

Table 41. Variation of the covalent bond orders for conformers of **III**

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	1.24	1.24	1.24
O2 – C5'	1.37	1.37	1.37
N1 – C2	0.89	0.90	0.89
N1 – C6	1.05	1.05	1.05
N3 – C2	1.02	1.01	1.02
N3 – C4	0.90	0.91	0.90
C4 – C4'	0.95	0.95	0.95
C4 – C5	0.95	0.96	0.95
C5 – C6	1.52	1.49	1.51
C6 – C6'	0.99	1.00	0.99
C5 – C5'	1.05	1.06	1.06
C5' – C5''	0.95	0.95	0.95
N1 – H1	0.79	0.79	0.79
N3 – H3	0.81	0.81	0.81
C4 – H4	0.89	0.90	0.89
C4' – H41	0.96	0.96	0.96
C4' – H42	0.95	0.96	0.95
C4' – H43	0.96	0.95	0.95
C6' – H61	0.94	0.92	0.93
C6' – H62	0.93	0.95	0.94
C6' – H63	0.94	0.93	0.93
C5'' – H51''	0.94	0.95	0.95
C5'' – H52''	0.95	0.94	0.95
C5'' – H53''	0.94	0.95	0.94