7	20	0	0.5941	1
16	5	7	20	180	-2.8995	2
16	5	7	20	0	0.6569	3
16	5	9	22	0	0.5941	1
16	5	9	22	180	-2.8995	2
16	5	9	22	0	0.6569	3
16	5	9	23	0	0.5941	1
16	5	9	23	180	-2.8995	2
16	5	9	23	0	0.6569	3
16	5	9	24	0	0.5941	1
16	5	9	24	180	-2.8995	2
16	5	9	24	0	0.6569	3
21	8	10	25	0	0.5941	1
21	8	10	25	180	-2.8995	2
21	8	10	25	0	0.6569	3

21	8	10	26	0	0.5941	1
21	8	10	26	180	-2.8995	2
21	8	10	26	0	0.6569	3
21	8	10	27	0	0.5941	1
21	8	10	27	180	-2.8995	2
21	8	10	27	0	0.6569	3
21	8	11	28	0	0.5941	1
21	8	11	28	180	-2.8995	2
21	8	11	28	0	0.6569	3
21	8	11	29	0	0.5941	1
21	8	11	29	180	-2.8995	2
21	8	11	29	0	0.6569	3
21	8	11	30	0	0.5941	1
21	8	11	30	180	-2.8995	2
21	8	11	30	0	0.6569	3



THY

label	*q*	σ_{ii} / Å	ϵ_{ii} / kJ mol^{-1}	#
C2	-0.32609	3.55005	0.29288	1
C	-0.00174	3.55005	0.29288	2
C	-0.51837	3.55005	0.29288	3
C	0.54077	3.55005	0.29288	4
C	-0.62065	3.55005	0.29288	5
C	0.51088	3.55005	0.29288	6
C	-0.62065	3.50000	0.27610	7
C	0.63080	3.50000	0.27610	8
C	-0.46905	3.50000	0.27610	9
C	-0.53629	3.50000	0.27610	10
O2	-0.64051	3.07000	0.70788	11
H	0.14172	2.50000	0.12552	12
H	0.12843	2.50000	0.12552	13
H	0.13852	2.50000	0.12552	14
H	-0.03549	2.50000	0.12552	15
H	0.09171	2.50000	0.12552	16
H	0.11706	2.50000	0.12552	17
H	0.10186	2.50000	0.12552	18
H	0.12642	2.42000	0.12552	19
H	0.19804	2.42000	0.12552	20
H	0.13668	2.50000	0.12552	21
H	0.13847	2.50000	0.12552	22
H	0.13970	2.50000	0.12552	23
H	0.20587	2.42000	0.12552	24
H2	0.43098	0.40000	0.19246	25

Bonds

Atom Numbers		r_{eq} /Å	k_r/ kJ mol^{-1} Å^{-2}
7	8	1.508	1282.1115
7	12	1.093	1435.0745
7	13	1.093	1435.0745
7	14	1.093	1435.0745
8	9	1.508	1282.1115
8	1	1.486	1492.5875
8	15	1.093	1435.0745
9	16	1.093	1435.0745
9	17	1.093	1435.0745
9	18	1.093	1435.0745
1	2	1.374	1678.0685
1	6	1.374	1678.0685
2	3	1.374	1678.0685
2	19	1.084	1597.673
3	4	1.374	1678.0685
3	20	1.084	1597.673
4	10	1.486	1492.5875
4	5	1.374	1678.0685
10	21	1.093	1435.0745
10	22	1.093	1435.0745
10	23	1.093	1435.0745
5	6	1.374	1678.0685
5	24	1.084	1597.673
6	11	1.376	1690.4155
11	25	0.973	2360.3745

