Table 9. Potential energy 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	-0.486	-0.488	-0.487	-0.487	-0.487	-0.488	-0.487
O1 - C5'	-1.325	-1.324	-1.325	-1.321	-1.320	-1.328	-1.324
O2 - C5'	-0.716	-0.694	-0.692	-0.710	-0.710	-0.700	-0.704
N1 - C2	-0.580	-0.581	-0.582	-0.580	-0.579	-0.582	-0.581
C2 - N3	-0.687	-0.684	-0.684	-0.688	-0.687	-0.683	-0.685
N3 - C4	-0.408	-0.404	-0.404	-0.409	-0.408	-0.405	-0.406
C4 - C5	-0.258	-0.257	-0.257	-0.259	-0.259	-0.257	-0.258
C5 - C6	-0.486	-0.486	-0.485	-0.486	-0.486	-0.486	-0.486
C6 - N1	-0.587	-0.594	-0.593	-0.587	-0.589	-0.592	-0.590
C4 - C4'	-0.244	-0.244	-0.243	-0.244	-0.245	-0.243	-0.244
C5 - C5'	-0.314	-0.315	-0.313	-0.314	-0.316	-0.312	-0.314
C6 - C6'	-0.276	-0.279	-0.279	-0.276	-0.275	-0.279	-0.277
O2 - C7	-0.497	-0.498	-0.498	-0.492	-0.492	-0.503	-0.497
C7 - C8	-0.263	-0.259	-0.259	-0.259	-0.259	-0.263	-0.261
N1 - H1	-0.531	-0.530	-0.530	-0.531	-0.531	-0.530	-0.531
N3 - H3	-0.524	-0.523	-0.523	-0.524	-0.524	-0.524	-0.524
C4 - H4	-0.321	-0.323	-0.323	-0.321	-0.321	-0.323	-0.322
C4' - H41'	-0.313	-0.313	-0.313	-0.313	-0.313	-0.313	-0.313
C4' - H42'	-0.311	-0.311	-0.311	-0.311	-0.311	-0.311	-0.311
C4' - H43'	-0.312	-0.313	-0.312	-0.312	-0.312	-0.312	-0.312
C6' - H61'	-0.307	-0.307	-0.307	-0.321	-0.320	-0.307	-0.311
C6' - H62'	-0.312	-0.311	-0.310	-0.307	-0.307	-0.310	-0.310
C6' - H63'	-0.322	-0.320	-0.321	-0.312	-0.313	-0.321	-0.318
C7 - H71	-0.318	-0.320	-0.320	-0.320	-0.320	-0.317	-0.319
C7 - H72	-0.318	-0.320	-0.320	-0.320	-0.320	-0.318	-0.319
C8 - H81	-0.313	-0.314	-0.313	-0.313	-0.314	-0.313	-0.313
C8 - H82	-0.313	-0.313	-0.314	-0.314	-0.313	-0.313	-0.313
C8 - H83	-0.312	-0.311	-0.311	-0.311	-0.310	-0.312	-0.311