

Table 19. Electron density curvature  $\lambda_1$  for conformers of **II** (a.u.)

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	-0.20	-0.20	-0.20	-0.20	-0.20	-0.20	-0.20
O – C5'	-1.03	-1.02	-1.03	-1.03	-1.03	-1.03	-1.03
N1 – C2	-0.65	-0.66	-0.65	-0.66	-0.65	-0.65	-0.65
N1 – C6	-0.60	-0.60	-0.60	-0.60	-0.60	-0.60	-0.60
N3 – C2	-0.75	-0.74	-0.74	-0.74	-0.76	-0.75	-0.75
N3 – C4	-0.46	-0.47	-0.47	-0.47	-0.46	-0.46	-0.47
C4 – C4'	-0.45	-0.45	-0.45	-0.45	-0.45	-0.45	-0.45
C4' – C4''	-0.44	-0.44	-0.44	-0.44	-0.44	-0.45	-0.44
C4 – C5	-0.48	-0.48	-0.47	-0.48	-0.48	-0.48	-0.48
C5 – C6	-0.69	-0.69	-0.69	-0.69	-0.69	-0.69	-0.69
C6 – C6'	-0.49	-0.49	-0.49	-0.49	-0.49	-0.48	-0.49
C5 – C5'	-0.55	-0.55	-0.55	-0.55	-0.54	-0.54	-0.55
C5' – C5''	-0.49	-0.49	-0.49	-0.49	-0.48	-0.48	-0.49
N1 – H1	-1.33	-1.33	-1.33	-1.33	-1.33	-1.33	-1.33
N3 – H3	-1.32	-1.32	-1.31	-1.31	-1.31	-1.31	-1.31
C4 – H4	-0.78	-0.76	-0.76	-0.76	-0.79	-0.78	-0.77
C4' – H41	-0.72	-0.71	-0.71	-0.70	-0.71	-0.70	-0.71
C4' – H42	-0.71	-0.71	-0.71	-0.71	-0.70	-0.73	-0.71
C4'' – H43	-0.70	-0.70	-0.70	-0.71	-0.72	-0.71	-0.70
C4'' – H44	-0.71	-0.71	-0.71	-0.70	-0.71	-0.70	-0.71
C4'' – H45	-0.70	-0.71	-0.71	-0.71	-0.70	-0.70	-0.70
C6' – H61	-0.71	-0.73	-0.73	-0.73	-0.71	-0.71	-0.72
C6' – H62	-0.71	-0.71	-0.71	-0.71	-0.71	-0.71	-0.71
C6' – H63	-0.74	-0.74	-0.73	-0.73	-0.74	-0.74	-0.74
C5'' – H51''	-0.73	-0.73	-0.73	-0.73	-0.71	-0.69	-0.72
C5'' – H52''	-0.71	-0.69	-0.70	-0.70	-0.69	-0.74	-0.70
C5'' – H53''	-0.69	-0.69	-0.69	-0.69	-0.74	-0.71	-0.70