ANALYSIS OF THE VIBRATIONAL SPECTRA OF $P_3N_3(OCH_2CF_3)_6$ AND $P_4N_4(OCH_2CF_3)_8$

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The cyclic phosphazene trimer $P_3N_3(OCH_2CF_3)_6$ and the related cyclic tetramer $P_4N_4(OCH_2CF_3)_8$ have been proposed as the major low-to-medium temperature pyrolysis products of the parent polyphosphazene $(PN(OCH_2CF_3)_2)_n$ [ab]. Recently, both molecules have been synthesized, isolated and their vapour-phase vibrational spectra recorded using a high-resolution FTIR instrument.

The interpretation of these spectra is achieved primarily by comparison with the results of high-quality density functional calculations, which enable the principal absorption features to be assigned and conclusions to be drawn regarding the geometries and conformations adopted by both molecules. These in turn allow interesting comparisons to be made with analogous cyclic halo-phosphazenes such as $P_3N_3Cl_6$ and $P_4N_4Cl_8$ [cd].

Work to record *in situ* the spectra of the vapour-phase pyrolysis products of $(PN(OCH_2CF_3)_2)_n$ and to analyse these results in terms of the tetramer and trimer spectra will also be presented.

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