

Table 30. Variation of atomic electronic energies (a.u.) for conformers of **II**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S	-398.704	-398.703	-398.702	-398.704	-398.703	-398.705	-398.704
O	-75.897	-75.902	-75.902	-75.903	-75.901	-75.899	-75.901
N1	-55.391	-55.398	-55.394	-55.407	-55.387	-55.401	-55.396
N3	-55.366	-55.357	-55.354	-55.356	-55.363	-55.366	-55.360
C2	-37.658	-37.663	-37.666	-37.658	-37.662	-37.652	-37.660
C4	-37.816	-37.807	-37.806	-37.800	-37.817	-37.810	-37.809
C4'	-37.988	-37.989	-37.988	-37.986	-37.983	-37.987	-37.987
C4''	-37.973	-37.974	-37.973	-37.976	-37.970	-37.974	-37.973
C5	-38.075	-38.079	-38.080	-38.075	-38.072	-38.068	-38.075
C5'	-37.448	-37.445	-37.446	-37.445	-37.446	-37.448	-37.446
C5''	-38.023	-38.026	-38.026	-38.026	-38.024	-38.023	-38.025
C6	-37.831	-37.833	-37.834	-37.829	-37.831	-37.827	-37.831
C6'	-37.994	-37.989	-37.990	-37.990	-37.995	-37.995	-37.992
H1	-0.461	-0.460	-0.460	-0.459	-0.462	-0.461	-0.461
H3	-0.465	-0.465	-0.465	-0.466	-0.464	-0.465	-0.465
H4	-0.619	-0.635	-0.635	-0.637	-0.616	-0.621	-0.627
H41	-0.623	-0.632	-0.629	-0.632	-0.633	-0.633	-0.630
H42	-0.632	-0.627	-0.632	-0.633	-0.633	-0.620	-0.629
H43	-0.623	-0.626	-0.628	-0.622	-0.618	-0.624	-0.624
H44	-0.621	-0.619	-0.623	-0.621	-0.627	-0.622	-0.622
H45	-0.626	-0.624	-0.620	-0.624	-0.624	-0.628	-0.624
H51''	-0.605	-0.606	-0.606	-0.606	-0.618	-0.615	-0.609
H52''	-0.619	-0.617	-0.615	-0.617	-0.616	-0.605	-0.615
H53''	-0.614	-0.613	-0.615	-0.613	-0.605	-0.619	-0.613
H61	-0.606	-0.597	-0.596	-0.597	-0.606	-0.606	-0.602
H62	-0.617	-0.626	-0.626	-0.627	-0.617	-0.618	-0.622
H63	-0.617	-0.600	-0.601	-0.600	-0.617	-0.617	-0.609
Σ	-934.512	-934.512	-934.510	-934.511	-934.510	-934.510	-934.511