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Development of new coarse-grained models for chromonic liquid crystals: insights from *top-down* approaches

Thomas D. Potter, Jos Tasche, Elin L. Barrett, Martin Walker & Mark R. Wilson

Supplementary Information

1. GROMACS topology file containing force field information for the MARTINI TP6EO2M model.

```
; TP6EO2M_GMX.top

[ defaults ]
; nbfunc      comb-rule      gen-pairs      fudgeLJ fudgeQQ
1            2                yes            0.5      0.8333
1 1

[ atomtypes ]
;name bond_type      mass      charge      ptype      sigma      epsilon      Amb
CC      CC            24.00000  0.00000    A          0.0        0.0
CO      CO            25.00000  0.00000    A          0.0        0.0
AI      AI            44.00000  0.00000    A          0.0        0.0
AO      AO            31.00000  0.00000    A          0.0        0.0
P4      P4            72.00000  0.00000    A          0.0        0.0
BP4     BP4            72.00000  0.00000    A          0.0        0.0
POL     POL            24.0      0.000      A 0.0 0.0
D       D             24.0      0.000      A 0.0 0.0

[ nonbond_params ]
;name name      fubct 4*(s^6) 4*(s^12)
P4 P4 1 0.21558E-00 0.23238E-02 ; attractive
BP4 BP4 1 0.21558E-00 0.23238E-02 ; attractive
CC CC 1 0.66375E-01 0.41957E-03 ; 75intermediate, s=0.43
CO CO 1 0.66375E-01 0.41957E-03 ; 75intermediate, s=0.43
AI AI 1 0.85338E-01 0.53946E-03 ; 75almost attractive, s=0.43
AO AO 1 0.85338E-01 0.53946E-03 ; 75almost attractive, s=0.43
P4 BP4 1 0.76824E-00 0.26348E-01 ; supra attractive, s=0.57
P4 CC 1 0.11642E-00 0.12549E-02 ; semi repulsive
P4 CO 1 0.11642E-00 0.12549E-02 ; semi repulsive
P4 AI 1 0.17246E-00 0.18590E-02 ; semi attractive
P4 AO 1 0.17246E-00 0.18590E-02 ; semi attractive
P4 CC 1 0.11642E-00 0.12549E-02 ; semi repulsive
BP4 CO 1 0.11642E-00 0.12549E-02 ; semi repulsive
BP4 AI 1 0.17246E-00 0.18590E-02 ; semi attractive
BP4 AO 1 0.17246E-00 0.18590E-02 ; semi attractive
CC CO 1 0.66375E-01 0.41957E-03 ; 75intermediate, s=0.43
CC AI 1 0.58789E-01 0.37162E-03 ; 75almost intermediate, s=0.43
CC AO 1 0.58789E-01 0.37162E-03 ; 75almost intermediate, s=0.43
CO AI 1 0.58789E-01 0.37162E-03 ; 75almost intermediate, s=0.43
CO AO 1 0.58789E-01 0.37162E-03 ; 75almost intermediate, s=0.43
AI AO 1 0.85338E-01 0.53946E-03 ; 75almost attractive, s=0.43
POL POL 1 0.17246E-00 0.18590E-02 ; semi attractive
POL CC 1 0.14336E-00 0.15454E-02 ; intermediate 95%
POL CO 1 0.14336E-00 0.15454E-02 ; intermediate 95%
POL AI 1 0.16384E-00 0.17660E-02 ; semi attractive 95%
POL AO 1 0.16384E-00 0.17660E-02 ; semi attractive 95%
D D 1 0.00000E-00 0.00000E-00 ; no LJ interaction
D CC 1 0.00000E-00 0.00000E-00 ; no LJ interaction
D CO 1 0.00000E-00 0.00000E-00 ; no LJ interaction
D AI 1 0.00000E-00 0.00000E-00 ; no LJ interaction
D AO 1 0.00000E-00 0.00000E-00 ; no LJ interaction

[ moleculetype ]
;name nrexcl
TP6EO2M 2

[ atoms ]
; nr type resi res atom cgnr charge mass ; qtot bond_type
1 CC 1 1 MOL CC 1 ; -0.02
2 CC 1 1 MOL CC 2 ; -0.02
3 CC 1 1 MOL CC 3 ; -0.02
4 CO 1 1 MOL CO 4 ; 0.0801
5 CO 1 1 MOL CO 5 ; 0.0801
6 CO 1 1 MOL CO 6 ; 0.0801
7 CO 1 1 MOL CO 7 ; 0.0801
8 CO 1 1 MOL CO 8 ; 0.0801
9 CO 1 1 MOL CO 9 ; 0.0801
10 AI 1 1 MOL AI 10 ; 0.1407
11 AI 1 1 MOL AI 11 ; -0.007
12 AO 1 1 MOL AO 12 ; -0.2038
13 AI 1 1 MOL AI 13 ; 0.1407
14 AI 1 1 MOL AI 14 ; -0.007
15 AO 1 1 MOL AO 15 ; -0.2038
16 AI 1 1 MOL AI 16 ; 0.1407
17 AI 1 1 MOL AI 17 ; -0.007
```

```

18  AO   1  MOL   AO   18   ; -0.2038
19  AI   1  MOL   AI   19   ;  0.1407
20  AI   1  MOL   AI   20   ; -0.007
21  AO   1  MOL   AO   21   ; -0.2038
22  AI   1  MOL   AI   22   ;  0.1407
23  AI   1  MOL   AI   23   ; -0.007
24  AO   1  MOL   AO   24   ; -0.2038
25  AI   1  MOL   AI   25   ;  0.1407
26  AI   1  MOL   AI   26   ; -0.007
27  AO   1  MOL   AO   27   ; -0.2038

