NC_6N AND NC_5NC: COUPLED CLUSTER CALCULATIONS AND IMPROVED ASSIGNMENTS OF IR AND RAMAN SPECTRA

P. BOTSCHWINA, R. OSWALD, *Institut für Physikalische Chemie, Universität Göttingen, Tammannstrasse 6, D-37077 Göttingen, Germany.*

On the basis of CCSD(T) calculations, accurate equilibrium structures have been established for NC_6N and its less stable isotopomer NC_5NC. The ground-state rotational constants are predicted to be 561.3(2) and 580.2(2) MHz, respectively. The equilibrium dipole moment of NC_5NC is calculated to be 1.38 D. The most intense stretching vibration of NC_6N is ν_5 with an integrated IR intensity of 19 km mol^{-1}. The ν_7 band is predicted at 885 cm^{-1}, with a low intensity of 0.3 km mol^{-1}. Only three intense vibrational transitions are calculated for NC_5NC in the wavenumber range 2000-2300 cm^{-1}. Inclusion of anharmonicity effects is mandatory to obtain this result; an unusual anharmonicity effect between the fundamentals ν_1 and ν_2 is predicted. Isotopic substitution significantly changes the intensities of the two stretching vibrational bands with highest wavenumber.