Table 3. Laplacian of electron density at the bond critical points (a.u.) for conformers of **I**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	-0.04	-0.04	-0.04	-0.04	-0.04	-0.04	-0.04
O1 - C5'	-0.31	-0.32	-0.31	-0.32	-0.32	-0.31	-0.31
O2 - C5'	-0.51	-0.52	-0.52	-0.52	-0.52	-0.51	-0.51
N1 - C2	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90
C2 - N3	-0.98	-0.98	-0.98	-0.98	-0.98	-0.98	-0.98
N3 - C4	-0.63	-0.62	-0.63	-0.63	-0.63	-0.63	-0.63
C4 - C5	-0.58	-0.57	-0.57	-0.58	-0.58	-0.57	-0.57
C5 - C6	-0.92	-0.92	-0.92	-0.92	-0.92	-0.92	-0.92
C6 - N1	-0.80	-0.80	-0.81	-0.80	-0.80	-0.80	-0.80
C4 - C4'	-0.54	-0.54	-0.53	-0.54	-0.54	-0.53	-0.54
C5 - C5'	-0.69	-0.69	-0.69	-0.69	-0.69	-0.68	-0.69
C6 - C6'	-0.61	-0.61	-0.61	-0.61	-0.61	-0.61	-0.61
O2 - C7	-0.32	-0.31	-0.31	-0.31	-0.31	-0.32	-0.32
C7 - C8	-0.60	-0.58	-0.58	-0.58	-0.58	-0.60	-0.59
N1 - H1	-1.72	-1.72	-1.72	-1.72	-1.72	-1.72	-1.72
N3 - H3	-1.68	-1.68	-1.68	-1.68	-1.68	-1.68	-1.68
C4 - H4	-0.99	-0.99	-0.99	-0.99	-0.99	-0.99	-0.99
C4' - H41'	-0.92	-0.92	-0.92	-0.92	-0.92	-0.92	-0.92
C4' - H42'	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90
C4' - H43'	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91
C6' - H61'	-0.89	-0.89	-0.89	-0.97	-0.96	-0.89	-0.91
C6' - H62'	-0.90	-0.90	-0.89	-0.89	-0.90	-0.89	-0.90
C6' - H63'	-0.97	-0.98	-0.98	-0.90	-0.91	-0.98	-0.95
C7 - H71	-0.98	-0.99	-0.99	-0.99	-1.00	-0.98	-0.99
C7 - H72	-0.98	-0.99	-0.99	-1.00	-0.99	-0.98	-0.99
C8 - H81	-0.91	-0.92	-0.91	-0.91	-0.92	-0.91	-0.92
C8 - H82	-0.91	-0.91	-0.92	-0.92	-0.91	-0.91	-0.92
C8 - H83	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90