Supporting Information

Volumetric Properties and Solubility Parameters of Cyclohexane + CO_2 Mixtures at High Pressures and their Modeling with the Sanchez-Lacombe Equation of State

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a. Reproducibility of the data

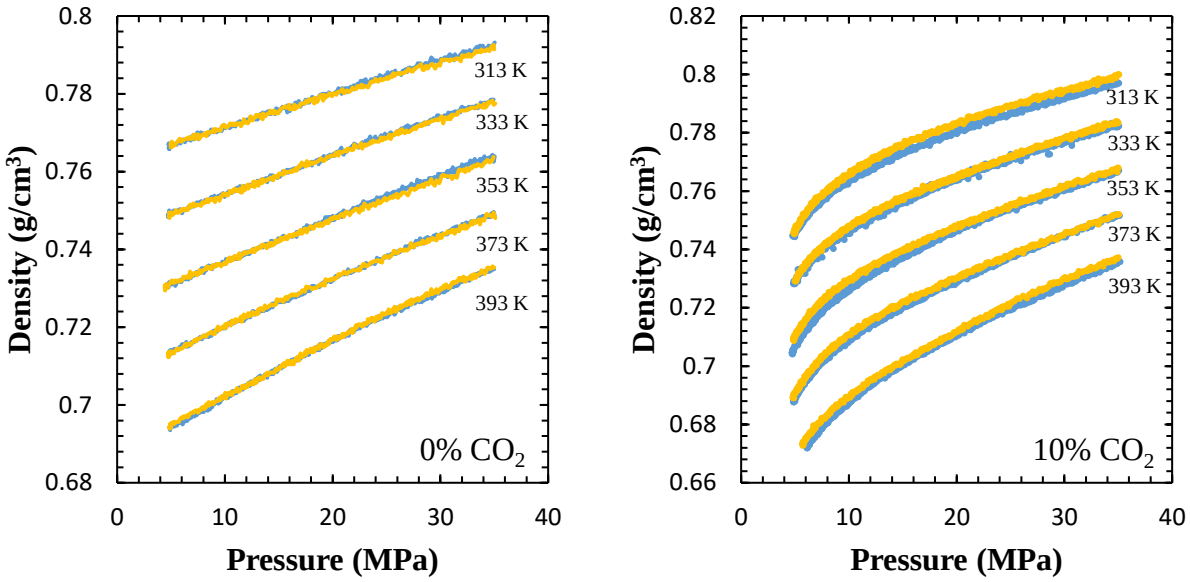
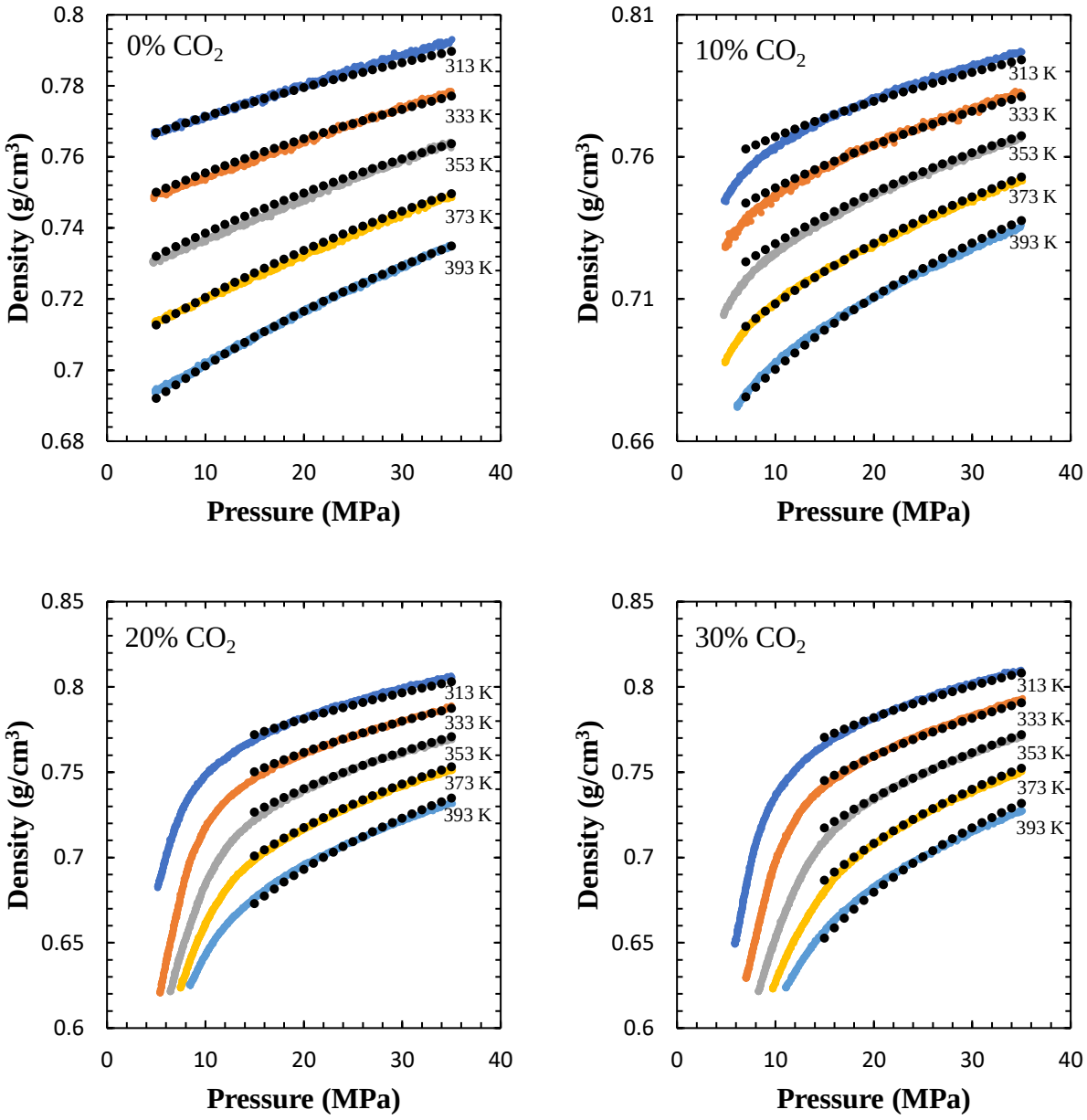


Figure S1. Density isotherms for pure cyclohexane (left) and for a mixture containing 10 wt % CO_2 (right) at 313, 333, 353, 373, and 393 K. The data at each temperture represent results from two independent runs (indicated by different colors).

b. Density of cyclohexane and mixtures with 10, 20, 30, 40, and 50 wt % CO_2 with their Sanchez-Lacombe (S-L) model descriptions