Angles

Atom Numbers			θ_{eq} / deg	k_θ / kJ mol^{-1} rad^{-2}
2	1	6	119.977	402.88
2	1	8	120.419	483.57
6	1	8	120.419	483.57
1	2	3	119.977	402.88
1	2	19	120.571	339.05
3	2	19	120.571	339.05
2	3	4	119.977	402.88
2	3	20	120.571	339.05
4	3	20	120.571	339.05
3	4	5	119.977	402.88
3	4	10	120.419	483.57
5	4	10	120.419	483.57
4	5	6	119.977	402.88
4	5	24	120.571	339.05
6	5	24	120.571	339.05
1	6	5	119.977	402.88
1	6	11	116.495	582.94
5	6	11	116.495	582.94
8	7	12	110.549	383
8	7	13	110.549	383
8	7	14	110.549	383
12	7	13	108.836	310.74
12	7	14	108.836	310.74
13	7	14	108.836	310.74
1	8	7	108.617	455.27
1	8	9	108.617	455.27
1	8	15	109.491	377.58
7	8	9	109.608	512.48
7	8	15	110.549	383
9	8	15	110.549	383
8	9	16	110.549	383
8	9	17	110.549	383
8	9	18	110.549	383
16	9	17	108.836	310.74
16	9	18	108.836	310.74
17	9	18	108.836	310.74
4	10	21	109.491	377.58
4	10	22	109.491	377.58
4	10	23	109.491	377.58
21	10	22	108.836	310.74
21	10	23	108.836	310.74
22	10	23	108.836	310.74
6	11	25	105.409	437.2

Dihedrals

Atom Numbers				δ / deg	k_ϕ / kJ mol^{-1}	m
1	2	3	4	180	14.644	2

1	2	3	20	180	14.644	2
1	6	5	4	180	14.644	2
1	6	5	24	180	14.644	2
1	6	11	25	180	5.8618	2
1	8	7	12	0	0.8159	3
1	8	7	13	0	0.8159	3
1	8	7	14	0	0.8159	3
1	8	9	16	0	0.8159	3
1	8	9	17	0	0.8159	3
1	8	9	18	0	0.8159	3
2	1	6	5	180	14.644	2
2	1	6	11	180	14.644	2
2	1	8	7	180	0.9414	2
2	1	8	9	180	0.9414	2
2	1	8	15	180	-0.8786	2
2	1	8	15	0	0.8201	3
2	3	4	5	180	14.644	2
2	3	4	10	180	14.644	2
3	2	1	6	180	14.644	2
3	2	1	8	180	14.644	2
3	4	5	6	180	14.644	2
3	4	5	24	180	14.644	2
3	4	10	21	180	-0.8786	2
3	4	10	21	0	0.8201	3
3	4	10	22	180	-0.8786	2
3	4	10	22	0	0.8201	3
3	4	10	23	180	-0.8786	2
3	4	10	23	0	0.8201	3
4	3	2	19	180	14.644	2
4	5	6	11	180	14.644	2
5	4	3	20	180	14.644	2
5	4	10	21	180	-0.8786	2
5	4	10	21	0	0.8201	3
5	4	10	22	180	-0.8786	2
5	4	10	22	0	0.8201	3
5	4	10	23	180	-0.8786	2
5	4	10	23	0	0.8201	3
5	6	1	8	180	14.644	2
5	6	11	25	180	5.8618	2
6	1	2	19	180	14.644	2
6	1	8	7	180	0.9414	2
6	1	8	9	180	0.9414	2
6	1	8	15	180	-0.8786	2
6	1	8	15	0	0.8201	3
6	5	4	10	180	14.644	2
7	8	9	16	0	1.3389	1
7	8	9	16	180	-1.318	2
7	8	9	16	0	0.5523	3
7	8	9	17	0	1.3389	1
7	8	9	17	180	-1.318	2
7	8	9	17	0	0.5523	3
7	8	9	18	0	1.3389	1
7	8	9	18	180	-1.318	2
7	8	9	18	0	0.5523	3
8	1	2	19	180	14.644	2
8	1	6	11	180	14.644	2
9	8	7	12	0	1.3389	1
9	8	7	12	180	-1.318	2
9	8	7	12	0	0.5523	3
9	8	7	13	0	1.3389	1
9	8	7	13	180	-1.318	2
9	8	7	13	0	0.5523	3
9	8	7	14	0	1.3389	1
9	8	7	14	180	-1.318	2
9	8	7	14	0	0.5523	3
10	4	3	20	180	14.644	2
10	4	5	24	180	14.644	2
11	6	5	24	180	14.644	2
12	7	8	15	0	0.5941	1
12	7	8	15	180	-2.8995	2
12	7	8	15	0	0.6569	3
13	7	8	15	0	0.5941	1
13	7	8	15	180	-2.8995	2
13	7	8	15	0	0.6569	3
14	7	8	15	0	0.5941	1
14	7	8	15	180	-2.8995	2

