Table 48. Laplacian of electron density at the bond critical points (a.u.) 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	-0.42	-0.31	-0.50	-0.12
O2 – C5'	-0.22	-0.03	-0.36	0.25
N1 – C2	-0.85	-0.94	-0.74	-0.89
N1 – C6	-0.82	-0.81	-0.78	-0.69
N3 – C2	-1.00	-1.07	-0.91	-1.05
N3 – C4	-0.63	-0.67	-0.56	-0.53
C4 – C4'	-0.53	-0.61	-0.47	-0.69
C4 – C5	-0.57	-0.64	-0.51	-0.71
C5 – C6	-0.90	-1.01	-0.82	-1.11
C6 – C6'	-0.60	-0.68	-0.54	-0.75
C5 – C5'	-0.66	-0.74	-0.60	-0.80
C5' – C5"	-0.58	-0.67	-0.51	-0.75
N1 – H1	-1.68	-1.85	-1.54	-2.03
N3 – H3	-1.64	-1.80	-1.51	-1.97
C4 – H4	-0.99	-1.07	-0.94	-1.14
C4' – H41	-0.90	-0.96	-0.85	-1.01
C4' – H42	-0.92	-0.99	-0.88	-1.05
C4' – H43	-0.90	-0.96	-0.86	-1.02
C6' – H61	-0.91	-0.97	-0.86	-1.03
C6' – H62	-0.95	-1.02	-0.90	-1.09
C6' – H63	-0.89	-0.95	-0.85	-1.01
C5" – H51"	-0.93	-1.00	-0.89	-1.05
C5" – H52"	-0.91	-0.97	-0.86	-1.04
C5" – H53"	-0.88	-0.94	-0.84	-1.00