Table 56. Variation of the covalent bond orders for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	1.24	1.14	1.30	1.00
O2 – C5'	1.37	1.32	1.41	1.25
N1 – C2	0.89	0.83	0.92	0.73
N1 – C6	1.05	1.00	1.08	0.93
N3 – C2	1.02	0.95	1.07	0.82
N3 – C4	0.90	0.87	0.91	0.82
C4 – C4'	0.95	0.95	0.95	0.94
C4 – C5	0.95	0.95	0.95	0.94
C5 – C6	1.52	1.55	1.50	1.59
C6 – C6'	0.99	0.99	0.99	0.97
C5 – C5'	1.05	1.03	1.07	0.99
C5' – C5"	0.95	0.94	0.95	0.93
N1 – H1	0.79	0.78	0.80	0.77
N3 – H3	0.81	0.80	0.82	0.79
C4 – H4	0.89	0.89	0.89	0.90
C4' – H41	0.96	0.96	0.96	0.96
C4' – H42	0.95	0.95	0.94	0.95
C4' – H43	0.96	0.96	0.95	0.96
C6' – H61	0.94	0.95	0.94	0.95
C6' – H62	0.93	0.94	0.93	0.94
C6' – H63	0.94	0.94	0.94	0.95
C5" – H51"	0.94	0.95	0.94	0.95
C5" – H52"	0.95	0.95	0.95	0.96
C5" – H53"	0.94	0.95	0.94	0.95