```

[bonds]

```

1 2 1 0.212 15000 ;core-core
1 3 1 0.212 15000 ;core-core
2 3 1 0.212 15000 ;core-core
1 4 1 0.212 15000 ;core-core
1 5 1 0.212 15000 ;core-core
2 8 1 0.212 15000 ;core-core
2 9 1 0.212 15000 ;core-core
3 6 1 0.212 15000 ;core-core
3 7 1 0.212 15000 ;core-core
4 5 1 0.212 15000 ;ocore-core
8 9 1 0.212 15000 ;ocore-core
6 7 1 0.212 15000 ;ocore-core
5 9 1 0.424 15000 ;core-adjcore
7 8 1 0.424 15000 ;core-adjcore
4 6 1 0.424 15000 ;core-adjcore

```

```

4 10 1 0.276 10000 ;core-arm
10 11 1 0.328 10000 ;arm-arm
11 12 1 0.282 10000 ;arm-arm
5 13 1 0.276 10000 ;core-arm
13 14 1 0.328 10000 ;arm-arm
14 15 1 0.282 10000 ;arm-arm
6 25 1 0.276 10000
25 26 1 0.328 10000
26 27 1 0.282 10000
7 22 1 0.276 10000
22 23 1 0.328 10000
23 24 1 0.282 10000
8 19 1 0.276 10000
19 20 1 0.328 10000
20 21 1 0.282 10000
9 16 1 0.276 10000
16 17 1 0.328 10000
17 18 1 0.282 10000

```

[angles]

```

;4 1 2 2 180.0 50
;4 1 3 2 120.0 50
;5 1 2 2 120.0 50
;5 1 3 2 180.0 50
;6 3 1 2 120.0 50
;6 3 2 2 180.0 50
;7 3 1 2 180.0 50
;7 3 2 2 120.0 50
;8 2 1 2 180.0 50
;8 2 3 2 120.0 50
;9 2 1 2 120.0 50
;9 2 3 2 180.0 50

```

```

3 7 22 2 180.0 85
7 22 23 2 130.0 85
22 23 24 2 130.0 85
3 6 25 2 180.0 85
6 25 26 2 130.0 85
25 26 27 2 130.0 85
1 4 10 2 180.0 85
4 10 11 2 130.0 85
10 11 12 2 130.0 85
1 5 13 2 180.0 85
5 13 14 2 130.0 85
13 14 15 2 130.0 85
2 8 19 2 180.0 85
8 19 20 2 130.0 85
19 20 21 2 130.0 85
2 9 16 2 180.0 85
9 16 17 2 130.0 85
16 17 18 2 130.0 85

