Table S1. Calculated Bond lengths (Å), for the title compound.

N	Intramolecular bond lenghts	X-Ray	B3LYP/ 6-311G(3df, 2p)
1	O1 – N1	1.205(3)	1.2247
2	O2 – N1	1.204(3)	1.2242
3	O3 – C5	1.356 (3)	1.3514
4	O3 – H31	0.96(3)	0.9892
5	N1 – C1	1.465(3)	1.4811
6	C1 – C2	1.377(3)	1.3896
7	C1 – C6	1.377(3)	1.3895
8	C2 – C3	1.376(4)	1.3929
9	C2 – H2	0.9300	1.0798
10	C3 – C4	1.373(3)	1.3901
11	C3 – H3	0.9300	1.0838
12	C4 – C5	1.382(3)	1.402
13	C4 – H4	0.9300	1.0834
14	C5 – C6	1.384 (3)	1.3987
15	C6 – H6	0.9300	1.0813
16	O4 – N2	1.325(2)	1.2939 1.2655
17	N2 – C7	1.331(3)	1.3655 1.3749
18	N2 – C11	1.337(3)	1.364 1.3749
19	C7 – C8	1.374(3)	1.3777

			1.3755
20	C7 – H7	0.9300	1.0808 1.0798
21	C8 – C9	1.376(3)	1.4038 1.4044
22	C8 – H8	0.9300	1.0824 1.0829
23	C9 – C10	1.383(3)	1.4046 1.4043
24	C9 – C9	1.496 (4)	1.4707
25	C10 – C11	1.365(3)	1.3766 1.3755
26	C10 – H10	0.9300	1.0823 1.0829
27	C11 – H11	0.9300	1.0799 1.0798
28	O4 – H31	1.65(3)	1.7043

Table S2. Calculated **Bond angles (º), for the title compound.**

N1	**bond angles**	**X - Ray**	**B3LYP** **6-311G (3df, 2p)**
1	C3 – C4 – C5	120.5(2)	120.4664
2	C3 – C4 – H4	119.7	121.1677
3	C5 – C4 – H4	119.7	118.3655
4	O3 – C5 – C4	118.4(2)	118.0568
5	C4 – C5 – C6	119.7(2)	119.3966

6	C1 – C6 – C5	118.4(2)	118.5479
7	C1 – C6 – H6	120.8	120.3608
8	C5 – C6 – H6	120.8	121.0903
9	O4 – N2 – C7	119.8(2)	121.5652 121.022
10	O4 – N2 – C11	120.1(2)	119.5053 121.0163
11	C7 – N2 – C11	120.05(19)	118.9295 117.9618
12	N2 – C7 – C8	120.4(2)	121.0264 121.5263
13	N2 – C7 – H7	119.8	114.7203 113.7147
14	C8 – C7 – H7	119.8	124.2505 124.7562
15	C7 – C8 – C9	121.5(2)	121.5219 121.5439
16	C7 – C8 – H8	119.3	117.5371 117.5238
17	C9 – C8 – H8	119.3	120.9146 120.9051
18	C8 – C9 – C10	116.02(19)	115.9016 115.8954
19	C8 – C9 – C9	121.9(2)	122.0573 122.0568

20	C10 – C9 – C9	122.1(2)	122.0412 122.0478
21	C11 – C10 – C9	121.3(2)	121.3565 121.5603
22	C11 – C10 – H10	119.4	117.6711 117.5393
23	C9 – C10 – H10	119.4	120.9529 120.8754
24	N2 – C11 – C10	120.7(2)	121.2638 121.5115
25	N2 – C11 – H11	119.6	114.0214 113.7135
26	C10 – C11 – H11	119.6	124.7122 124.7724
27	O3 – C5 – C6	121.9(2)	122.5459
28	C5 – O3 – H31	111.7(18)	110.5437
29	O2 – N1 – O1	122.1(2)	124.495
30	O2 - N1 – C1	119.2(2)	117.704
31	O1 – N1 – C1	118.7(2)	117.8008
32	C2 – C1 – C6	122.7(2)	123.0826
33	C2 – C1 – N1	119.1(2)	118.7577
34	C6 – C1 – N1	118.2(2)	118.159
35	C3 – C2 –C1	117.9(2)	117.5613
36	C3 – C2 – H2	121.0	122.4631
37	C1 – C2 – H2	121.0	119.9757
38	C4 – C3 – C2	120.8(3)	120.9447

39	C4 – C3 – H3	119.6	119.5113
40	C2 – C3 – H3	119.6	119.5439