

Table 67. Characteristics of N1 atom for conformers of **I – III**

Conformer	Valence index	Volume	Charge	Electronic energy
<b>I</b> (1R, 1S)	2.83	13.892	-1.13	-55.391
<b>I</b> (2R, 2S)	2.83	13.873	-1.13	-55.395
<b>I</b> (3R, 3S)	2.83	13.884	-1.13	-55.395
<b>I</b> (4R, 4S)	2.83	13.936	-1.13	-55.390
<b>I</b> (5R, 5S)	2.83	13.894	-1.13	-55.391
<b>I</b> (6R, 6S)	2.83	13.879	-1.13	-55.394
<b>II</b> (1R, 1S)	2.83	13.790	-1.12	-55.391
<b>II</b> (2R, 2S)	2.83	13.801	-1.13	-55.398
<b>II</b> (3R, 3S)	2.83	13.740	-1.13	-55.394
<b>II</b> (4R, 4S)	2.83	13.692	-1.13	-55.407
<b>II</b> (5R, 5S)	2.83	13.731	-1.12	-55.387
<b>II</b> (6R, 6S)	2.83	13.749	-1.13	-55.401
<b>III</b> (1R, 1S)	2.72	14.183	-1.12	-55.422
<b>III</b> (2R, 2S)	2.73	14.173	-1.13	-55.430
Mean value	2.82	13.873	-1.13	-55.399