```

[dihedrals]

```

;5 1 2 9 2 0.0 20.0
;8 2 3 7 2 0.0 20.0
;6 3 1 4 2 0.0 20.0
;3 7 22 23 2 180.0 5.0
;7 22 23 24 2 180.0 2.5
;3 6 25 26 2 180.0 5.0
;6 25 26 27 2 180.0 2.5
;1 4 10 11 2 180.0 5.0
;4 10 11 12 2 180.0 2.5
;1 5 13 14 2 180.0 5.0
;5 13 14 15 2 180.0 2.5
;2 8 19 20 2 180.0 5.0
;8 19 20 21 2 180.0 2.5
;2 9 16 17 2 180.0 5.0

```

;9 16 17 18 2 180.0 2.5

[dihedrals] ; impropers

i	j	k	l	func	eo	ke
; 1	2	3	5	2	0.00	8.0
; 1	2	3	4	2	0.00	8.0
; 2	1	3	9	2	0.00	8.0
; 2	3	1	8	2	0.00	8.0
; 3	2	1	7	2	0.00	8.0
; 3	2	1	6	2	0.00	8.0
; 4	5	3	1	2	0.00	8.0
; 4	5	2	1	2	0.00	8.0
; 8	9	1	2	2	0.00	8.0
; 8	9	3	2	2	0.00	8.0
; 6	7	1	3	2	0.00	8.0
; 6	7	2	3	2	0.00	8.0

[dihedrals] ; mark

; 4	1	3	6	2	0.00	30.0
; 5	1	2	9	2	0.00	30.0
; 7	3	2	8	2	0.00	30.0
; 1	2	5	4	2	0.00	30.0
; 1	3	4	5	2	0.00	30.0
; 2	1	8	9	2	0.00	30.0
; 2	3	8	9	2	0.00	30.0
; 3	1	6	7	2	0.00	30.0
; 3	2	6	7	2	0.00	30.0
; 5	1	2	9	2	0.00	30.0
; 7	3	2	8	2	0.00	30.0
; 4	1	3	6	1	180.00	30.0 1
; 5	1	2	9	1	180.00	30.0 1
; 7	3	2	8	1	180.00	30.0 1
4	1	3	2	1	0.00	30.0 1
5	1	2	3	1	0.00	30.0 1
6	3	1	2	1	0.00	30.0 1
7	3	2	1	1	0.00	30.0 1
8	2	3	1	1	0.00	30.0 1
9	2	1	3	1	0.00	30.0 1

;;;;; POLARIZABLE WATER

[moleculetype]

; molname nrexcl
W 1

[atoms]

id	type	resnr	residu	atom	cgnr	charge
1	P4	1	W	W	1	0

[moleculetype]

; molname nrexcl
AW 1

[atoms]

id	type	resnr	residu	atom	cgnr	charge
1	BP4	1	AW	AW	1	0

[system]

TP6E02M in water

[molecules]

