

Table 66. Characteristics of C6 – N1 bond for conformers of **I – III**

Conformer	$\rho(\mathbf{r})$	$\nabla^2 \rho(\mathbf{r})$	λ_1	λ_2	λ_3	ε	$g(\mathbf{r})$	$v(\mathbf{r})$	$h(\mathbf{r})$	n
I (1R, 1S)	0.30	-0.80	-0.60	-0.56	0.35	0.07	0.193	-0.587	-0.394	1.03
I (2R, 2S)	0.30	-0.80	-0.60	-0.56	0.36	0.06	0.196	-0.594	-0.398	1.03
I (3R, 3S)	0.30	-0.81	-0.60	-0.56	0.36	0.06	0.196	-0.593	-0.397	1.03
I (4R, 4S)	0.30	-0.80	-0.60	-0.56	0.35	0.07	0.193	-0.587	-0.394	1.03
I (5R, 5S)	0.30	-0.80	-0.60	-0.56	0.36	0.07	0.194	-0.589	-0.395	1.03
I (6R, 6S)	0.30	-0.80	-0.60	-0.56	0.36	0.06	0.196	-0.592	-0.397	1.03
II (1R, 1S)	0.30	-0.80	-0.60	-0.56	0.35	0.08	0.192	-0.586	-0.394	1.04
II (2R, 2S)	0.30	-0.80	-0.60	-0.56	0.37	0.06	0.200	-0.600	-0.400	1.04
II (3R, 3S)	0.30	-0.80	-0.60	-0.56	0.36	0.06	0.199	-0.598	-0.399	1.04
II (4R, 4S)	0.30	-0.80	-0.60	-0.57	0.37	0.06	0.203	-0.605	-0.403	1.04
II (5R, 5S)	0.30	-0.80	-0.60	-0.56	0.35	0.08	0.192	-0.586	-0.393	1.04
II (6R, 6S)	0.30	-0.81	-0.60	-0.56	0.36	0.08	0.196	-0.593	-0.398	1.04
III (1R, 1S)	0.30	-0.82	-0.61	-0.57	0.36	0.07	0.195	-0.595	-0.400	1.05
III (2R, 2S)	0.30	-0.81	-0.61	-0.58	0.37	0.05	0.203	-0.609	-0.406	1.05
Mean value	0.30	-0.80	-0.60	-0.56	0.36	0.07	0.196	-0.594	-0.398	1.04