

NVT) at 300 K, followed by EM.

Molecule:

$\rho = 1.36 \text{ g cm}^{-3}$ (experimental range 1.2-1.4 g cm^{-3} (Diallo et al., 2001)),
solubility parameter = $19.2 \text{ J}^{1/2} \text{ cm}^{-3/2}$ (experimental estimate (Diallo et al., 2001)).

spectrum comparable to experimental spectra:

