

Table 68. Characteristics of C2 atom for conformers of **I – III**

Conformer	Valence index	Volume	Charge	Electronic energy
I (1R, 1S)	3.72	8.509	0.58	-37.654
I (2R, 2S)	3.72	8.492	0.58	-37.656
I (3R, 3S)	3.73	8.543	0.58	-37.655
I (4R, 4S)	3.72	8.490	0.58	-37.654
I (5R, 5S)	3.72	8.468	0.58	-37.655
I (6R, 6S)	3.72	8.525	0.58	-37.655
II (1R, 1S)	3.72	8.477	0.58	-37.658
II (2R, 2S)	3.72	8.510	0.57	-37.663
II (3R, 3S)	3.73	8.563	0.57	-37.666
II (4R, 4S)	3.71	8.305	0.58	-37.658
II (5R, 5S)	3.72	8.474	0.58	-37.662
II (6R, 6S)	3.71	8.347	0.59	-37.652
III (1R, 1S)	3.15	4.905	1.78	-37.036
III (2R, 2S)	3.15	4.883	1.77	-37.039
Mean value	3.64	7.964	0.75	-37.569