

Table 10. Electronic energy density  $h(\mathbf{r})$  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	-0.248	-0.248	-0.248	-0.248	-0.248	-0.248	-0.248
O1 - C5'	-0.701	-0.701	-0.702	-0.700	-0.700	-0.703	-0.701
O2 - C5'	-0.422	-0.411	-0.411	-0.420	-0.419	-0.413	-0.416
N1 - C2	-0.402	-0.403	-0.403	-0.402	-0.402	-0.404	-0.403
C2 - N3	-0.466	-0.464	-0.464	-0.466	-0.466	-0.464	-0.465
N3 - C4	-0.282	-0.280	-0.280	-0.283	-0.282	-0.281	-0.281
C4 - C5	-0.201	-0.200	-0.200	-0.201	-0.202	-0.200	-0.201
C5 - C6	-0.358	-0.358	-0.358	-0.357	-0.357	-0.358	-0.358
C6 - N1	-0.394	-0.398	-0.397	-0.394	-0.395	-0.397	-0.396
C4 - C4'	-0.189	-0.189	-0.189	-0.189	-0.189	-0.189	-0.189
C5 - C5'	-0.243	-0.243	-0.242	-0.243	-0.244	-0.242	-0.243
C6 - C6'	-0.214	-0.216	-0.216	-0.214	-0.213	-0.216	-0.215
O2 - C7	-0.289	-0.288	-0.288	-0.285	-0.286	-0.291	-0.288
C7 - C8	-0.207	-0.202	-0.202	-0.202	-0.202	-0.207	-0.204
N1 - H1	-0.481	-0.480	-0.480	-0.481	-0.481	-0.480	-0.481
N3 - H3	-0.472	-0.472	-0.472	-0.472	-0.472	-0.472	-0.472
C4 - H4	-0.285	-0.286	-0.286	-0.285	-0.284	-0.286	-0.285
C4' - H41'	-0.272	-0.271	-0.271	-0.271	-0.272	-0.271	-0.271
C4' - H42'	-0.268	-0.268	-0.268	-0.268	-0.268	-0.268	-0.268
C4' - H43'	-0.270	-0.270	-0.270	-0.270	-0.270	-0.270	-0.270
C6' - H61'	-0.265	-0.264	-0.264	-0.282	-0.280	-0.264	-0.270
C6' - H62'	-0.269	-0.268	-0.267	-0.265	-0.266	-0.267	-0.267
C6' - H63'	-0.282	-0.282	-0.283	-0.269	-0.270	-0.283	-0.278
C7 - H71	-0.282	-0.284	-0.284	-0.284	-0.284	-0.281	-0.283
C7 - H72	-0.281	-0.284	-0.284	-0.284	-0.284	-0.282	-0.283
C8 - H81	-0.271	-0.273	-0.270	-0.270	-0.273	-0.271	-0.271
C8 - H82	-0.270	-0.270	-0.272	-0.273	-0.270	-0.271	-0.271
C8 - H83	-0.269	-0.267	-0.268	-0.267	-0.267	-0.269	-0.268