Table 15. Variation of atomic electronic energies (a.u.) for conformers of **I**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S1	-398.686	-398.685	-398.685	-398.686	-398.686	-398.685	-398.685
O1	-75.929	-75.941	-75.942	-75.932	-75.931	-75.939	-75.936
O2	-75.893	-75.879	-75.880	-75.886	-75.886	-75.887	-75.885
N1	-55.391	-55.395	-55.395	-55.390	-55.391	-55.394	-55.393
N3	-55.357	-55.354	-55.355	-55.358	-55.357	-55.355	-55.356
C2	-37.654	-37.656	-37.655	-37.654	-37.655	-37.655	-37.655
C4	-37.797	-37.793	-37.794	-37.798	-37.797	-37.794	-37.795
C4'	-37.998	-37.998	-37.998	-37.998	-37.998	-37.998	-37.998
C5	-38.061	-38.061	-38.060	-38.061	-38.063	-38.060	-38.061
C5'	-37.140	-37.140	-37.137	-37.140	-37.142	-37.137	-37.139
C6	-37.825	-37.829	-37.829	-37.825	-37.825	-37.830	-37.827
C6'	-37.993	-37.997	-38.000	-37.994	-37.991	-38.000	-37.996
C7	-37.748	-37.745	-37.746	-37.748	-37.747	-37.745	-37.747
C8	-37.981	-37.986	-37.986	-37.987	-37.987	-37.981	-37.985
H1	-0.461	-0.460	-0.460	-0.461	-0.461	-0.460	-0.460
H3	-0.465	-0.465	-0.465	-0.465	-0.465	-0.465	-0.465
H4	-0.621	-0.625	-0.625	-0.621	-0.621	-0.625	-0.623
H41'	-0.611	-0.615	-0.615	-0.612	-0.611	-0.615	-0.613
H42'	-0.621	-0.621	-0.622	-0.621	-0.621	-0.621	-0.621
H43'	-0.621	-0.619	-0.619	-0.621	-0.621	-0.619	-0.620
H61'	-0.605	-0.605	-0.607	-0.604	-0.605	-0.607	-0.606
H62'	-0.619	-0.619	-0.617	-0.605	-0.604	-0.616	-0.613
H63'	-0.605	-0.595	-0.593	-0.620	-0.621	-0.593	-0.604
H71	-0.620	-0.615	-0.626	-0.626	-0.615	-0.621	-0.620
H72	-0.620	-0.626	-0.615	-0.614	-0.627	-0.620	-0.620
H81	-0.618	-0.614	-0.620	-0.620	-0.614	-0.619	-0.617
H82	-0.620	-0.620	-0.614	-0.614	-0.619	-0.619	-0.618
H83	-0.616	-0.617	-0.617	-0.616	-0.617	-0.617	-0.617
Σ	-1009.777	-1009.777	-1009.774	-1009.775	-1009.775	-1009.776	-1009.776