Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

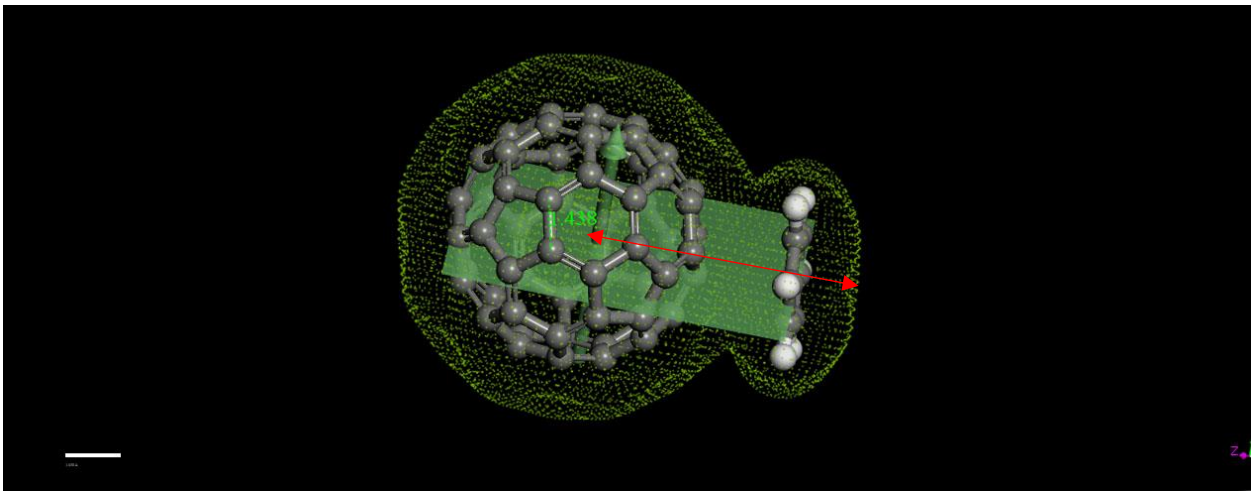
Supporting Information:

1. DFT calculations of clathrate inner radius:

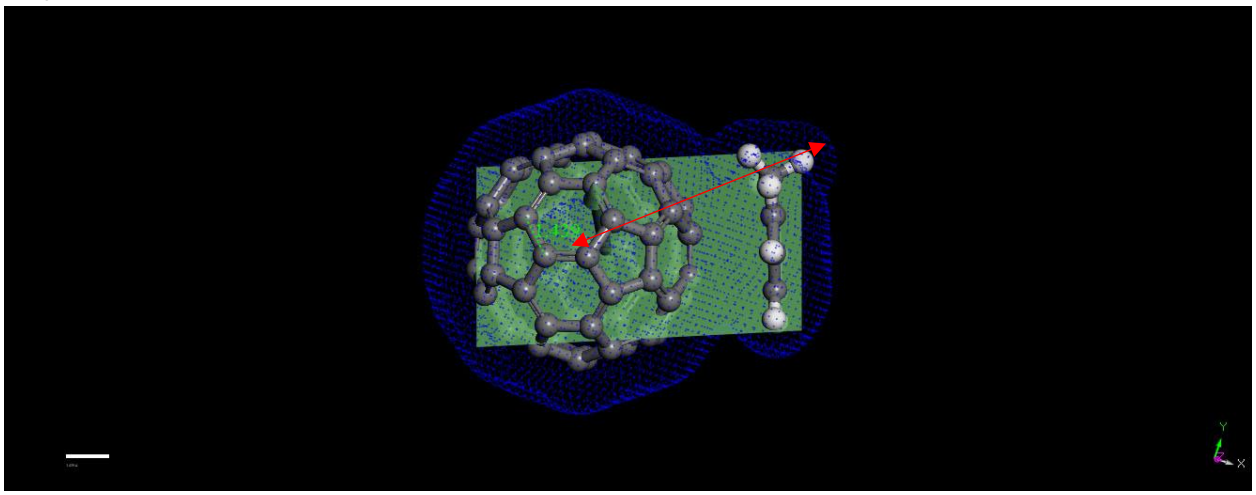
DMOl3 (Materials Studio) DFT calculations were conducted with fine quality using LDA/PWC functions to achieve geometry optimization utilizing structural symmetry. DFT-D correction method for OBS was also applied to our calculations. The acceptable tolerances were set at 1e-5 (Ha) for energy, 0.002 (Ha/Å) for maximum force, and 0.005 Å for maximum displacement during geometry optimization. Once structural geometry was optimized, the DOS (Density of States), and ED (Electron Density) were calculated. After plotting the ED for each of the three cases calculated (namely, C_{60} interacting with benzene, toluene, and chlorobenzene) the best fit plane was determined and the length along the plane from the C_{80} molecule till the end of the electron cloud was taken as the inner radius for the C_{60}/solvent clathrate (see figures below).