14	7	8	15	0	0.6569	3
15	8	9	16	0	0.5941	1
15	8	9	16	180	-2.8995	2
15	8	9	16	0	0.6569	3
15	8	9	17	0	0.5941	1
15	8	9	17	180	-2.8995	2
15	8	9	17	0	0.6569	3
15	8	9	18	0	0.5941	1
15	8	9	18	180	-2.8995	2
15	8	9	18	0	0.6569	3
19	2	3	20	180	14.644	2

Improper

	Atom Numbers			**ϕ_0 / deg**	**k_ϕ / kJ mol^{-1}**
1	2	6	8	0	24.0915
2	3	1	19	0	9.0291
3	4	2	20	0	9.0291
4	10	3	5	0	24.0915
8	7	1	9	0	0
8	7	1	15	0	0
6	5	1	11	0	28.9031
7	12	8	13	0	0
7	12	8	14	0	0
9	16	8	17	0	0
9	16	8	18	0	0
10	21	4	22	0	0
10	21	4	23	0	0
5	6	4	24	0	9.0291

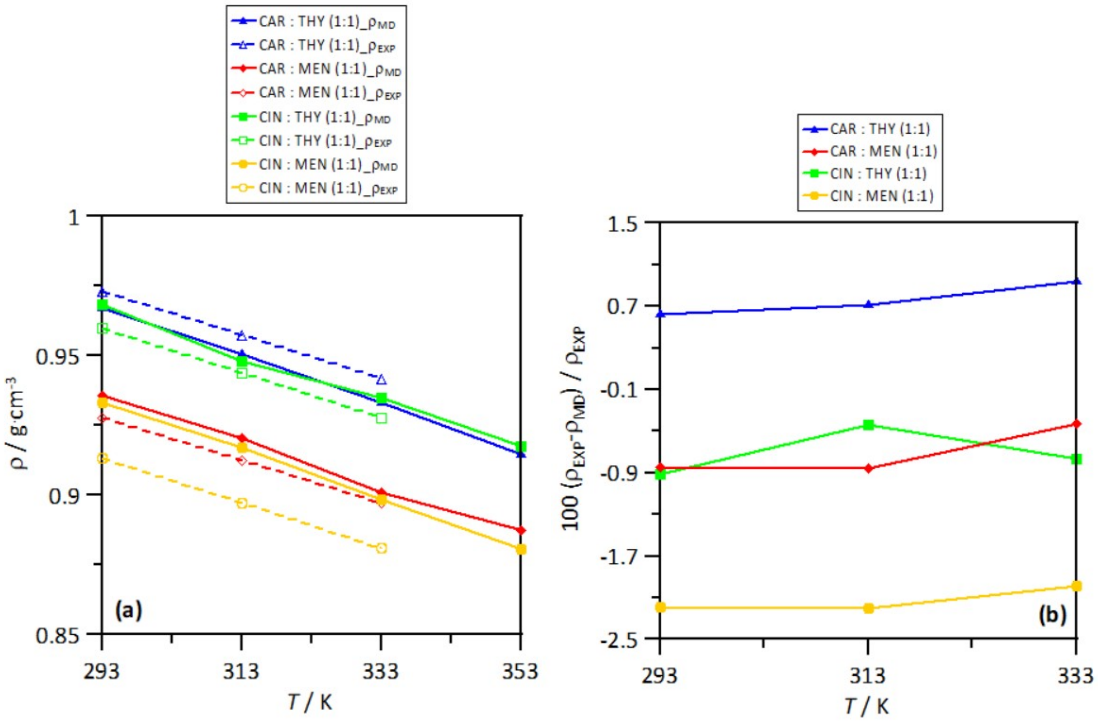


Figure S1. Comparison of experimental, ρ_{EXP}, and predicted by using MD density, ρ_{MD}, for the studied DESs at different temperatures and 0.1 MPa. 100 (ρ_{EXP} - ρ_{MD})/ρ_{EXP} stands for density deviations (%).

