

Table 72. Characteristics of C6 atom for conformers of **I – III**

Conformer	Valence index	Volume	Charge	Electronic energy
I (1R, 1S)	3.56	9.038	0.39	-37.825
I (2R, 2S)	3.54	8.948	0.39	-37.829
I (3R, 3S)	3.55	8.975	0.39	-37.829
I (4R, 4S)	3.56	9.093	0.39	-37.825
I (5R, 5S)	3.55	9.027	0.39	-37.825
I (6R, 6S)	3.55	8.987	0.39	-37.830
II (1R, 1S)	3.55	9.157	0.37	-37.831
II (2R, 2S)	3.53	8.911	0.39	-37.833
II (3R, 3S)	3.53	8.914	0.39	-37.834
II (4R, 4S)	3.52	8.818	0.39	-37.829
II (5R, 5S)	3.55	9.137	0.37	-37.831
II (6R, 6S)	3.55	9.048	0.38	-37.827
III (1R, 1S)	3.56	9.130	0.38	-37.852
III (2R, 2S)	3.53	8.893	0.40	-37.855
Mean value	3.54	9.006	0.39	-37.833