

Table 1. Optimized geometrical parameters (ROHF/6-311G**) in singlet state as well as triplet state compared with the observed geometry in ref. 4.

Bondlength in Angstrom	Expt	Calculated for S	Calculated for T
Dihedral angle, degree	1.20	3.63	1.02
C1 – C14	3.79	3.782	3.810
N5 – O6	1.277	1.175	1.247
N2 – O7	1.276	1.186	1.269
N2 – C1	1.351	1.338	1.274
N5 – C1	1.353	1.355	1.403
N2 – C3	1.494	1.502	1.492
N5 – C4	1.505	1.503	1.475
C3 – C4	1.553	1.551	1.562

Ref. 12

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