

Table 61. Characteristics of N1 – C2 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)	0.31	-0.90	-0.65	-0.60	0.36	0.09	0.178	-0.580	-0.402	1.02
I (2R, 2S)	0.31	-0.90	-0.66	-0.60	0.36	0.09	0.178	-0.581	-0.403	1.03
I (3R, 3S)	0.31	-0.90	-0.66	-0.60	0.36	0.09	0.178	-0.582	-0.403	1.03
I (4R, 4S)	0.31	-0.90	-0.65	-0.60	0.36	0.09	0.178	-0.580	-0.402	1.02
I (5R, 5S)	0.31	-0.90	-0.65	-0.60	0.36	0.09	0.178	-0.579	-0.402	1.02
I (6R, 6S)	0.31	-0.90	-0.66	-0.60	0.36	0.09	0.178	-0.582	-0.404	1.03
II (1R, 1S)	0.31	-0.89	-0.65	-0.60	0.35	0.09	0.177	-0.576	-0.400	1.02
II (2R, 2S)	0.31	-0.90	-0.66	-0.60	0.36	0.10	0.178	-0.581	-0.403	1.03
II (3R, 3S)	0.31	-0.90	-0.65	-0.60	0.35	0.10	0.176	-0.576	-0.400	1.03
II (4R, 4S)	0.31	-0.91	-0.66	-0.60	0.36	0.10	0.180	-0.587	-0.407	1.03
II (5R, 5S)	0.30	-0.89	-0.65	-0.59	0.35	0.09	0.174	-0.570	-0.396	1.01
II (6R, 6S)	0.31	-0.90	-0.65	-0.60	0.36	0.09	0.179	-0.582	-0.403	1.02
III (1R, 1S)	0.29	-0.85	-0.64	-0.57	0.36	0.11	0.150	-0.512	-0.362	0.89
III (2R, 2S)	0.30	-0.86	-0.65	-0.58	0.36	0.12	0.151	-0.517	-0.366	0.90
Mean value	0.31	-0.89	-0.65	-0.60	0.36	0.10	0.174	-0.570	-0.397	1.00