

Table 71. Characteristics of C5 atom for conformers of **I – III**

Conformer	Valence index	Volume	Charge	Electronic energy
I (1R, 1S)	3.50	10.663	-0.01	-38.061
I (2R, 2S)	3.49	10.621	-0.01	-38.061
I (3R, 3S)	3.50	10.648	-0.01	-38.060
I (4R, 4S)	3.50	10.626	-0.01	-38.061
I (5R, 5S)	3.50	10.640	-0.01	-38.063
I (6R, 6S)	3.49	10.642	-0.01	-38.060
II (1R, 1S)	3.52	10.703	-0.03	-38.075
II (2R, 2S)	3.51	10.710	-0.04	-38.079
II (3R, 3S)	3.50	10.487	-0.04	-38.080
II (4R, 4S)	3.51	10.552	-0.04	-38.075
II (5R, 5S)	3.51	10.619	-0.03	-38.072
II (6R, 6S)	3.52	10.597	-0.03	-38.068
III (1R, 1S)	3.52	10.813	-0.03	-38.102
III (2R, 2S)	3.51	10.803	-0.04	-38.106
Mean value	3.50	10.652	-0.02	-38.073