Supplementary Data: Ion-induced soot nucleation using a new potential for curved aromatics

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1. Corannulene geometry and charges

Corannulene elements, geometry (x, y, z in nm) and charges, in the curPAHIP potential. The element X represents the virtual mass-less atoms used to describe the flexoelectric effect, which are held above and parallel to the pentagon ring using intramolecular forces.

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35
CORANNULENE with curPAHIP charges
C          0.103   0.064   0.085    0.020
C          0.093  -0.078   0.085    0.020
C         -0.045  -0.112   0.085    0.020
C         -0.121   0.008   0.085    0.020
C         -0.030   0.117   0.085    0.020
C          0.205   0.129   0.022    0.177
C          0.310   0.049  -0.032   -0.201
C          0.300  -0.090  -0.032   -0.201
C          0.187  -0.156   0.022    0.177
C          0.143  -0.279  -0.032   -0.201
C          0.007  -0.313  -0.033   -0.201
C         -0.090  -0.225   0.022    0.177
C         -0.242   0.016   0.022    0.177
C         -0.296  -0.103  -0.032   -0.201
C         -0.222  -0.222  -0.032   -0.201
C         -0.280   0.142  -0.031   -0.201
C         -0.190   0.250  -0.031   -0.201
C         -0.059   0.235   0.023    0.177
C          0.049   0.310  -0.032   -0.201
C          0.178   0.258  -0.032   -0.201
H         -0.221   0.345  -0.072    0.133
H          0.031   0.408  -0.072    0.133
H          0.259   0.317  -0.073    0.133
H          0.398   0.097  -0.072    0.133
H          0.380  -0.149  -0.075    0.133
H          0.215  -0.348  -0.073    0.133
H         -0.024  -0.408  -0.074    0.133
H         -0.265  -0.312  -0.073    0.133
H         -0.396  -0.103  -0.074    0.133
H         -0.378   0.155  -0.073    0.133
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X          0.103    0.064    0.132    -0.063
X          0.093   -0.078    0.132    -0.063
X         -0.045   -0.113    0.132    -0.063
X         -0.121    0.008    0.133    -0.063
X         -0.030    0.117    0.133    -0.063
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2. curPAHIP parameters in SI units

Table S1: Parameters of curPAHIP in SI units

Atom pair	ρ (nm)	α (nm^{-1})	C_6 (kJmol^{-1}nm^6)
C C	0.2993	35.49	0.0017458
C H	0.2610	33.18	0.00072665
H H	0.2180	26.54	0.00030083

3. K^+ interaction parameters in SI units

σ = 0.51 nm and ϵ = 0.00009 kJ/mol