

**Table 4. (Supplementary Material) The Puckering (Cremer & Pople, 1975) and Asymmetric (Duax et al., 1976) Parameters**

Heterocyclic Rings	Molecules	Cremer & Pople Puckering Parameters	Asymmetric Parameters\$ (°)
Cyclohexene <b>(Ring-A)</b>			
	(I)	$q_2 = 0.349(2) \text{ \AA}$ , $q_3 = 0.300(2) \text{ \AA}$ , $\phi_2 = 166.7(3)^\circ$ , $\theta_2 = 49.4(2)^\circ$ , total puckering amplitude $Q = 0.460(2) \text{ \AA}$	$\Delta C_s (\text{C3B}) = 10.38$ $\Delta C_2 (\text{C3B-C7A}) = 12.17$
	(II)	$q_2 = 0.316(2) \text{ \AA}$ , $q_3 = 0.271(2) \text{ \AA}$ , $\phi_2 = 170.9(3)^\circ$ , $\theta_2 = 49.3(2)^\circ$ , total puckering amplitude $Q = 0.417(2) \text{ \AA}$	$\Delta C_s (\text{C3B}) = 6.66$ $\Delta C_2 (\text{C3B-C7A}) = 14.39$
	(III)	$q_2 = 0.312(1) \text{ \AA}$ , $q_3 = 0.271(1) \text{ \AA}$ , $\phi_2 = 171.5(3)^\circ$ , $\theta_2 = 49.0(2)^\circ$ , total puckering amplitude $Q = 0.414(2) \text{ \AA}$	$\Delta C_s (\text{C3B}) = 6.13$ $\Delta C_2 (\text{C3B-C7A}) = 14.67$
Dihydrofuran <b>(Ring-B)</b>			
	(I)	$q_2 = 0.111(2) \text{ \AA}$ , $\phi_2 = 320.5(8)^\circ$	$\Delta C_s (\text{C8A}) = 0.29$
	(II)	Planar	
	(III)	Planar	
Pyrrolidine <b>(Ring-C)</b>			
	(I)	$q_2 = 0.166(2) \text{ \AA}$ , $\phi_2 = 292.2(5)^\circ$	$\Delta C_s (\text{C3A}) = 2.01$
	(II)	Planar	
	(III)	Planar	
Cyclohexane (N-Substituent)			
	(I)	$q_2 = 0.032(2) \text{ \AA}$ , $q_3 = 0.573(2) \text{ \AA}$ , $\phi_2 = 38(3)^\circ$ , $\theta_2 = 3.2(2)^\circ$ , total puckering amplitude $Q = 0.574(2) \text{ \AA}$	$\Delta C_s (\text{C12}) = 2.20$ $\Delta C_2 (\text{C13-C14}) = 3.25$

\$Both  $\Delta C_s$  and  $\Delta C_2$  asymmetric parameters for cyclohexene have been provided since its conformation for (I)-(III) is in-between half-chair ( $C_2$ ) and sofa ( $C_s$ ) form.