

Table 18. Laplacian of electron density at the bond critical points (a.u.) for conformers of **II**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	-0.04	-0.03	-0.03	-0.03	-0.04	-0.04	-0.04
O – C5'	-0.22	-0.22	-0.22	-0.22	-0.22	-0.22	-0.22
N1 – C2	-0.89	-0.90	-0.90	-0.91	-0.89	-0.90	-0.90
N1 – C6	-0.80	-0.80	-0.80	-0.80	-0.80	-0.81	-0.80
N3 – C2	-0.99	-0.98	-0.98	-0.97	-0.99	-0.98	-0.98
N3 – C4	-0.62	-0.63	-0.63	-0.62	-0.61	-0.61	-0.62
C4 – C4'	-0.53	-0.52	-0.52	-0.51	-0.52	-0.52	-0.52
C4' – C4''	-0.53	-0.53	-0.53	-0.53	-0.53	-0.54	-0.53
C4 – C5	-0.57	-0.57	-0.57	-0.56	-0.57	-0.57	-0.57
C5 – C6	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91
C6 – C6'	-0.60	-0.61	-0.61	-0.61	-0.60	-0.60	-0.61
C5 – C5'	-0.66	-0.66	-0.66	-0.66	-0.65	-0.65	-0.66
C5' – C5''	-0.58	-0.58	-0.58	-0.58	-0.58	-0.58	-0.58
N1 – H1	-1.72	-1.73	-1.73	-1.73	-1.72	-1.72	-1.72
N3 – H3	-1.69	-1.69	-1.68	-1.68	-1.68	-1.68	-1.68
C4 – H4	-0.99	-0.97	-0.97	-0.97	-1.00	-0.99	-0.98
C4' – H41	-0.93	-0.91	-0.92	-0.90	-0.91	-0.90	-0.91
C4' – H42	-0.91	-0.92	-0.91	-0.91	-0.91	-0.93	-0.91
C4'' – H43	-0.90	-0.89	-0.90	-0.91	-0.92	-0.91	-0.90
C4'' – H44	-0.91	-0.91	-0.91	-0.90	-0.91	-0.90	-0.91
C4'' – H45	-0.90	-0.91	-0.91	-0.91	-0.90	-0.90	-0.90
C6' – H61	-0.89	-0.92	-0.93	-0.92	-0.89	-0.89	-0.91
C6' – H62	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91
C6' – H63	-0.95	-0.93	-0.92	-0.93	-0.95	-0.95	-0.94
C5'' – H51''	-0.94	-0.94	-0.94	-0.94	-0.91	-0.88	-0.92
C5'' – H52''	-0.91	-0.89	-0.89	-0.89	-0.88	-0.94	-0.90
C5'' – H53''	-0.88	-0.88	-0.89	-0.88	-0.94	-0.91	-0.90