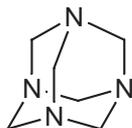


Table 5 . Average C-N bond distances along with the puckering parameters of the six-membered C-N-C-N-C-N rings of the HMT



T=300 K

Average C-N=1.474(3)Å

Q₂=0.014(2)Å

Q₃=0.592(2)Å

Q_T=0.593(2)Å

θ=0.4(2)^o

Average C-N=1.474(3)Å

Q₂=0.014(2)Å

Q₃=0.592(2)Å

Q_T=0.593(2)Å

θ=0.4(2)^o

Average C-N=1.471(3)Å

Q₂=0.008(2)Å

Q₃=0.598(2)Å

Q_T=0.598(2)Å

θ=1.6(2)^o

Average C-N=1.469(3)Å

Q₂=0.004(2)Å

Q₃=0.584(2)Å

Q_T=0.585(2)Å

θ=1.1(2)^o

T=143 K

Average C-N=1.480(3)Å

Q₂=0.009(3)Å

Q₃=0.596(3)Å

Q_T=0.596(3)Å

θ=0.0(3)^o

Average C-N=1.480(3)Å

Q₂=0.017(3)Å

Q₃=0.600(3)Å

Q_T=0.600(3)Å

θ=1.8(3)^o

Average C-N=1.479(3)Å

Q₂=0.007(2)Å

Q₃=0.597(2)Å

Q_T=0.597(3)Å

θ=2.1(3)^o

Average C-N=1.473(3)Å

Q₂=0.009(3)Å

Q₃=0.578(3)Å

Q_T=0.578(3)Å

θ=0.0(3)^o

Note : All the rings adopt a chair conformation.