

Table 70. Characteristics of C4 atom for conformers of **I – III**

Conformer	Valence index	Volume	Charge	Electronic energy
<b>I (1R, 1S)</b>	3.69	6.550	0.38	-37.797
<b>I (2R, 2S)</b>	3.69	6.573	0.38	-37.793
<b>I (3R, 3S)</b>	3.69	6.519	0.38	-37.794
<b>I (4R, 4S)</b>	3.69	6.535	0.37	-37.798
<b>I (5R, 5S)</b>	3.69	6.580	0.37	-37.797
<b>I (6R, 6S)</b>	3.69	6.558	0.38	-37.794
<b>II (1R, 1S)</b>	3.65	6.430	0.36	-37.816
<b>II (2R, 2S)</b>	3.68	6.454	0.36	-37.807
<b>II (3R, 3S)</b>	3.68	6.515	0.36	-37.806
<b>II (4R, 4S)</b>	3.68	6.538	0.36	-37.800
<b>II (5R, 5S)</b>	3.65	6.515	0.36	-37.817
<b>II (6R, 6S)</b>	3.66	6.468	0.36	-37.810
<b>III (1R, 1S)</b>	3.69	6.496	0.38	-37.827
<b>III (2R, 2S)</b>	3.71	6.573	0.38	-37.818
Mean value	3.68	6.522	0.37	-37.805