

Table 45. Variation of atomic electronic energies (a.u.) for conformers of **III**

Atom	Conformer		Mean value
	1R, 1S	2R, 2S	
O1	-75.963	-75.965	-75.964
O2	-75.956	-75.961	-75.958
N1	-55.422	-55.430	-55.426
N3	-55.386	-55.375	-55.381
C2	-37.036	-37.039	-37.038
C4	-37.827	-37.818	-37.822
C4'	-38.028	-38.030	-38.029
C5	-38.102	-38.106	-38.104
C6	-37.852	-37.855	-37.853
C6'	-38.025	-38.020	-38.023
C5'	-37.479	-37.476	-37.478
C5''	-38.053	-38.056	-38.054
H1	-0.466	-0.464	-0.465
H3	-0.470	-0.471	-0.471
H4	-0.622	-0.638	-0.630
H41	-0.623	-0.622	-0.623
H42	-0.612	-0.622	-0.617
H43	-0.623	-0.619	-0.621
H61	-0.618	-0.599	-0.608
H62	-0.618	-0.628	-0.623
H63	-0.608	-0.600	-0.604
H51''	-0.606	-0.607	-0.606
H52''	-0.621	-0.619	-0.620
H53''	-0.615	-0.614	-0.615
$\Sigma$	-572.232	-572.233	-572.232