

Table 63. Characteristics of N3 – C4 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)	0.25	-0.63	-0.47	-0.45	0.29	0.04	0.126	-0.408	-0.282	0.89
I (2R, 2S)	0.25	-0.62	-0.47	-0.45	0.30	0.04	0.124	-0.404	-0.280	0.89
I (3R, 3S)	0.25	-0.63	-0.47	-0.45	0.30	0.04	0.124	-0.404	-0.280	0.89
I (4R, 4S)	0.25	-0.63	-0.47	-0.45	0.29	0.04	0.126	-0.409	-0.283	0.89
I (5R, 5S)	0.25	-0.63	-0.47	-0.45	0.29	0.04	0.126	-0.408	-0.282	0.89
I (6R, 6S)	0.25	-0.63	-0.47	-0.45	0.30	0.04	0.124	-0.405	-0.281	0.89
II (1R, 1S)	0.25	-0.62	-0.46	-0.44	0.29	0.04	0.129	-0.412	-0.283	0.89
II (2R, 2S)	0.25	-0.63	-0.47	-0.45	0.30	0.04	0.124	-0.405	-0.281	0.89
II (3R, 3S)	0.25	-0.63	-0.47	-0.45	0.30	0.04	0.123	-0.403	-0.280	0.89
II (4R, 4S)	0.25	-0.62	-0.47	-0.45	0.30	0.04	0.124	-0.403	-0.280	0.89
II (5R, 5S)	0.25	-0.61	-0.46	-0.44	0.29	0.04	0.129	-0.411	-0.282	0.89
II (6R, 6S)	0.25	-0.61	-0.46	-0.44	0.29	0.05	0.129	-0.410	-0.282	0.89
III (1R, 1S)	0.25	-0.63	-0.47	-0.45	0.29	0.04	0.127	-0.412	-0.285	0.90
III (2R, 2S)	0.25	-0.64	-0.48	-0.46	0.30	0.03	0.122	-0.404	-0.282	0.91
Mean value	0.25	-0.62	-0.47	-0.45	0.29	0.04	0.125	-0.407	-0.282	0.89