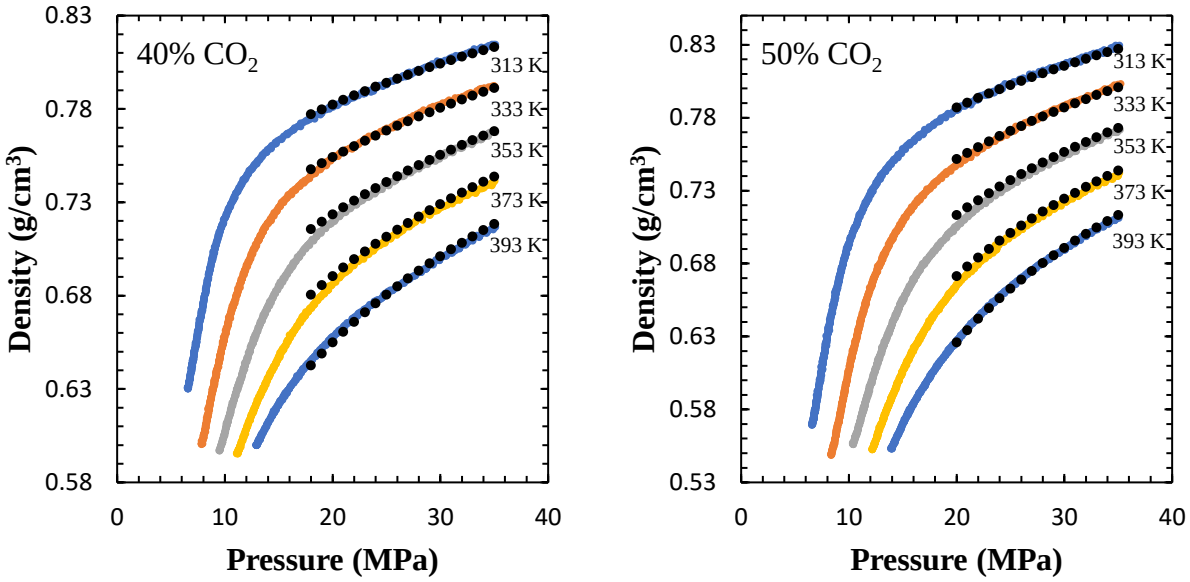
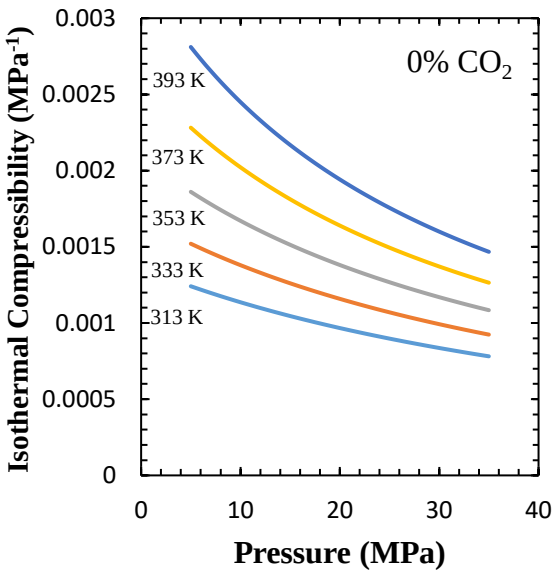
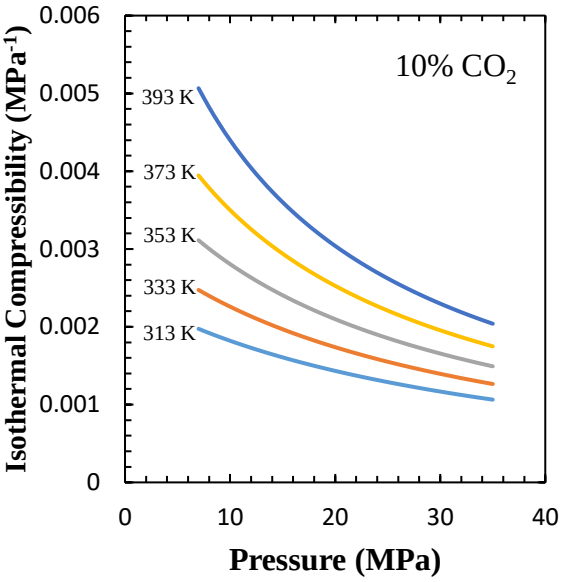
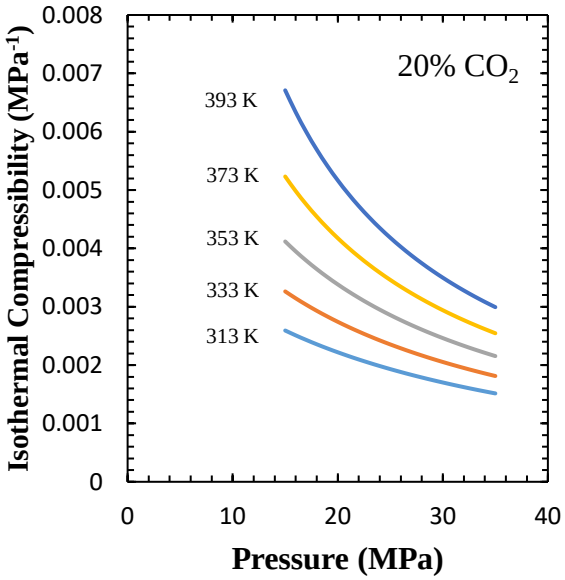


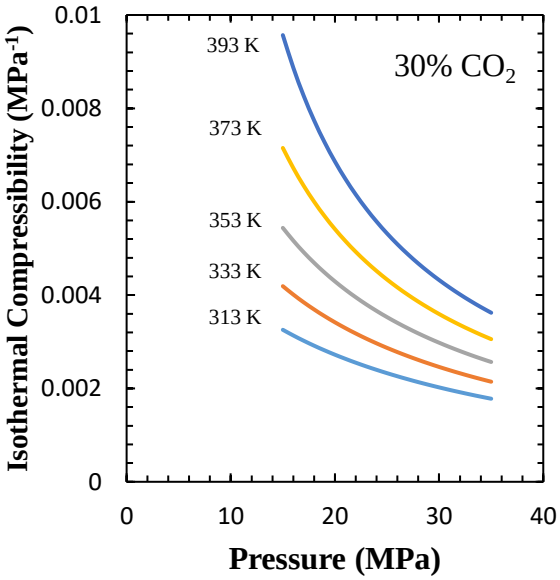
Figure S2. Density isotherms at 313, 333, 353, 373, and 393 K for pure cyclohexane and mixtures of cyclohexane and CO_2. Figures show the experimental data (solid colored curves) and their respective Sanchez-Lacombe EOS model fits (black dotted curves).

c. Isothermal Compressibility of cyclohexane and mixtures with 10, 20, 30, 40, and 50 wt % CO_2


0% CO2
393 K
373 K
353 K
333 K
313 K
Isothermal Compressibility (MPa-1)
Pressure (MPa)
0.003
0.0025
0.002
0.0015
0.001
0.0005
0
0
10
20
30
40


10% CO2
393 K
373 K
353 K
333 K
313 K
Isothermal Compressibility (MPa-1)
Pressure (MPa)
0.006
0.005
0.004
0.003
0.002
0.001
0
0
10
20
30
40


20% CO2
393 K
373 K
353 K
333 K
313 K
Isothermal Compressibility (MPa-1)
Pressure (MPa)
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
0
10
20
30
40


30% CO2
393 K
373 K
353 K
333 K
313 K
Isothermal Compressibility (MPa-1)
Pressure (MPa)
0.01
0.008
0.006
0.004
0.002
0
0
10
20
30
40

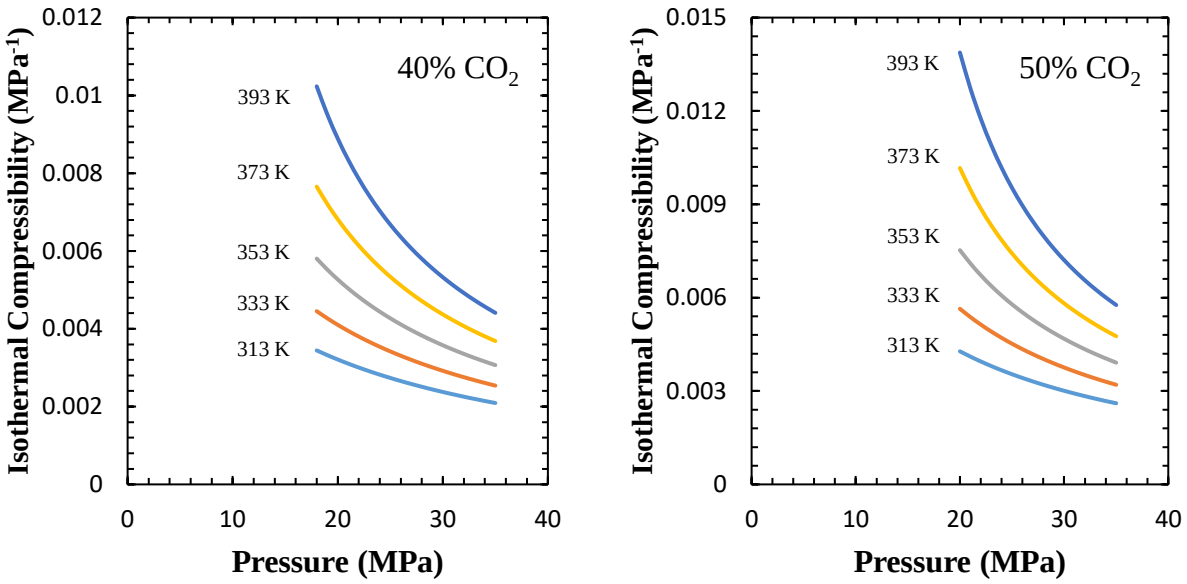
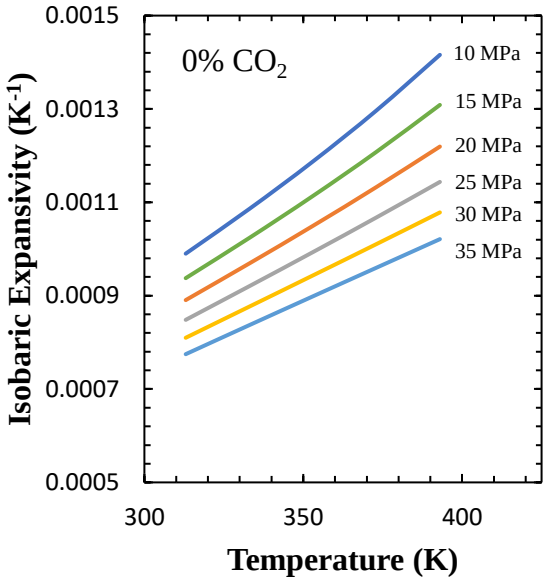
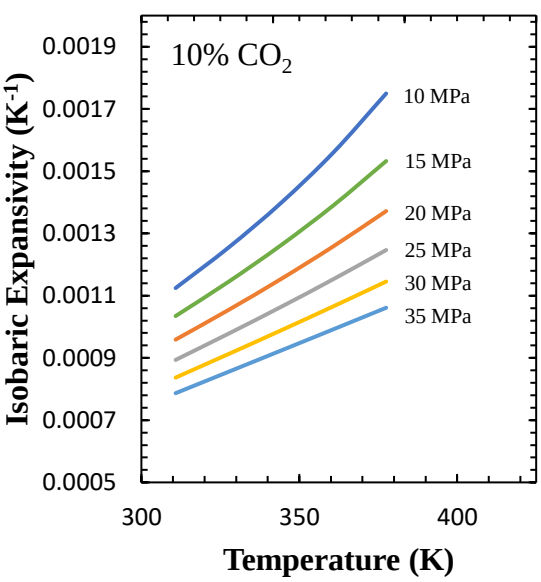
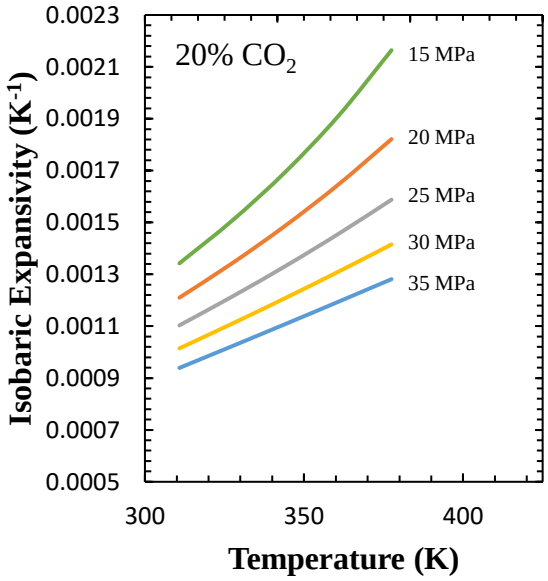


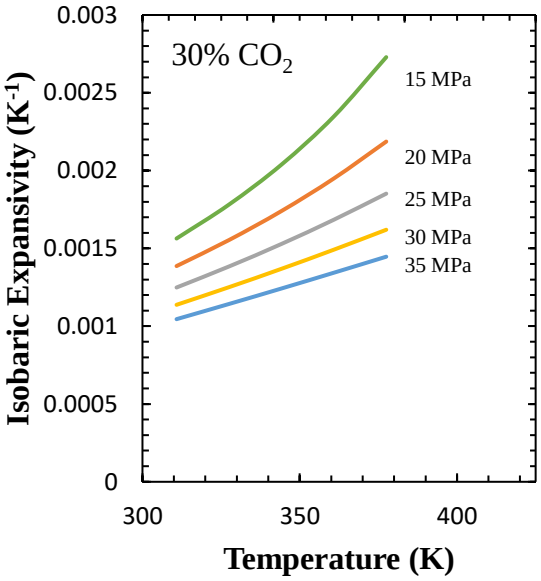
Figure S3. Variation of isothermal compressibility with pressure for cyclohexane (0% CO_2) and for mixtures containing 10, 20, 30, 40, and 50 wt % CO_2 at 313, 333, 353, 373 and 393 K.

d. Isobaric expansivity of cyclohexane and mixtures with 10, 20, 30, 40, and 50 wt % CO_2


0% CO2
10 MPa
15 MPa
20 MPa
25 MPa
30 MPa
35 MPa
Isobaric Expansivity (K-1)
Temperature (K)
0.0015
0.0013
0.0011
0.0009
0.0007
0.0005
300
350
400


10% CO2
10 MPa
15 MPa
20 MPa
25 MPa
30 MPa
35 MPa
Isobaric Expansivity (K-1)
Temperature (K)
0.0019
0.0017
0.0015
0.0013
0.0011
0.0009
0.0007
0.0005
300
350
400


20% CO2
15 MPa
20 MPa
25 MPa
30 MPa
35 MPa
Isobaric Expansivity (K-1)
Temperature (K)
0.0023
0.0021
0.0019
0.0017
0.0015
0.0013
0.0011
0.0009
0.0007
0.0005
300
350
400


30% CO2
15 MPa
20 MPa
25 MPa
30 MPa
35 MPa
Isobaric Expansivity (K-1)
Temperature (K)
0.003
0.0025
0.002
0.0015
0.001
0.0005
0
300
350
400

