

Table 65. Characteristics of C5 – C6 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)	0.33	-0.92	-0.70	-0.51	0.30	0.36	0.129	-0.486	-0.358	1.53
I (2R, 2S)	0.33	-0.92	-0.70	-0.52	0.30	0.37	0.128	-0.486	-0.358	1.52
I (3R, 3S)	0.33	-0.92	-0.70	-0.52	0.30	0.37	0.128	-0.485	-0.358	1.52
I (4R, 4S)	0.33	-0.92	-0.70	-0.51	0.30	0.36	0.128	-0.486	-0.357	1.53
I (5R, 5S)	0.33	-0.92	-0.70	-0.51	0.30	0.36	0.128	-0.486	-0.357	1.52
I (6R, 6S)	0.33	-0.92	-0.70	-0.52	0.30	0.37	0.128	-0.486	-0.358	1.52
II (1R, 1S)	0.32	-0.91	-0.69	-0.51	0.30	0.35	0.128	-0.484	-0.356	1.52
II (2R, 2S)	0.32	-0.91	-0.69	-0.52	0.30	0.34	0.126	-0.480	-0.354	1.49
II (3R, 3S)	0.32	-0.91	-0.69	-0.52	0.30	0.34	0.126	-0.479	-0.353	1.49
II (4R, 4S)	0.32	-0.91	-0.69	-0.51	0.30	0.35	0.126	-0.479	-0.353	1.49
II (5R, 5S)	0.32	-0.91	-0.69	-0.51	0.30	0.34	0.128	-0.482	-0.354	1.52
II (6R, 6S)	0.32	-0.91	-0.69	-0.51	0.30	0.35	0.128	-0.482	-0.354	1.52
III (1R, 1S)	0.32	-0.90	-0.69	-0.51	0.30	0.35	0.128	-0.482	-0.354	1.52
III (2R, 2S)	0.32	-0.91	-0.69	-0.51	0.30	0.35	0.126	-0.478	-0.352	1.49
Mean value	0.33	-0.91	-0.70	-0.51	0.30	0.35	0.127	-0.483	-0.355	1.51