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Validating an optimized GAFF force field for liquid crystals: T_{NI} predictions for bent-core mesogens and the first atomistic predictions of a dark conglomerate phase

Nicola Jane Boyd[a] and Mark R. Wilson *[a]

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Supplementary Material

[a] *Department of Chemistry, Durham University, South Road, Durham, DH1 3LE, United Kingdom.*
∗ *Author for correspondence. E-mail: mark.wilson@durham.ac.uk*
† Electronic Supplementary Information (ESI) available: force field parameters and chemical structures of fragment molecules studied. See DOI: 10.1039/b000000x/

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Table S 1 Optimized Ryckaert-Bellemans (RB) parameters used in GAFF-LCFF. [a]GAFFlipid RB parameters.[1] [b]From current study. All other RB parameters taken from Boyd and Wilson.[2]

Dihedral	Molecule	C_0	C_1	C_2	C_3	C_4	C_5
dihedral φ_1	phenyl benzoate	7.335350	0.000000	-7.335350	0.000000	0.000000	0.000000
dihedral φ_2	phenyl benzoate	6.000000	0.000000	0.000000	0.000000	-6.000000	0.000000
dihedral ϕ_1	ODBP	4.000000	0.000000	-4.000000	0.00000	0.000000	0.000000
C-C-C-C[a]	*n*-alkane	0.56568	1.69703	0.00000	-2.26271	0.000000	0.000000
C_{ar}-OCH_2[b]	ethoxybenzene	11.5312	0.000000	-11.5312	0.000000	0.000000	0.000000

Table S 2 Optimized Lennard Jones (LJ) parameters used in GAFF-LCFF. [a]Original GAFF LC parameters. [b] GAFFlipid LJ parameters.[1] [c]Modified GAFFlipid parameters. All other LJ parameters taken from Boyd and Wilson.[2]

Atom / description	GAFF atom types	σ / nm	ε / kJ mol^{-1}
O (sp^2O in carbonyl)	o	0.295992[a]	0.478608
C (sp^2 C in aromatic ring)	ca	0.339967[a]	0.289824
O (sp^3O in ester)	os	0.300001[a]	0.611280
N (inner sp^2 N in conjugated ring)	nd	0.325000[a]	0.411280
C (inner sp^2 C in conjugated ring)	cc	0.369967[a]	0.429824
C (long *n*-alkanes)	c3	0.358140[b]	0.230120[b]
H (long *n*-alkanes)	hc	0.238760[b]	0.100420[b]
C (medium *n*-alkanes)	c3	0.353600[c]	0.287020[c]
H (medium *n*-alkanes)	hc	0.245310[c]	0.091730[c]

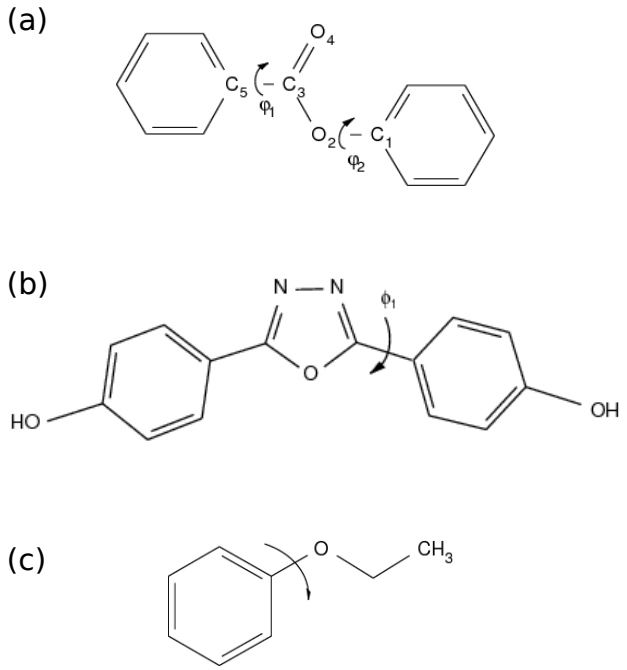

Fig. S 1 Chemical structures and dihedrals of fragments used for deriving new RB coefficients.

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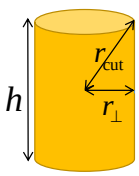
a) Normalization for $g_\perp$



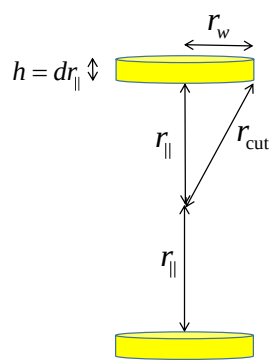
$$h = 2(r_{\text{cut}}^2 - r_\perp{}^2)^{1/2}$$

$$V_{\text{shell}} = h\pi(r_\perp + dr_\perp/2)^2 - h\pi(r_\perp - dr_\perp/2)^2$$

$$\Rightarrow V_{\text{shell}} = h\pi\left[(r_\perp^2 + r_\perp dr_\perp + dr_\perp^2/4) - (r_\perp^2 - r_\perp dr_\perp + dr_\perp^2/4)\right]$$

$$\Rightarrow V_{\text{shell}} = h\pi\left[(2r_\perp dr_\perp)\right]$$

b) Normalization for $g_\parallel$



$$V_{\text{shell}} = 2V_{\text{cyl}} = 2(\pi r_w^2 dr_\parallel)$$

$$r_w = (r_{\text{cut}}^2 - r_\parallel^2)^{1/2}$$

Fig. S 2 Figure illustrating the respective volumes, V_{shell}, used to normalize $g_\perp$ and $g_\parallel$.