IR and NMR properties of Ionic Liquids:
Do they tell us the same thing?

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Supporting material

Derived and used relations between spectroscopic properties:

\[ \chi_D = A - B \cdot \left( \delta^1 H \right)^3 \] with \( A = 230,495 \text{ kHz} \) and \( B = 0,0564605 \text{ kHz/ppm}^3 \)

\[ r_{CH} = A + B \cdot \left( \delta^1 H \right)^3 \] with \( A = 107,373 \text{ pm} \) and \( B = 1,56423 \text{ A/ppm}^3 \)

\[ \nu_{CH} = A - B \cdot \left( \delta^1 H \right)^3 \] with \( A = 3258,3 \text{ cm}^{-1} \) and \( B = 0,227893 \text{ cm}^{-1}/\text{ppm}^3 \)

NMR relaxation rates:

\[ R_{13C} = \left( \frac{1}{T_1}_D \right)_{13C} = \frac{4}{3} \left( \frac{\mu_0}{4\pi} \right)^2 \gamma^C_n^2 \gamma^C_e^2 h^2 I(I+1) \frac{1}{r_{CH}^6} \cdot \tau_c \]

\[ R_D = \left( \frac{1}{T_1}_D \right) = \frac{3}{2} \pi^2 \left( 1 + \frac{\eta^D_D}{3} \right) \chi^D \cdot \tau_c \]

Calibration of the nuclear quadrupole moment:

The deuteron quadrupole \( \chi_D = (eQeQ/h) \) coupling constants were obtained by multiplying the calculated electric field gradients, eq, with a calibrated nuclear quadrupole moment, eQ. The calibrated NQM is obtained by plotting measured gas phase quadrupole coupling constants from microwave spectroscopy versus calculated electric field gradients for small molecules such as CD₄, CD₃OD, DNCO etc. as described by Huber et al.[25,26] The slope gives a reasonable NQM (295.5 fm²) which should be used for calculating deuteron quadrupole coupling constants at the B3LYP/6-31+G* level of theory no matter whether we investigate gas phase molecules, hydrogen bonded clusters or ionic liquid complexes.