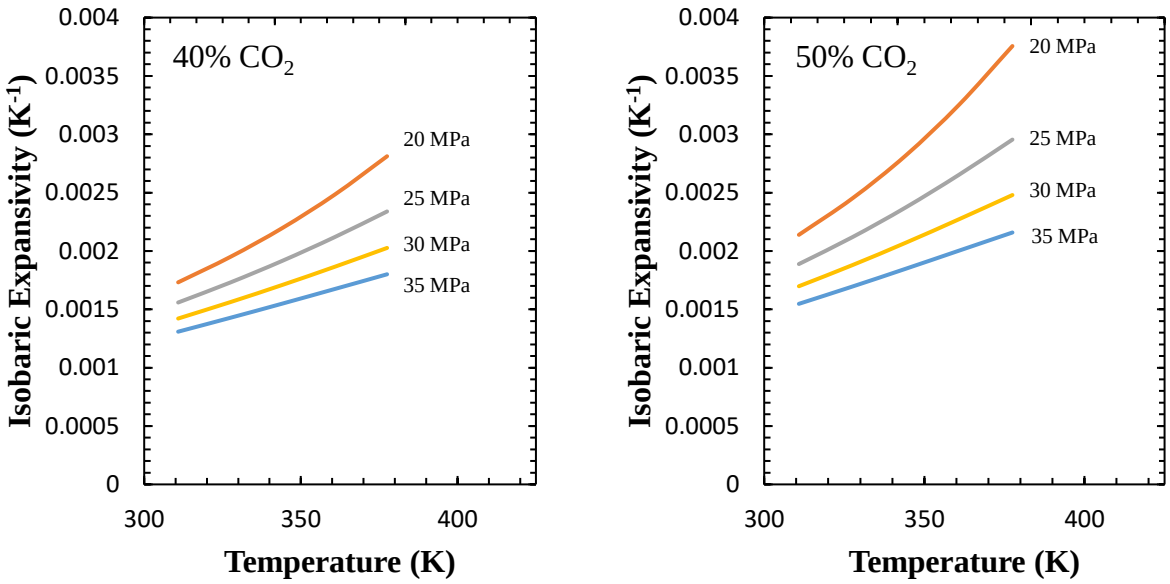
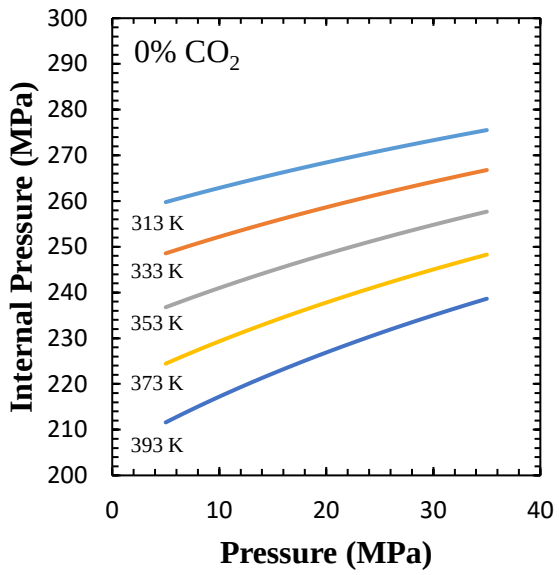
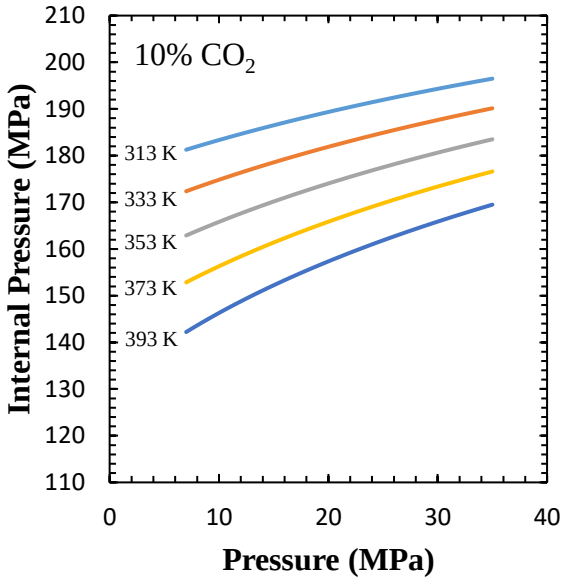
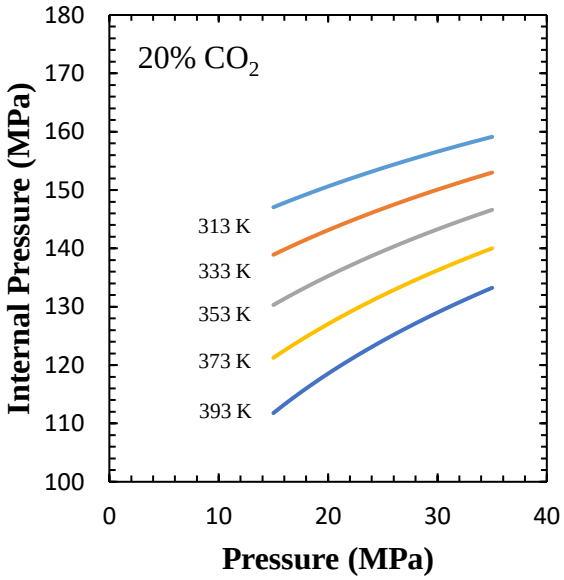


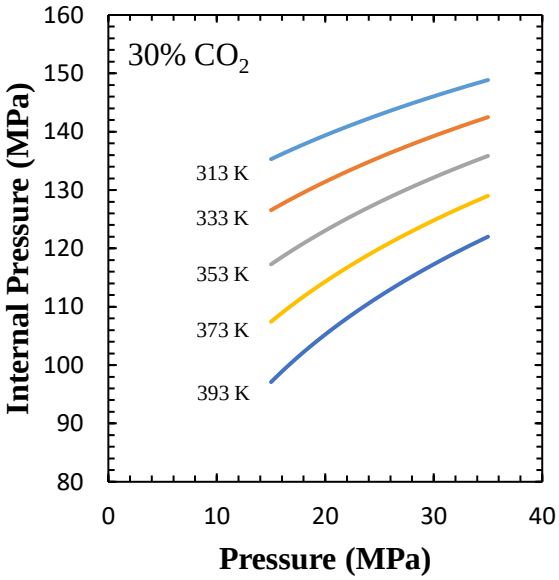
Figure S4. The variation of isobaric expansivity with temperature at selected pressures in cyclohexane (0 wt% CO_2) and mixtures containing 10, 20, 30, 40, and 50 wt % CO_2.

e. Internal pressure of cyclohexane and mixtures with 10, 20, 30, 40, and 50 wt % CO_2


0% CO2
313 K
333 K
353 K
373 K
393 K
Internal Pressure (MPa)
Pressure (MPa)
300
290
280
270
260
250
240
230
220
210
200
0
10
20
30
40


10% CO2
313 K
333 K
353 K
373 K
393 K
Internal Pressure (MPa)
Pressure (MPa)
210
200
190
180
170
160
150
140
130
120
110
0
10
20
30
40


20% CO2
313 K
333 K
353 K
373 K
393 K
Internal Pressure (MPa)
Pressure (MPa)
180
170
160
150
140
130
120
110
100
0
10
20
30
40


30% CO2
313 K
333 K
353 K
373 K
393 K
Internal Pressure (MPa)
Pressure (MPa)
160
150
140
130
120
110
100
90
80
0
10
20
30
40

