

Table 26. Variation of the covalent bond orders for conformers of **II**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	1.55	1.56	1.56	1.55	1.56	1.55	1.56
O – C5'	1.38	1.38	1.38	1.38	1.38	1.38	1.38
N1 – C2	1.02	1.03	1.03	1.03	1.01	1.02	1.02
N1 – C6	1.04	1.04	1.04	1.04	1.04	1.04	1.04
N3 – C2	1.15	1.13	1.14	1.13	1.15	1.15	1.14
N3 – C4	0.89	0.89	0.89	0.89	0.89	0.89	0.89
C4 – C4'	0.93	0.93	0.93	0.93	0.93	0.93	0.93
C4' – C4''	0.99	0.99	0.99	0.99	0.99	0.99	0.99
C4 – C5	0.95	0.96	0.96	0.96	0.95	0.95	0.96
C5 – C6	1.52	1.49	1.49	1.49	1.52	1.52	1.51
C6 – C6'	0.99	1.00	1.00	1.00	0.99	0.99	0.99
C5 – C5'	1.05	1.06	1.05	1.05	1.04	1.05	1.05
C5' – C5''	0.95	0.95	0.95	0.95	0.95	0.95	0.95
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	0.88	0.89	0.89	0.89	0.88	0.89	0.89
C4' – H41	0.93	0.93	0.93	0.94	0.93	0.94	0.93
C4' – H42	0.94	0.93	0.94	0.93	0.94	0.93	0.93
C4'' – H43	0.96	0.96	0.95	0.95	0.95	0.95	0.95
C4'' – H44	0.96	0.96	0.95	0.96	0.95	0.96	0.96
C4'' – H45	0.96	0.95	0.96	0.95	0.96	0.95	0.96
C6' – H61	0.94	0.92	0.92	0.92	0.94	0.94	0.93
C6' – H62	0.94	0.95	0.95	0.95	0.94	0.95	0.95
C6' – H63	0.93	0.93	0.93	0.93	0.93	0.93	0.93
C5'' – H51''	0.94	0.95	0.95	0.95	0.95	0.94	0.95
C5'' – H52''	0.95	0.94	0.94	0.94	0.94	0.94	0.94
C5'' – H53''	0.94	0.95	0.95	0.95	0.94	0.95	0.95