Below, are the figures and the determined values for the inner radii:

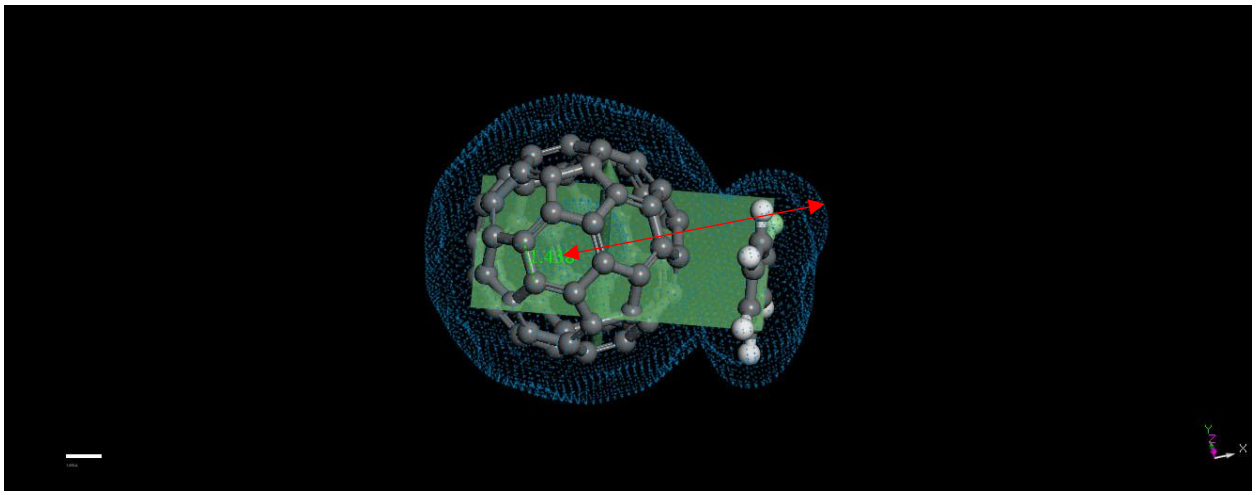
a. C_{60}/Benzene: r_i=0.8 nm



b. C_{60}/Toluene: r_i=0.85 nm



c. C_{60}/Chlorobenzene: r_i=1.05 nm



2. Example calculations of the outer radius of the toluene solvent clathrate (spherical shell).

Maximum evaporation rate occurred at C_{60} mole fraction of 1.48×10^{-4} (see Fig. 3),
Mole fraction= #C_{60}/#(Solvent + C_{60})
For 1 fullerene molecule,
solvent= (1/mole fraction) – 1
= (1/1.48e-4)-1 = 6755 molecule.

toluene mole= # molecules/Avogardros No.
= 6755/6.022e23 = 1.12e-20 mole

Volume of toluene shell= # toluene moles*toluene molar volume
= 1.12e-20 (mol)*92.14 (cm^3/mol.)
= 1.034e-18 (cm^3)

This volume is a spherical shell around the fullerene solvent clathrate
Shell volume = $Shell\ Volume = \frac{4}{3}\pi(r_o^3 - r_i^3)$
Using r_i from DFT calculations as 0.85 nm, and solving for r_o gives;
r_o=6.6 nm