RS•C
ROYAL SOCIETY OF CHEMISTRY

5th World Congress of Theoretically Oriented Chemists

WATOC '99

IMPERIAL COLLEGE, LONDON
1-6 AUGUST 1999

BOOK OF ABSTRACTS

On Some Characteristic Points of the Potential Energy Surface of the Molecular System CN<sub>2/sub>OS

Gy. Dömötör(*)(+), L. L. Stachó, M. I. Bán
Institute of Physical Chemistry, József Att

The global path-following algorithm DDRP[1] interfaced with the ab initio program TEXAS 90 [2] was used to calculate some parts of the potential energy surface and the characteristic points (saddle points, etc.) of reaction paths between some stable species of the open chain and ring isomers of the molecular system CN<sub>/2sub>OS. The results have been compared to those obtained for the same system by a different method [3]. Our aim with the calculations was double: i) to gain an ab initio level practice with the DDRP method and ii) to check the DDRP method itself with results of known examples having a large number of different structures and conformational isomers. [1] Gy. Dömötör, M. I. Bán and L. L. Stachó J. Comput. Chem. 14(1993) 1491. [2] P. Pulay: TX90 ab initio program system. [3] T. Pasinszki, N. P. C. Westwood, J. Chem. Soc. Faraday Trans. 92(1996) 333.