Table 11. Variation of the covalent bond orders for conformers of **I**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	1.55	1.56	1.56	1.55	1.55	1.56	1.56
O1 - C5'	1.27	1.27	1.28	1.27	1.27	1.28	1.28
O2 - C5'	0.87	0.86	0.87	0.87	0.87	0.86	0.87
N1 - C2	1.02	1.03	1.03	1.02	1.02	1.03	1.02
C2 - N3	1.14	1.14	1.14	1.14	1.14	1.14	1.14
N3 - C4	0.89	0.89	0.89	0.89	0.89	0.89	0.89
C4 - C5	0.95	0.95	0.96	0.95	0.95	0.96	0.95
C5 - C6	1.53	1.52	1.52	1.53	1.52	1.52	1.52
C6 - N1	1.03	1.03	1.03	1.03	1.03	1.03	1.03
C4 - C4'	0.95	0.95	0.95	0.95	0.95	0.95	0.95
C5 - C5'	1.02	1.02	1.02	1.02	1.02	1.02	1.02
C6 - C6'	0.99	1.00	1.00	0.99	0.99	1.00	1.00
O2 - C7	0.82	0.82	0.82	0.82	0.82	0.82	0.82
C7 - C8	0.98	0.98	0.98	0.98	0.98	0.98	0.98
N1 - H1	0.77	0.77	0.77	0.77	0.77	0.77	0.77
N3 - H3	0.79	0.79	0.79	0.79	0.79	0.79	0.79
C4 - H4	0.89	0.89	0.89	0.89	0.89	0.89	0.89
C4' - H41'	0.95	0.95	0.95	0.95	0.95	0.95	0.95
C4' - H42'	0.96	0.96	0.96	0.96	0.96	0.96	0.96
C4' - H43'	0.95	0.95	0.95	0.95	0.95	0.95	0.95
C6' - H61'	0.94	0.94	0.94	0.92	0.92	0.94	0.93
C6' - H62'	0.95	0.95	0.95	0.94	0.94	0.95	0.95
C6' - H63'	0.92	0.91	0.91	0.95	0.95	0.91	0.93
C7 - H71	0.91	0.90	0.92	0.92	0.90	0.91	0.91
C7 - H72	0.91	0.92	0.90	0.90	0.93	0.91	0.91
C8 - H81	0.96	0.95	0.96	0.96	0.95	0.96	0.96
C8 - H82	0.96	0.96	0.95	0.95	0.96	0.96	0.95
C8 - H83	0.96	0.96	0.96	0.96	0.96	0.96	0.96