

Table 69. Characteristics of N3 atom for conformers of **I – III**

Conformer	Valence index	Volume	Charge	Electronic energy
I (1R, 1S)	2.83	13.758	-1.10	-55.357
I (2R, 2S)	2.82	13.721	-1.10	-55.354
I (3R, 3S)	2.82	13.724	-1.10	-55.355
I (4R, 4S)	2.83	13.753	-1.10	-55.358
I (5R, 5S)	2.83	13.768	-1.10	-55.357
I (6R, 6S)	2.82	13.695	-1.10	-55.355
II (1R, 1S)	2.82	13.454	-1.10	-55.366
II (2R, 2S)	2.81	13.440	-1.09	-55.357
II (3R, 3S)	2.82	13.628	-1.09	-55.354
II (4R, 4S)	2.82	13.412	-1.10	-55.356
II (5R, 5S)	2.83	13.604	-1.10	-55.363
II (6R, 6S)	2.82	13.480	-1.10	-55.366
III (1R, 1S)	2.73	14.092	-1.10	-55.386
III (2R, 2S)	2.72	13.987	-1.09	-55.375
Mean value	2.81	13.680	-1.10	-55.361