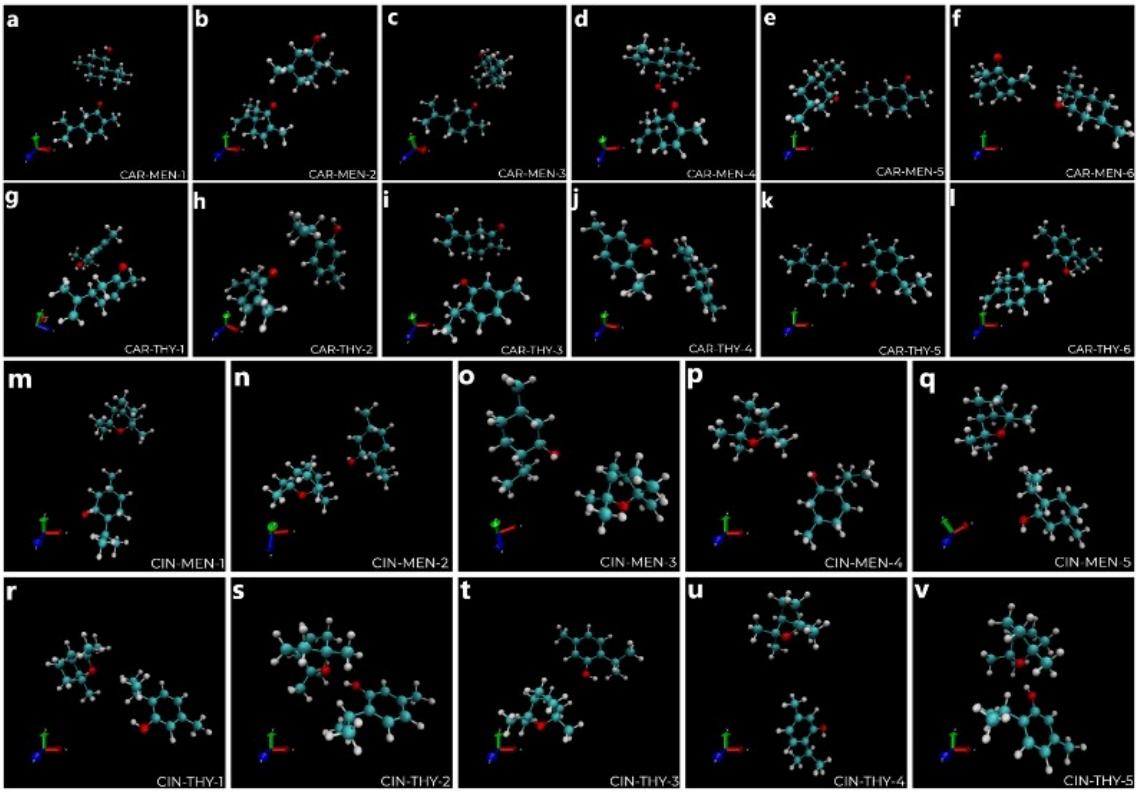


Figure S2. Studied NADES structures at various different spatial positions; (a-f) CAR:MEN, (g-i) CAR:THY, (m-q) CIN:MEN, and (r-v) CIN:THY cases.

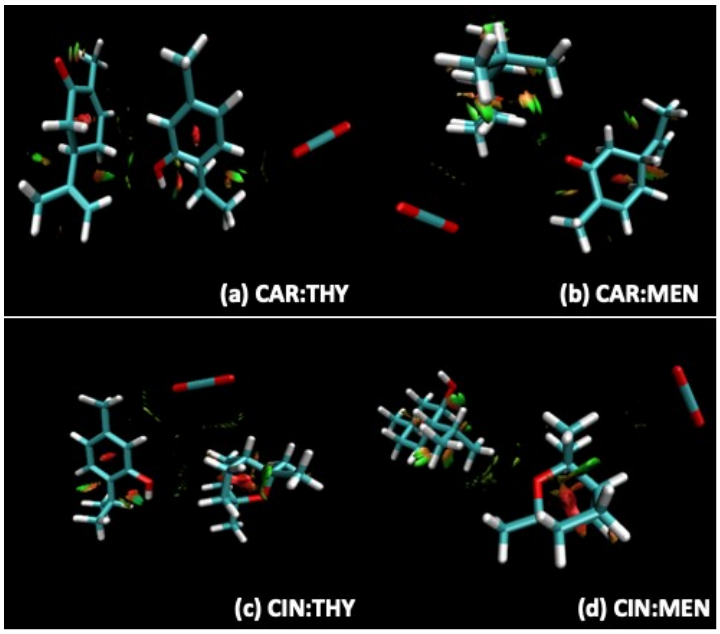


Figure S3. Reduced density gradient (RDG) isosurfaces of studied NADES+CO_2 systems.