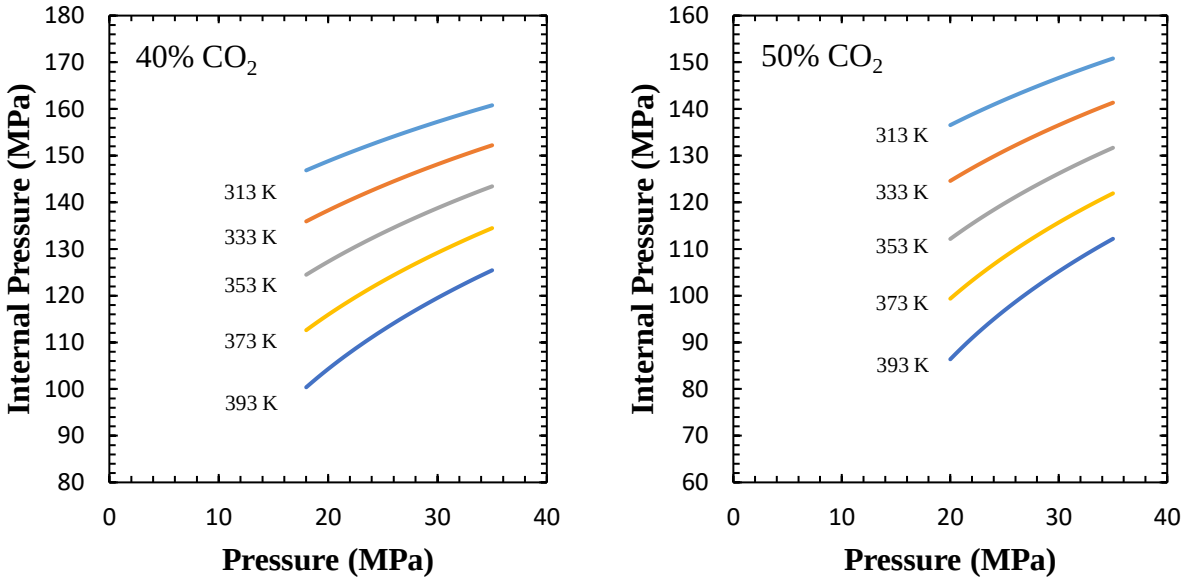
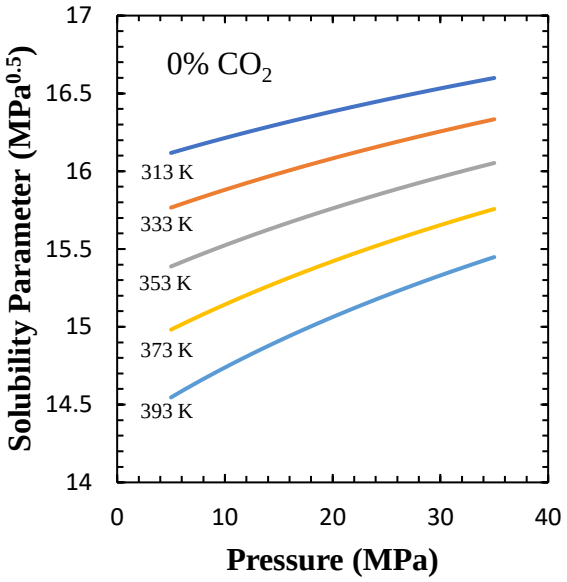
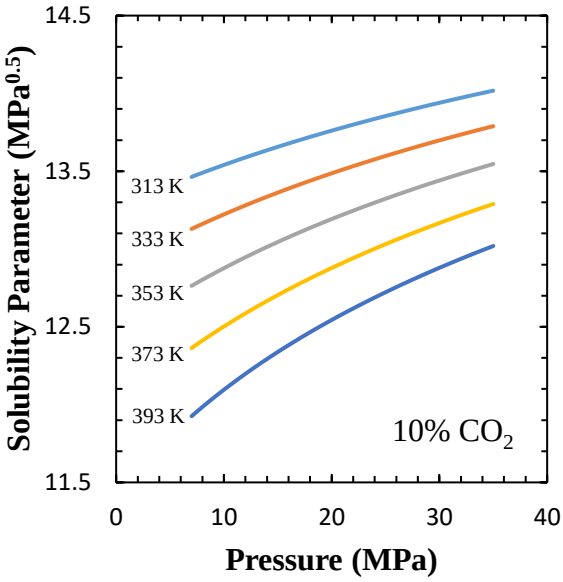
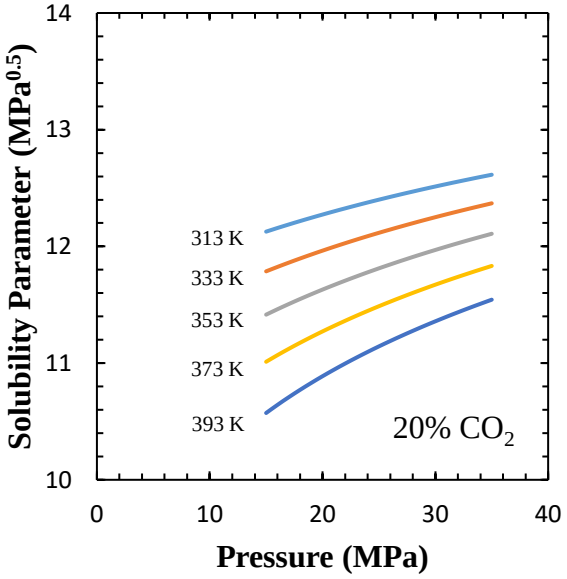


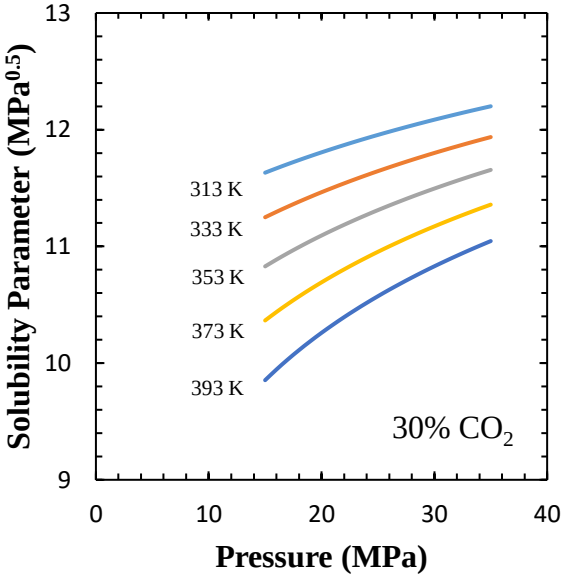
Figure S5. The variation of internal pressure with pressure for cylohexane and for its mixtures containing 30 and 50 wt % CO_2 at different temperatures**.**

f. Solubility parameters of cyclohexane and mixtures with 10, 20, 30, 40, and 50 wt % CO_2


0% CO2
313 K
333 K
353 K
373 K
393 K
Solubility Parameter (MPa0.5)
Pressure (MPa)
17
16.5
16
15.5
15
14.5
14
0
10
20
30
40


10% CO2
313 K
333 K
353 K
373 K
393 K
Solubility Parameter (MPa0.5)
Pressure (MPa)
14.5
13.5
12.5
11.5
0
10
20
30
40


20% CO2
313 K
333 K
353 K
373 K
393 K
Solubility Parameter (MPa0.5)
Pressure (MPa)
14
13
12
11
10
0
10
20
30
40


30% CO2
313 K
333 K
353 K
373 K
393 K
Solubility Parameter (MPa0.5)
Pressure (MPa)
13
12
11
10
9
0
10
20
30
40

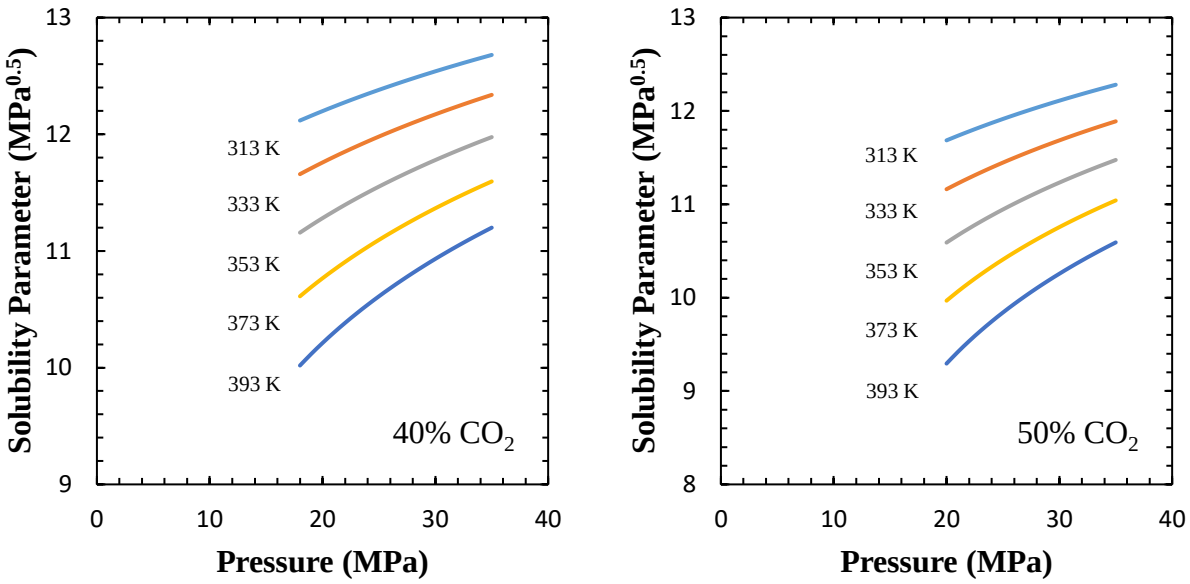
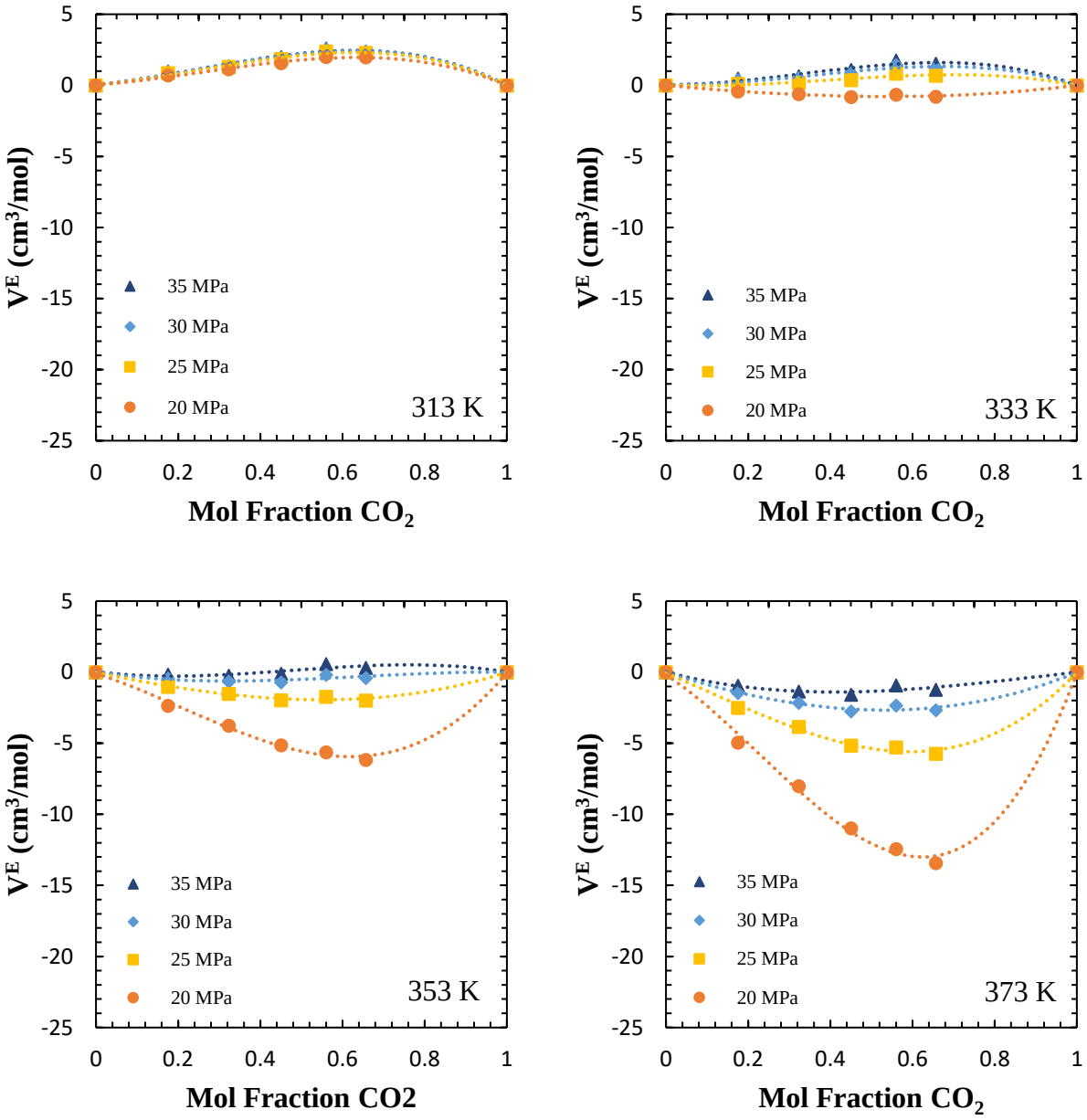


Figure S6. The variation of the solubility parameter of cyclohexane and its mixtures with 10, 20, 30, 40 and 50 wt % CO_2 with pressure at different temperatures.

g. Excess volume of mixtures of cyclohexane and CO_2 at 10, 20, 30, 40, and 50 wt % CO_2


5
0
-5
-10
-15
-20
-25
0
0.2
0.4
0.6
0.8
1
V^E (cm^3/mol)
Mol Fraction CO_2
35 MPa
30 MPa
25 MPa
20 MPa
313 K
333 K
353 K
373 K
Mol Fraction CO2

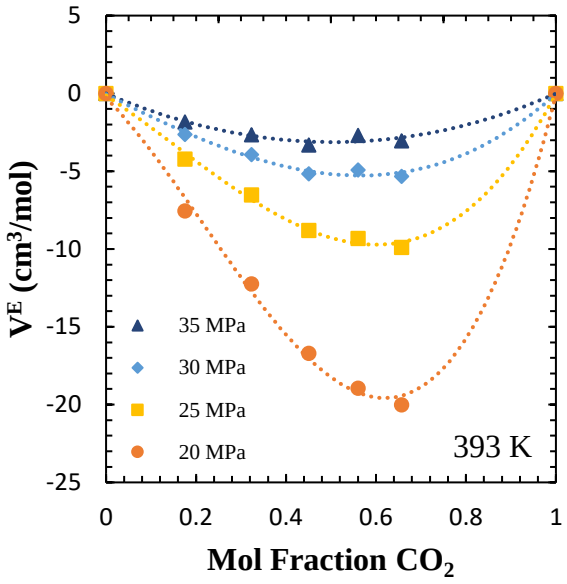


Figure S7. Comparisons of the variation of molar excess volume with carbon dioxide content at 20, 25, 30, and 35 MPa at 313, 333, 353, 373 and 393 K.

