

Table 64. Characteristics of C4 – C5 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	-0.58	-0.48	-0.45	0.36	0.07	0.057	-0.258	-0.201	0.95
I (2R, 2S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.257	-0.200	0.95
I (3R, 3S)	0.25	-0.57	-0.48	-0.45	0.36	0.07	0.057	-0.257	-0.200	0.96
I (4R, 4S)	0.25	-0.58	-0.48	-0.45	0.36	0.07	0.057	-0.259	-0.201	0.95
I (5R, 5S)	0.25	-0.58	-0.48	-0.45	0.36	0.07	0.057	-0.259	-0.202	0.95
I (6R, 6S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.257	-0.200	0.96
II (1R, 1S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.258	-0.201	0.95
II (2R, 2S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.058	-0.258	-0.200	0.96
II (3R, 3S)	0.25	-0.57	-0.47	-0.45	0.36	0.05	0.058	-0.257	-0.199	0.96
II (4R, 4S)	0.25	-0.56	-0.48	-0.45	0.36	0.06	0.058	-0.256	-0.199	0.96
II (5R, 5S)	0.25	-0.57	-0.48	-0.45	0.36	0.05	0.057	-0.257	-0.199	0.95
II (6R, 6S)	0.25	-0.57	-0.48	-0.45	0.36	0.07	0.057	-0.255	-0.198	0.95
III (1R, 1S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.256	-0.199	0.95
III (2R, 2S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.256	-0.199	0.96
Mean value	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.257	-0.200	0.95