; Compound nmols
TP6E02M 10
W 3917
AW 435

2. SAFT fits to thermodynamic data

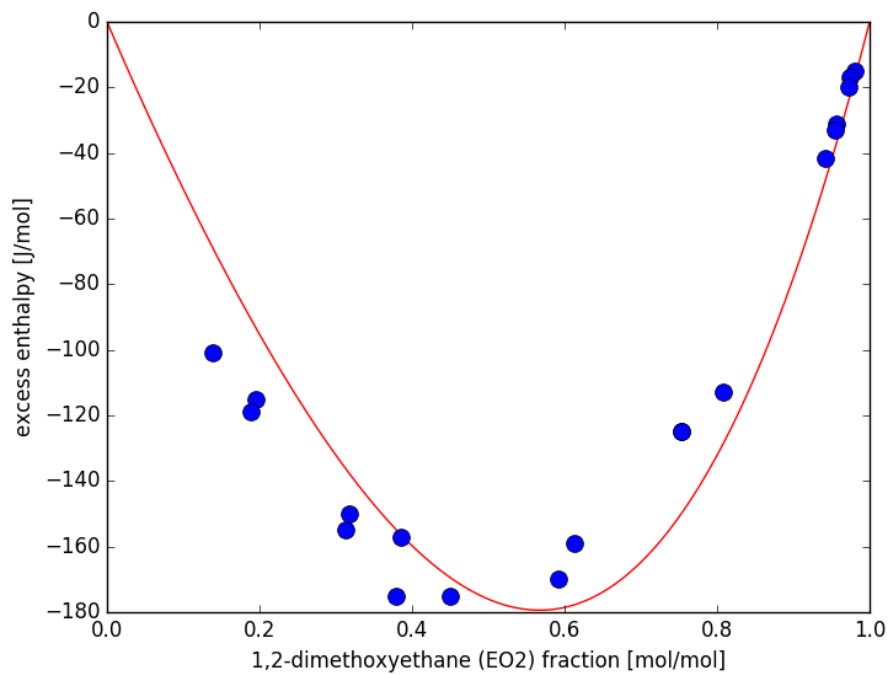


Figure 1. Enthalpies of mixing (excess enthalpies) of 1,2-dimethoxyethane (EO2) and benzene at 298.15 K. The SAFT model (lines) with fitted interaction of $\epsilon_{EO,Ar} = 323.4$ K to the experimental data (symbols)[1, 2]. Benzene is modelled in the SAFT calculations as a chain, the EO2 model is made of 2 beads fitted to properties of EO4 by Lobanova[3].

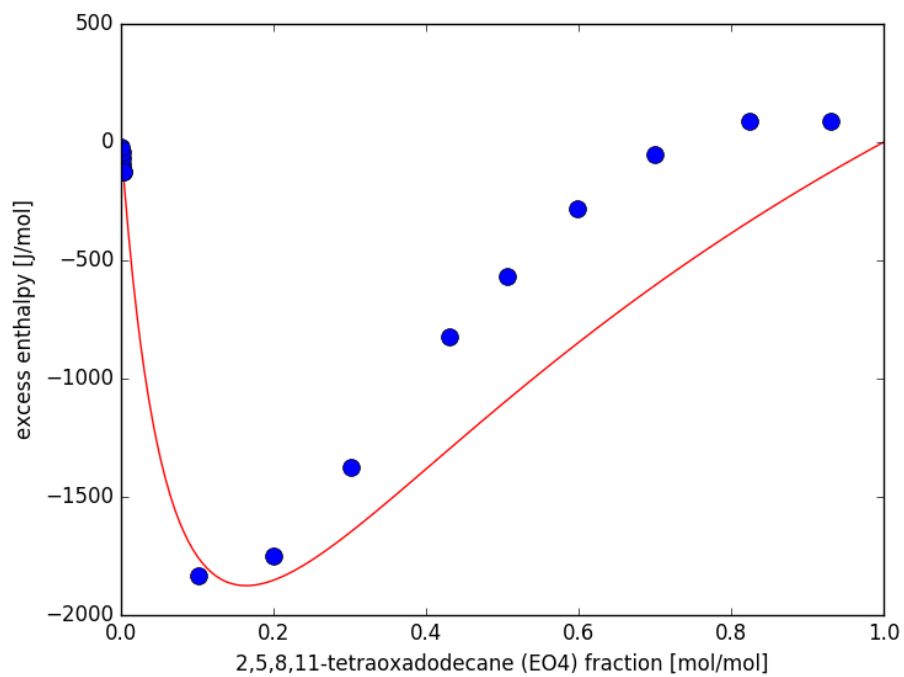


Figure 2. Enthalpies of mixing (excess enthalpies) of 2,5,8,11-tetraoxadodecane (EO4) and water at 298.15 K. The SAFT model (lines) with fitted interaction of $\epsilon_{EO,W} = 465$ K to the experimental data (symbols)[4, 5].

