Exploring Polymorphism of Benzene and Naphthalene with Free Energy Based Enhanced Molecular Dynamics. Supporting Information

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1. Force Field Parameters

Table S1. Dispersion parameters from OPLS-AA (Jorgensen *et al.*, 1996) for initial packing and Williams99 parameters (Williams, 2001) for UPACK minimization and MD simulations.

	OPLS-AA		Williams99		
	C12 [kJ/molÅ^{-12}]	C6 [kJ/molÅ^{-6}]	A [kJ/mol]	B [Å^{-1}]	C [kJ/molÅ^{-6}]
C	3248063	1167.98	3030.6	3.56	66.53
H	4841	24.10	64618.3	3.60	406.72

Table S2. Atomic charges for Benzene and Naphthalene.

	q Benzene
C	-0.1298
H	0.1298

	q Naphthalene
C1	-0.119
C2	-0.2975
C3	0.219
H1	0.1386
H2	0.1684

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Table S3. Harmonic parameters for bond and bend intramolecular interaction and intramolecular torsional parameter, $V_2(1-\cos(2\phi))$.

Bond	k_r [kJ/molÅ^{-2}]	r_0 [Å]
C-C	200162.6	1.387
C-H	144055.1	1.087
Bend	k_θ [kJ/mol]	θ_0
C-C-C	281.1	119.97
C-C-H	202.8	120.01
Torsion	V_2 [kJ/mol]	
C-C-C-C	15.1670	
C-C-C-H	15.1670	
H-C-C-H	15.1670	

2. Structural Details for Benzene Polymorphs

Table S4. Predicted unit cell parameters for benzene structures from the Crystal-AFED simulation. SG is the space group for each structure, P is the simulation pressure, and V_m is the molecular volume in Å^3.

Polymorph	SG	P	a	b	c	β	V_m
I	*Pbca*	1 bar	7.28	7.63	9.43	90.0	131.00
I(HP)	$P21/n$	2 GPa	5.51	6.51	6.28	103.6	109.29
II	$P21/c$	2 GPa	5.35	5.43	7.68	106.0	107.24
V'	$P21/c$	2 GPa	10.12	6.11	7.07	97.3	108.42

Structural information, including the atomic coordinates for predicted phases I(HP) and V', is found in the additional supporting information files.

Figure S1. Predicted structures Benzene II (left) and Benzene I (right).

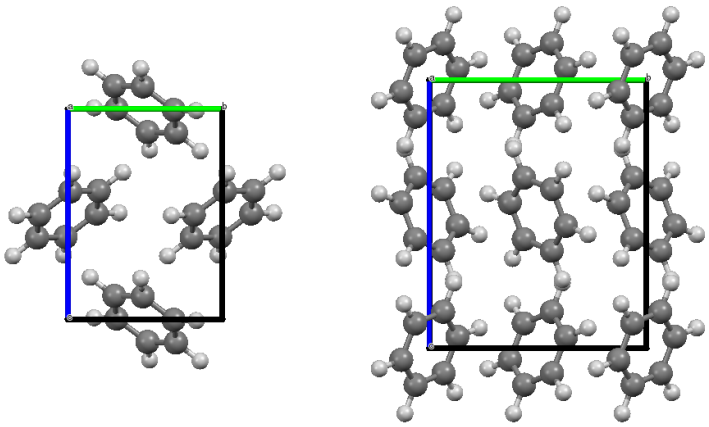
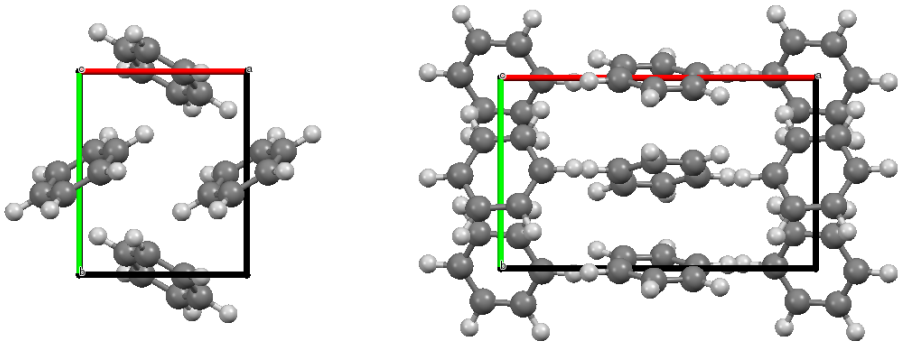


Figure S2. Predicted structures Benzene I(HP) (left) and Benzene V' (right).



3. Mixed Domain Naphthalene Structures

An animation showing the prevalence of the mixed domains in high pressure naphthalene structures is included as an additional supporting information file.

References

Jorgensen, W. L., Maxwell, D. S. & Tirado-Rives, J. (1996). *Journal of the American Chemical Society*, **118**(45), 11225–11236.
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