

Table 13. Variation of the atomic volumes (\AA^3) for conformers of **I**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S1	37.448	37.390	37.405	37.389	37.419	37.411	37.410
O1	18.944	18.560	18.554	18.773	18.790	18.720	18.724
O2	14.044	14.240	14.176	14.060	14.103	14.204	14.138
N1	13.892	13.873	13.884	13.936	13.894	13.879	13.893
N3	13.758	13.721	13.724	13.753	13.768	13.695	13.737
C2	8.509	8.492	8.543	8.490	8.468	8.525	8.504
C4	6.550	6.573	6.519	6.535	6.580	6.558	6.552
C4'	10.003	10.002	10.033	10.018	10.016	10.045	10.019
C5	10.663	10.621	10.648	10.626	10.640	10.642	10.640
C5'	5.969	6.024	6.125	6.012	5.982	6.105	6.036
C6	9.038	8.948	8.975	9.093	9.027	8.987	9.011
C6'	10.208	10.218	10.258	10.133	10.017	10.283	10.186
C7	7.581	7.790	7.832	7.788	7.830	7.578	7.733
C8	10.141	10.262	10.282	10.218	10.201	10.195	10.216
H1	4.385	4.380	4.409	4.374	4.358	4.410	4.386
H3	4.501	4.508	4.506	4.497	4.489	4.501	4.500
H4	6.476	6.459	6.437	6.461	6.483	6.434	6.458
H41'	7.125	7.192	7.161	7.155	7.131	7.210	7.162
H42'	7.629	7.630	7.637	7.619	7.626	7.624	7.628
H43'	7.565	7.521	7.509	7.550	7.560	7.519	7.537
H61'	7.267	7.275	7.316	6.083	6.240	7.309	6.915
H62'	7.335	7.401	7.405	7.278	7.229	7.406	7.342
H63'	6.141	5.895	5.771	7.332	7.308	5.777	6.371
H71	7.003	6.606	7.267	7.252	6.584	7.099	6.969
H72	7.039	7.268	6.590	6.593	7.275	6.972	6.956
H81	7.518	7.191	7.556	7.577	7.189	7.532	7.427
H82	7.576	7.572	7.195	7.159	7.552	7.519	7.429
H83	7.537	7.590	7.585	7.584	7.587	7.558	7.574
Σ	271.844	271.203	271.301	271.336	271.348	271.697	271.455