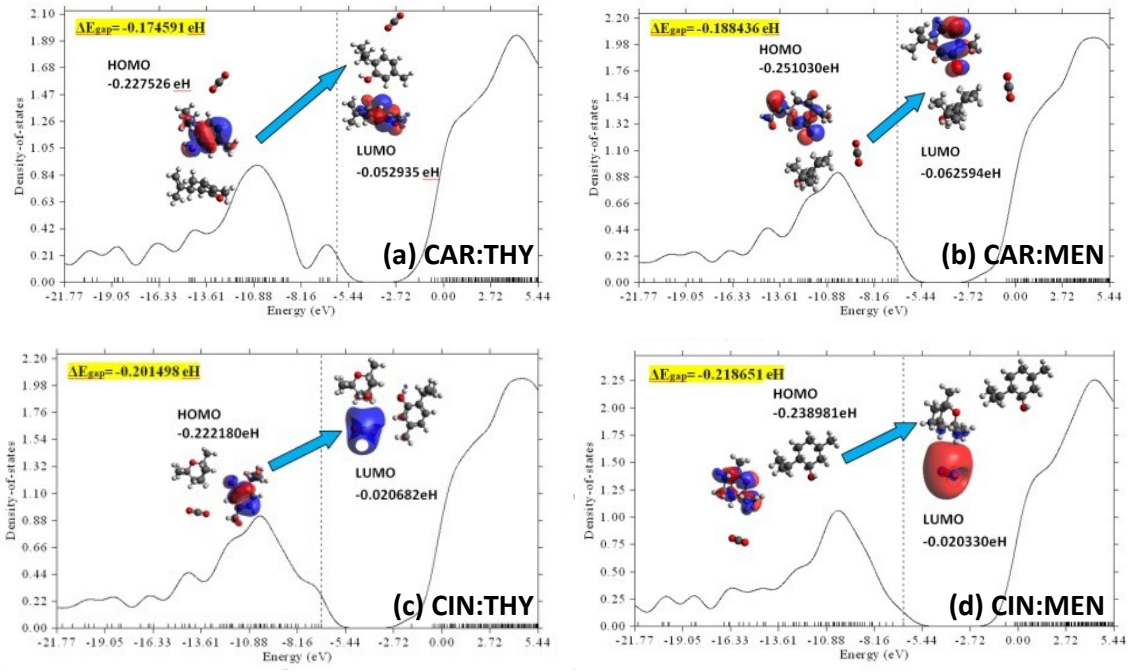


Figure S4. Density of states (DOS) plots and Homo-Lumo energy gaps for the studied NADES+CO_2 systems.

