

Appendix

Optimized structures and their (harmonic) vibrational spectra were obtained from GAUSSIAN 03W, Version 6.1 (Frisch et al., 2004), with GAUSSVIEW 6.1 (Dennington et al., 2003) used as the user interface. The DFT method was used for the calculations with the 6-31G+(d):B3LYP basis set:functional combination. The detailed structure of this type of calculation varies with the particular basis set:functional used. Standard convergence criteria were used for the optimizations, and quadratically convergent SCF was used as needed. The latter does not change either the optimized structures found or their minimized energies or their vibrational spectra. The symmetries imposed on the optimizations are indicated in the text. None of the symmetry-restrained optimized structures are those that would be found if no symmetry were imposed, and therefore as expected, negative (imaginary) frequencies were found in the lower frequency range of the calculated vibrational spectra.

Mulliken charges are those for the optimized structures from the GAUSSIAN output. The Mulliken gross charge on an atom (Q_A) is related to "net" charge on an atom (Q_{AA}) by the formula (Mulliken 1955; Namba et al. 2003):

$$Q_A = Q_{AA} + 1/2 \sum Q_{AB} \quad (S1)$$

and $1/2 \sum Q_{AB}$ = the total overlap population.

Atoms in Molecules (AIM) charges which are based on in principle, observable electron densities (Bader, 2005), were calculated using the AIMAll suite of programs (Keith, 2016). Formatted checkpoint files for use as input for the AIMQB sub-program of AIMAll, were obtained from standard checkpoint files outputted by GAUSSIAN via the FormChk utility of that program.