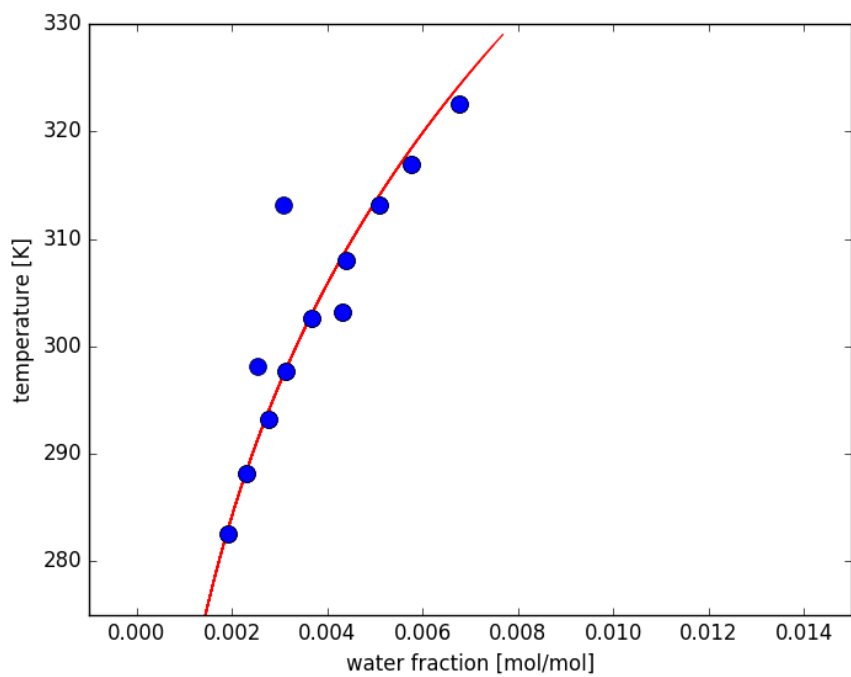


Figure 3. Solubility limit of water in benzene. The experimental data was measured at 1 bar, the SAFT calculations were performed at 5 bar to keep the water model from boiling, which does not significantly influence the solubility. The SAFT model (lines) are with a fitted interaction of $\epsilon_{A_r,W} = 195$ K to the experimental data (symbols)[6–8].





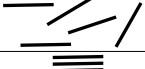


$k_{Ar/EO}$	$k_{Ar/W}$	$k_{EO/W}$	Morphology
↑	↑	↑	conglomerate 
↑	↑	=	chromonic stack 
↑	=	↑	chromonic stack with additional aggregation 
=	↑	↑	conglomerate of short stacks 
↑	=	=	monomers only 
=	↑	=	chromonic stack 
=	=	↑	chromonic stack with additional aggregation 

Figure 4. The influence of unfavourable cross-interactions on chromonic stacking. Results are shown for the final revised SAFT model with the same bond lengths as used in the MARTINI model. Up arrows indicate interactions that are less favourable than mixing rules with $k_{ij} = 0.2$. Equals signs indicate $k_{ij} = 0$. For the case where pure combining rules are used ($k_{ij} = 0$ for all cross-interactions), only monomers and transient self-assembled dimers are seen.

References

- [1] Koldobskaya LL, Gaile AA, Semenov L, Zhmaev E, Kuznetsova SY, Rumyantseva N. Enthalpy of Mixing of Hydrocarbons with Oxygen and Nitrogen Containing Polar Solvents. 1987;:1–17.
- [2] Kehiaian H, Sosnkows, Hryniewir. Enthalpy of Mixing of Ethers with Hydrocarbons at 25 Degrees C and Its Analysis in Terms of Molecular Surface Interactions. J Chim Phys-Chim Biol. 1971;68(6):922–934; wOS:A1971J711400014.
- [3] Lobanova O. Development of coarse-grained force fields from a molecular based equation of state for thermodynamic and structural properties of complex fluids [dissertation]. Imperial College London; 2014; Available from: <http://hdl.handle.net/10044/1/26139>.
- [4] Burgdorf R. Untersuchungen thermophysikalischer Eigenschaften ausgewählter organischer Flüssigkeitsgemische. Als ms. gedr ed. Berichte aus der Verfahrenstechnik; Aachen: Shaker; 1995; oCLC: 75622577.
- [5] Dohnal V, Roux AH, Hynek V. Limiting partial molar excess enthalpies by flow calorimetry: Some organic solvents in water. Journal of Solution Chemistry. 1994 Aug;23(8):889–900; Available from: <http://link.springer.com/10.1007/BF00972752>.
- [6] Bittrich H, Gedan H, Feix G. Influencing the solubility of hydrocarbons in water. Z Phys Chem Leipzig. 1979;260(5):1009–1013.
- [7] Moule DC, Thurston WM. A Method for the Determination of Water in Nonpolar Liquids; The Solubility of Water in Benzene. Canadian Journal of Chemistry. 1966 Jun;44(12):1361–1367; Available from: <http://www.nrcresearchpress.com/doi/abs/10.1139/v66-204>.
- [8] Tare J, Thurston S, Kher M. Studies in Ternary Phase (Liquid) Equilibrium. 1976;18(4):27–30.