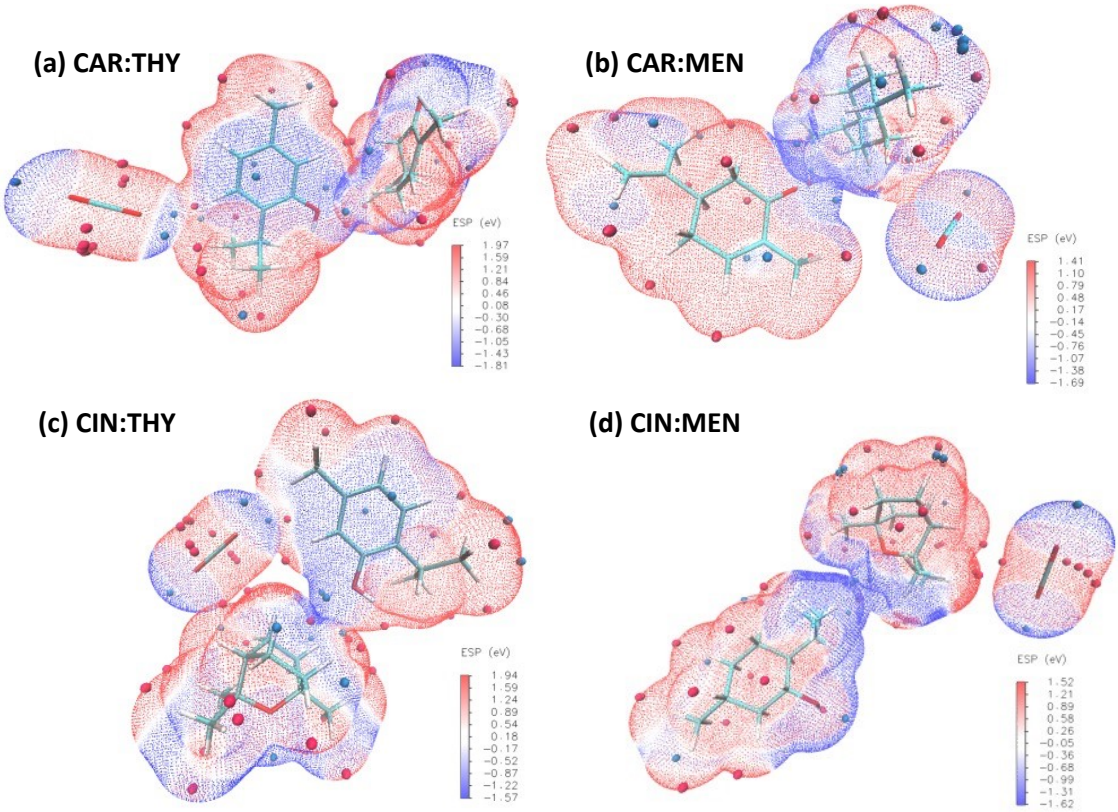


Figure S5. Electrostatic potential isosurfaces on studied NADES+CO_2 systems.

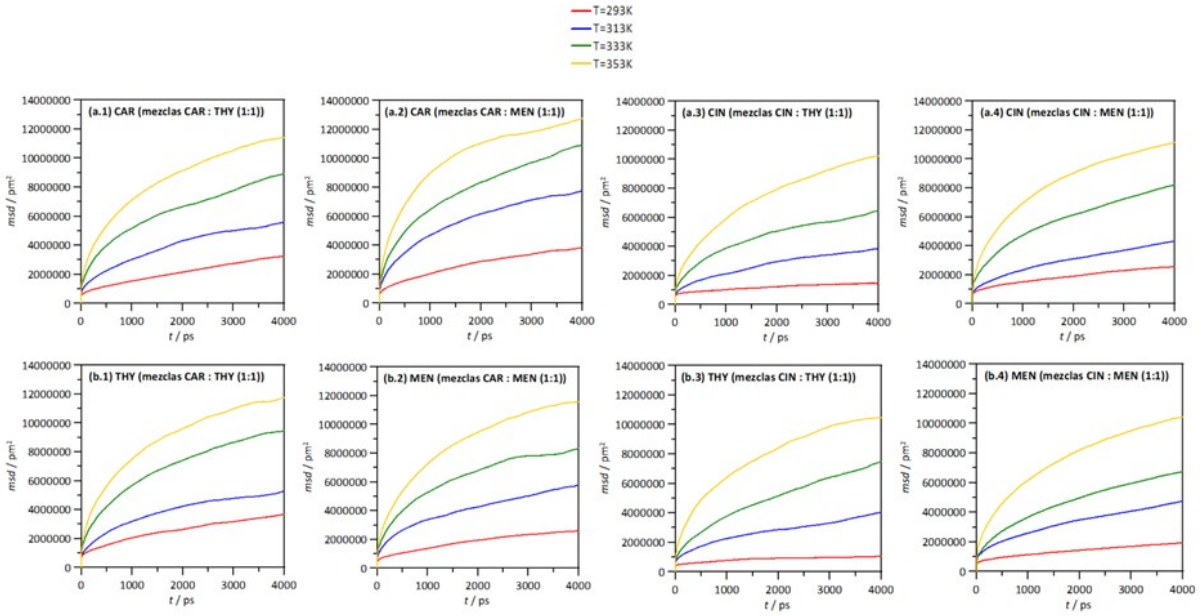


Figure S6. Mean square displacements, *msd*, for (a) HBA and (b) HBD for the studied DESs at different temperatures and 0.1 MPa.