

Inertia defects of urea

Campos-Vallete, M. M.

Toro-Labbe, A.

R. Contreras, R.

G. Diaz, F.

By means of an iterative consistency method it has been determined a complete potential field for the urea molecule. The force constants set which interpretes well the vibrational spectra of urea and its deuterio derivatives has been used to evaluate rovibrational constants. The calculated inertia defects should confirm a non-planar structure for urea in gaseous phase. © 1986.