Nitrogen and Oxygen Catenation Projects

Structure and Properties of XN_nY

Ab initio studies of the structure, vibrational frequencies, and intensities have been carried out on the open-chain species HN_nH, HN_nF, and FN_nF (n=3,4). Particular attention has been focused on the species HN_3H, which is isoelectronic with NO_2 and exhibits many of the same features in its electronic structure. HN_3H is shown to have a planar trans structure with R(N-N)=1.252 Angstroms, indicating considerable double-bond character. HN_3H also exhibits a low-lying doublet A_2 state separated from the ground state by about 36 kcal/mol. Replacement of one or more of the hydrogens in HN_3H by fluorines alters the electron distribution, spin density, and geometry, most importantly the NNN angle. The biradical species N_4 in its trans planar structure is shown to be of significantly higher energy than two N_2 molecules

Structure and Properties of XO_nY

Ab initio studies of the structure, vibrational frequencies, and intensities have been carried out on the open-chain species HO_nH, HO_nF, and FO_nF (n=2,4). Particular attention has been focused on the species HO_2F and HO_3H, which are isoelectronic. The former species has never been prepared experimentally but is of considerable interest as being intermediate between HO_2H and FO_2F which are both known but which have drastically different properties. As with most fluorine containing molecules a very high level calculation, at the QCISD level is needed. HO_2F behaves relatively normally in its bonding compared to FO_2F

Structure and Properties of O_n

Ab initio studies of the structure, vibrational frequencies, and intensities have been carried out on the open-chain species O_n (n=2,5). Particular attention has been focused on the species O_5, in both a cyclic and open-chain form. An equilibrium structure and vibrational frequencies have been obtained for O_5 in its lowest triplet state. Further calculations are in progress.