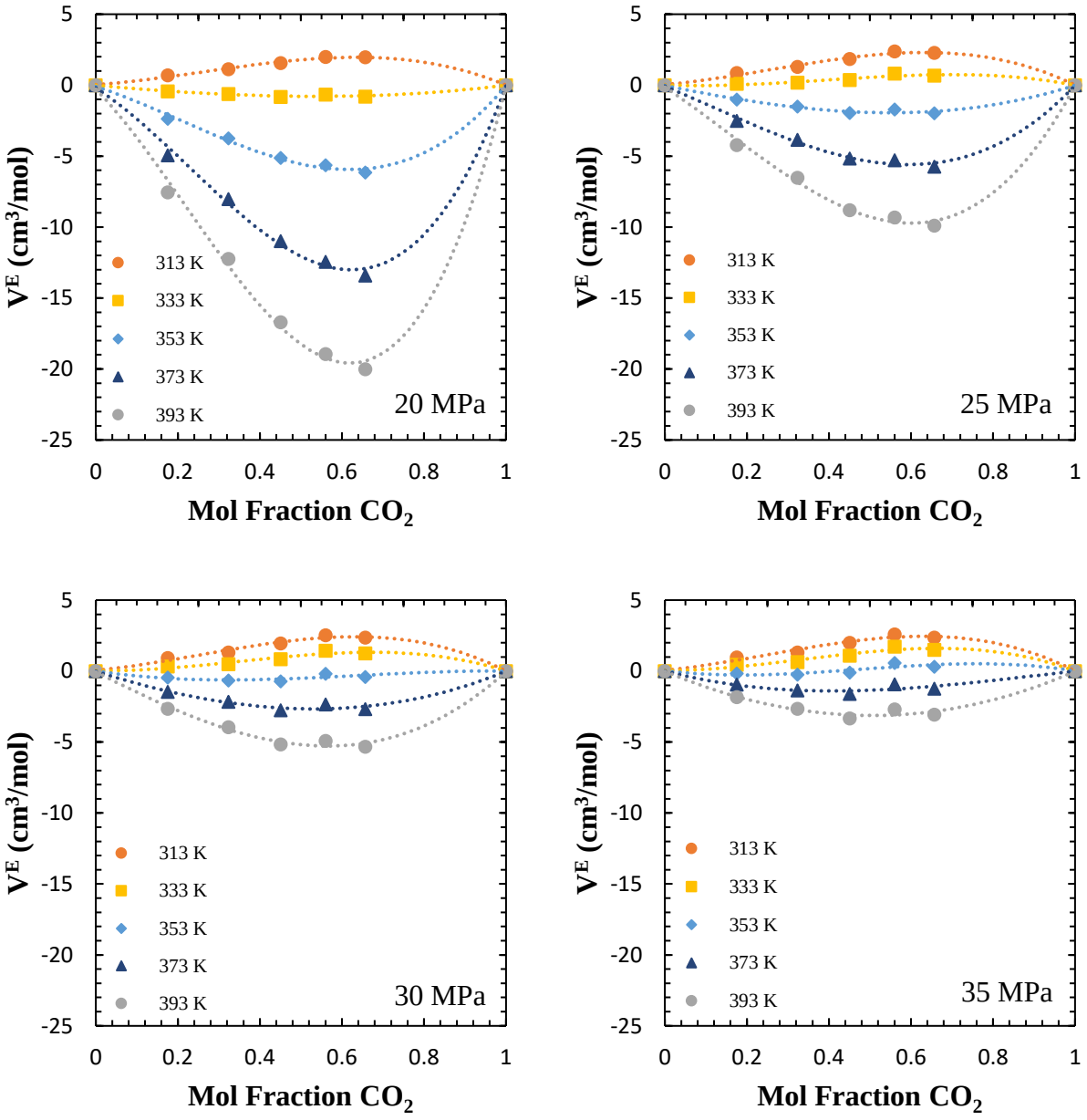
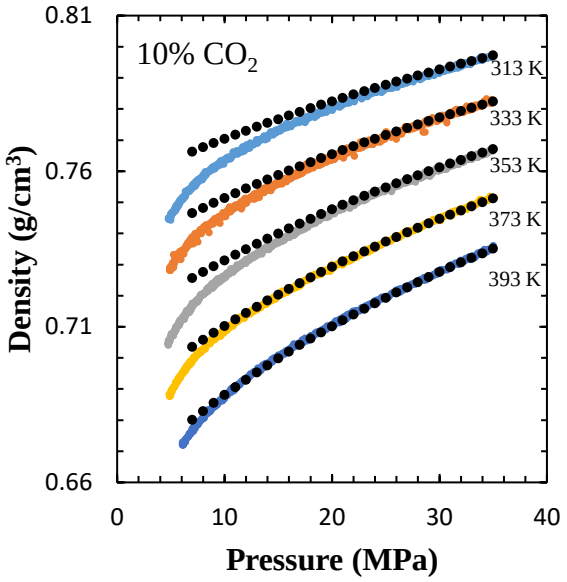
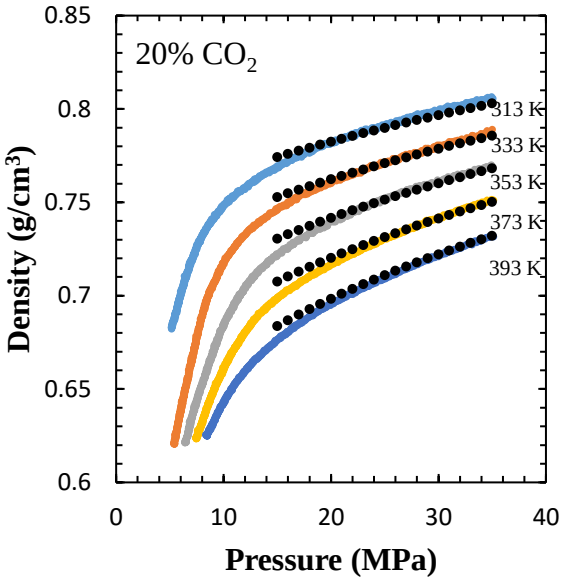
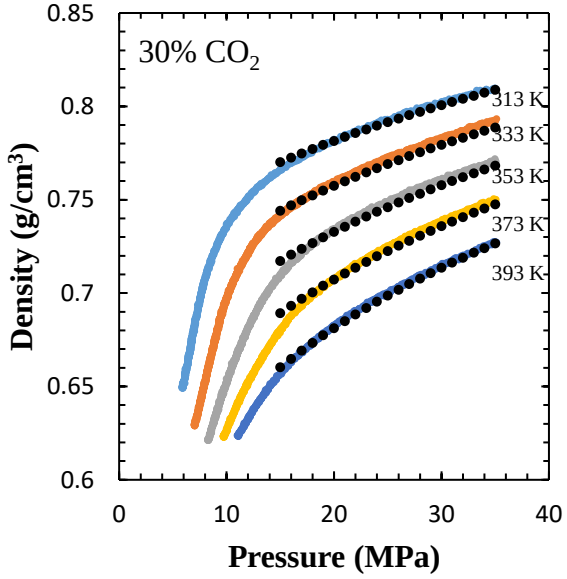


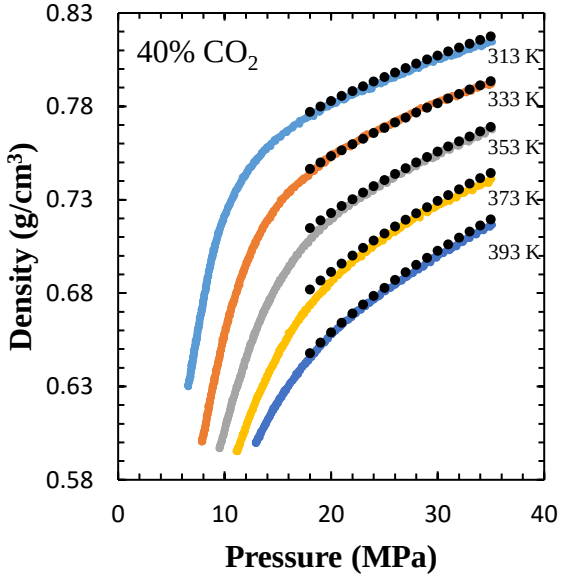
Figure S8. Comparisons of the variation of molar excess volume with carbon dioxide content at 313, 333, 353, 373 and 393 K at 20, 25, 30, and 35 MPa.

h. Modeling of the density of mixtures of cyclohexane containing 10, 20, 30, 40, and 50 wt % CO_2 using the S-L model parameters of pure CO_2 and cyclohexane using mixing rules


10% CO2
313 K
333 K
353 K
373 K
393 K
Density (g/cm3)
Pressure (MPa)
0.81
0.76
0.71
0.66
0
10
20
30
40


20% CO2
313 K
333 K
353 K
373 K
393 K
Density (g/cm3)
Pressure (MPa)
0.85
0.8
0.75
0.7
0.65
0.6
0
10
20
30
40


30% CO2
313 K
333 K
353 K
373 K
393 K
Density (g/cm3)
Pressure (MPa)
0.85
0.8
0.75
0.7
0.65
0.6
0
10
20
30
40


40% CO2
313 K
333 K
353 K
373 K
393 K
Density (g/cm3)
Pressure (MPa)
0.83
0.78
0.73
0.68
0.63
0.58
0
10
20
30
40

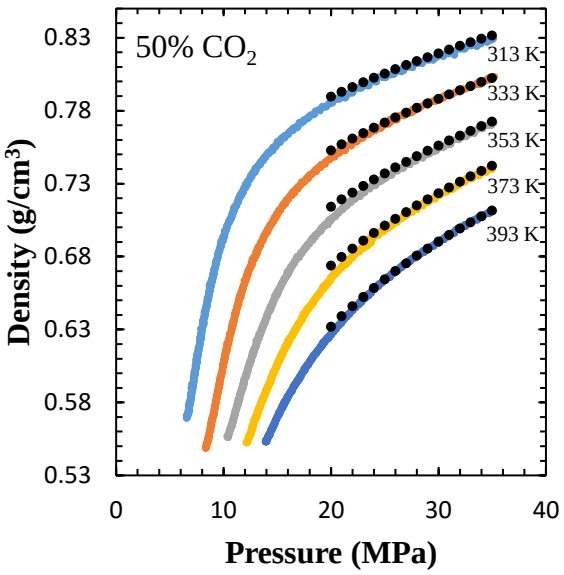


Figure S9. Comparisons of the experimental values of density (solid colored curves) with those predicted by the S-L EOS (black dotted curves) using the mixing rules (Equations 21-29) for mixtures with different mass % CO_2.

i. Tables S1-S3 present experimental density values and the predictions by the Sanchez-Lacombe equation of state by treating the mixtures as pseudo-pure compounds or by using mixing rules for pure cyclohexane, CO_2 (NIST data), and mixtures containing 10, 20, 30, 40 and 50 wt % CO_2. The model predictions are given only for the homogeneous conditions.

Table S1. Experimental values of the density (g/cm^3) of cyclohexane and its mixtures with carbon dioxide at selected P/T conditions.

