

Table 24. Potential energy 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	-0.487	-0.489	-0.490	-0.488	-0.487	-0.485	-0.488
O – C5'	-1.285	-1.284	-1.284	-1.284	-1.287	-1.284	-1.285
N1 – C2	-0.576	-0.581	-0.576	-0.587	-0.570	-0.582	-0.579
N1 – C6	-0.586	-0.600	-0.598	-0.605	-0.586	-0.593	-0.595
N3 – C2	-0.692	-0.678	-0.678	-0.683	-0.693	-0.698	-0.687
N3 – C4	-0.412	-0.405	-0.403	-0.403	-0.411	-0.410	-0.407
C4 – C4'	-0.242	-0.240	-0.237	-0.236	-0.238	-0.238	-0.238
C4' – C4''	-0.243	-0.243	-0.244	-0.244	-0.243	-0.244	-0.244
C4 – C5	-0.258	-0.258	-0.257	-0.256	-0.257	-0.255	-0.257
C5 – C6	-0.484	-0.480	-0.479	-0.479	-0.482	-0.482	-0.481
C6 – C6'	-0.271	-0.278	-0.278	-0.277	-0.271	-0.270	-0.274
C5 – C5'	-0.304	-0.309	-0.307	-0.307	-0.302	-0.303	-0.305
C5' – C5''	-0.261	-0.259	-0.259	-0.259	-0.261	-0.260	-0.260
N1 – H1	-0.530	-0.531	-0.531	-0.532	-0.530	-0.531	-0.531
N3 – H3	-0.526	-0.526	-0.523	-0.523	-0.523	-0.523	-0.524
C4 – H4	-0.320	-0.320	-0.321	-0.321	-0.321	-0.321	-0.321
C4' – H41	-0.315	-0.314	-0.314	-0.312	-0.314	-0.312	-0.313
C4' – H42	-0.313	-0.313	-0.313	-0.314	-0.313	-0.315	-0.314
C4'' – H43	-0.311	-0.311	-0.313	-0.313	-0.314	-0.313	-0.313
C4'' – H44	-0.313	-0.313	-0.313	-0.313	-0.314	-0.313	-0.313
C4'' – H45	-0.313	-0.313	-0.313	-0.313	-0.313	-0.313	-0.313
C6' – H61	-0.307	-0.310	-0.311	-0.310	-0.307	-0.307	-0.309
C6' – H62	-0.312	-0.314	-0.314	-0.315	-0.312	-0.313	-0.313
C6' – H63	-0.321	-0.312	-0.311	-0.312	-0.322	-0.322	-0.317
C5'' – H51''	-0.314	-0.315	-0.314	-0.315	-0.313	-0.309	-0.313
C5'' – H52''	-0.314	-0.310	-0.311	-0.311	-0.309	-0.314	-0.312
C5'' – H53''	-0.309	-0.308	-0.309	-0.308	-0.315	-0.314	-0.310