T (K)	P (MPa)	Cyclohexane	10 wt % CO_2	20 wt % CO_2	30 wt % CO_2	40 wt % CO_2	50 wt % CO_2	100 wt % CO_2*
313	10	0.7712	0.7637	0.7490	0.7360	0.7220	0.6932	0.6286
	15	0.7759	0.7731	0.7688	0.7665	0.7637	0.7588	0.7802
	20	0.7800	0.7797	0.7823	0.7821	0.7812	0.7852	0.8398
	25	0.7841	0.7867	0.7911	0.7924	0.7931	0.8029	0.8795
	30	0.7879	0.7915	0.7989	0.8026	0.8054	0.8179	0.9099
	35	0.7932	0.7971	0.8058	0.8099	0.8147	0.8288	0.9348
333	10	0.7542	0.7464	0.7171	0.6973	0.6598	0.6064	0.2900
	15	0.7594	0.7570	0.7469	0.7421	0.7274	0.7089	0.6041
	20	0.7640	0.7646	0.7603	0.7595	0.7550	0.7481	0.7237
	25	0.7686	0.7727	0.7718	0.7730	0.7698	0.7701	0.7866
	30	0.7737	0.7770	0.7807	0.7835	0.7822	0.7885	0.8297
	35	0.7785	0.7823	0.7891	0.7927	0.7922	0.8029	0.8629
353	10	0.7362	0.7258	0.6832	0.6520	0.6075	-	0.2216
	15	0.7422	0.7370	0.7226	0.7099	0.6856	0.6560	0.4272
	20	0.7476	0.7467	0.7397	0.7334	0.7206	0.7056	0.5939
	25	0.7545	0.7541	0.7519	0.7490	0.7394	0.7337	0.6862
	30	0.7594	0.7607	0.7607	0.7615	0.7532	0.7541	0.7456
	35	0.7640	0.7671	0.7690	0.7709	0.7676	0.7709	0.7890
373	10	0.7197	0.7089	0.6608	0.6268	-	-	0.1886
	15	0.7264	0.7204	0.6990	0.6812	0.6476	0.6072	0.3324
	20	0.7319	0.7290	0.7168	0.7078	0.6862	0.6659	0.4805
	25	0.7382	0.7376	0.7311	0.7245	0.7098	0.6990	0.5885
	30	0.7439	0.7451	0.7417	0.7388	0.7274	0.7223	0.6619
	35	0.7486	0.7516	0.7509	0.7503	0.7415	0.7414	0.7153
393	10	0.7024	0.6880	0.6427	-	-	-	0.1673
	15	0.7094	0.7004	0.6767	0.6568	0.6228	0.5701	0.2804
	20	0.7169	0.7108	0.6964	0.6823	0.6582	0.6268	0.4012
	25	0.7232	0.7192	0.7093	0.7005	0.6810	0.6642	0.5056
	30	0.7293	0.7279	0.7211	0.7159	0.7005	0.6896	0.5852
	35	0.7349	0.7361	0.7317	0.7277	0.7167	0.7117	0.6455

*Values from NIST database

Table S2. Density values (g/cm^3) predicted by the Sanchez-Lacombe EOS treating the mixtures as pseudo-pure compounds at the same P/T conditions as in Table S1**.**

T (K)	P (MPa)	Cyclohexane	10 wt % CO_2	20 wt % CO_2	30 wt % CO_2	40 wt % CO_2	50 wt % CO_2	100 wt % CO_2
313	10	0.7714	0.7671	-	-	-	-	0.6436
	15	0.7756	0.7737	0.7719	0.7704	-	-	0.7737
	20	0.7795	0.7796	0.7812	0.7819	0.7823	0.7869	0.8338
	25	0.7831	0.7849	0.7893	0.7918	0.7940	0.8024	0.8756
	30	0.7865	0.7897	0.7965	0.8005	0.8042	0.8156	0.9081
	35	0.7897	0.7941	0.8029	0.8081	0.8132	0.8270	0.9350
333	10	0.7555	0.7491	-	-	-	-	0.2537
	15	0.7605	0.7570	0.7502	0.7451	-	-	0.6060
	20	0.7651	0.7641	0.7615	0.7593	0.7541	0.7517	0.7219
	25	0.7694	0.7704	0.7712	0.7713	0.7683	0.7709	0.7848
	30	0.7734	0.7760	0.7797	0.7816	0.7805	0.7869	0.8294
	35	0.7771	0.7812	0.7873	0.7906	0.7912	0.8007	0.8643
353	10	0.7386	0.7295	-	-	-	-	0.2069
	15	0.7444	0.7390	0.7266	0.7172	-	-	0.4120
	20	0.7498	0.7474	0.7402	0.7347	0.7235	0.7132	0.5938
	25	0.7548	0.7548	0.7518	0.7492	0.7408	0.7371	0.6864
	30	0.7594	0.7614	0.7619	0.7614	0.7554	0.7565	0.7463
	35	0.7637	0.7674	0.7707	0.7720	0.7680	0.7728	0.7909
373	10	0.7204	0.7083	-	-	-	-	0.1806
	15	0.7274	0.7197	0.7009	0.6865	-	-	0.3195
	20	0.7337	0.7296	0.7174	0.7082	0.6904	0.6713	0.4759
	25	0.7394	0.7383	0.7312	0.7255	0.7115	0.7010	0.5883
	30	0.7447	0.7460	0.7429	0.7399	0.7289	0.7243	0.6629
	35	0.7497	0.7529	0.7531	0.7523	0.7437	0.7436	0.7172
393	10	0.7012	0.6852	-	-	-	-	0.1625
	15	0.7093	0.6990	0.6729	0.6526	-	-	0.2720
	20	0.7166	0.7107	0.6930	0.6795	0.6549	0.6259	0.3948
	25	0.7233	0.7207	0.7093	0.7003	0.6805	0.6627	0.5033
	30	0.7293	0.7296	0.7229	0.7173	0.7011	0.6907	0.5852
	35	0.7350	0.7376	0.7347	0.7316	0.7183	0.7133	0.6468

Table S3. Density values (g/cm^3) of the mixtures predicted by Sanchez-Lacombe EOS using pure component parameters with mixing rules at the same P/T conditions as in Table S1.

T (K)	P (MPa)	10 wt % CO_2	20 wt % CO_2	30 wt % CO_2	40 wt % CO_2	50 wt % CO_2
313	10	0.7704	-	-	-	-
	15	0.7767	0.7741	0.7701	-	-
	20	0.7824	0.7824	0.7815	0.7828	0.7896
	25	0.7877	0.7898	0.7916	0.7958	0.8054
	30	0.7926	0.7966	0.8006	0.8073	0.8193
	35	0.7972	0.8029	0.8088	0.8176	0.8316
333	10	0.7514	-	-	-	-
	15	0.7588	0.7527	0.7442	-	-
	20	0.7655	0.7623	0.7575	0.7533	0.7527
	25	0.7716	0.7709	0.7691	0.7685	0.7718
	30	0.7772	0.7786	0.7794	0.7818	0.7880
	35	0.7824	0.7857	0.7887	0.7935	0.8023
353	10	0.7313	-	-	-	-
	15	0.7400	0.7305	0.7172	-	-
	20	0.7477	0.7416	0.7327	0.7229	0.7141
	25	0.7547	0.7514	0.7460	0.7406	0.7369
	30	0.7612	0.7602	0.7578	0.7557	0.7560
	35	0.7671	0.7681	0.7682	0.7691	0.7724
373	10	0.7102	-	-	-	-
	15	0.7203	0.7075	0.6893	-	-
	20	0.7293	0.7202	0.7073	0.6914	0.6738
	25	0.7373	0.7314	0.7225	0.7120	0.7011
	30	0.7446	0.7413	0.7358	0.7293	0.7233
	35	0.7513	0.7502	0.7475	0.7443	0.7421
393	10	0.6881	-	-	-	-
	15	0.6998	0.6837	0.6602	-	-
	20	0.7101	0.6983	0.6812	0.6590	0.6317
	25	0.7193	0.7110	0.6986	0.6828	0.6643
	30	0.7275	0.7221	0.7135	0.7026	0.6901
	35	0.7350	0.7321	0.7266	0.7195	0.7116