

Conformer stabilization of N-(5,7-dinitro-8-quinolinyl)-N-(4-nitrophenyl)amine

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Table S1. Bond lengths (Å) in **1** (X-ray data, conformers **A** and **B**, conformers **A** and **B** in SCRF(PCM) model).

	X-Ray	B	A	B (SCRF)	A (SCRF)
N1-C1	1.320(4)	1.318	1.316	1.320	1.318
C1-C2	1.401(5)	1.405	1.406	1.406	1.407
C2-C3	1.364(5)	1.377	1.375	1.377	1.376
C3-C4	1.417(4)	1.418	1.417	1.417	1.416
C4-C5	1.433(4)	1.435	1.433	1.436	1.434
C5-C6	1.357(4)	1.371	1.368	1.371	1.369
C6-C7	1.403(4)	1.401	1.401	1.401	1.401
C7-C8	1.401(3)	1.400	1.414	1.406	1.415
C8-C9	1.457(3)	1.459	1.456	1.459	1.457
C9-C4	1.413(4)	1.423	1.428	1.422	1.425
C9-N1	1.362(3)	1.350	1.348	1.348	1.348
C5-N2	1.469(3)	1.460	1.461	1.449	1.450
N2-O1	1.220(3)	1.229	1.229	1.231	1.231
N2-O2	1.230(4)	1.225	1.225	1.230	1.230
C7-N3	1.459(3)	1.456	1.450	1.447	1.440
N3-O3	1.231(3)	1.226	1.221	1.230	1.227
N3-O4	1.231(3)	1.226	1.243	1.229	1.241
C8-N4	1.353(3)	1.353	1.352	1.350	1.351
N4-C10	1.409(3)	1.398	1.408	1.396	1.406
C10-C11	1.389(4)	1.402	1.402	1.404	1.404
C11-C12	1.387(4)	1.386	1.384	1.385	1.384
C12-C13	1.379(5)	1.391	1.394	1.395	1.397
C13-C14	1.365(6)	1.392	1.390	1.395	1.393
C14-C15	1.382(5)	1.385	1.388	1.384	1.387
C15-C10	1.399(4)	1.403	1.400	1.405	1.401
C13-N5	1.467(4)	1.462	1.462	1.451	1.451
N5-O5	1.239(7)	1.225	1.226	1.230	1.230
N5-O6	1.248(6)	1.226	1.226	1.230	1.230

Table S2. Bond angles (°) in **1** (X-ray data, conformers **A** and **B**, conformers **A** and **B** in SCRF(PCM) model).

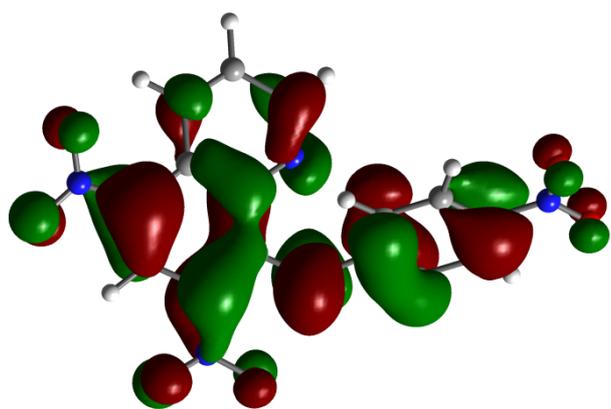
	X-Ray	B	A	B (SCRF)	A (SCRF)
N1-C1-C2	122.8(3)	122.4	122.8	122.4	122.9
C1-C2-C3	119.8(3)	119.4	119.1	119.3	119.1
C2-C3-C4	119.6(3)	119.8	119.715	119.7	119.6
C3-C4-C5	126.8(3)	127.0	125.8	126.7	125.8
C4-C5-C6	121.6(2)	120.5	120.8	120.9	121.1
C5-C6-C7	121.1(2)	122.1	121.69	121.6	121.3
C6-C7-C8	121.7(2)	121.3	121.5	121.3	121.4
C7-C8-C9	116.1(2)	116.3	116.3	116.4	116.4
C8-C9-N1	114.3(2)	114.5	115.6	114.7	115.6
C4-C5-N2	122.7(2)	123.5	123.3	123.0	122.8
O1-N2-O2	123.6(3)	123.8	124.0	123.0	123.2
C6-C7-N3	115.4(2)	115.7	115.7	115.6	115.8
O3-N3-O4	123.6(2)	125.0	122.8	123.7	122.1
C7-C8-N4	128.3(2)	129.4	121.4	128.7	122.1
C8-N4-C10	128.2(2)	132.4	131.2	131.7	129.9
N4-C10-C11	121.2(2)	123.0	122.5	122.7	122.1
C10-C11-C12	119.7(3)	120.1	120.0	120.0	119.9
C11-C12-C13	118.4(3)	119.2	119.2	119.2	119.2
C12-C13-C14	122.9(3)	121.7	121.7	121.7	121.7
C13-C14-C15	119.3(3)	118.9	118.8	118.9	118.8
C12-C13-N5	118.6(4)	119.2	119.1	119.1	119.1
O5-N5-O6	124.9(2)	124.9	124.8	123.4	123.4

Table S3. Energy values (H) obtained by B3PW91/6-31G(d,p) geometry optimizations.

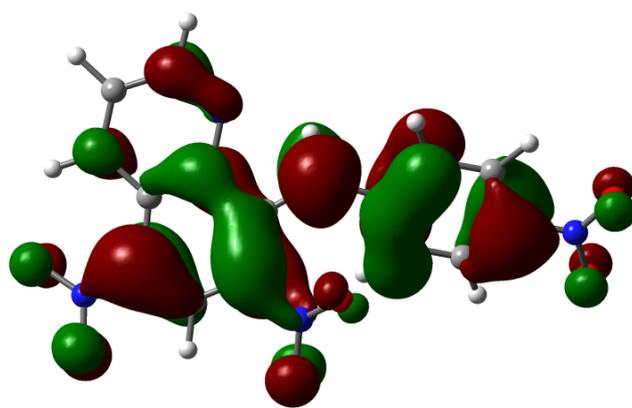
	A	B
Total energy	-1301.3537086	-1301.3534555
ZPE correction	0.242054	0.242449
TS energy*	-1301.3353293	
Total energy, SCRF model	-1301.3811217	-1301.3837788
TS energy*, SCRF model	-1301.3690278	

*Transition stage energy of isolated molecule was obtained by the maximum search (Gaussian03 keyword opt=ts) starting from the point of PES scan with highest energy. The corresponding value of energy in SCRF(PCM) model was obtained by single point calculation using the transition state geometry of isolated molecule.

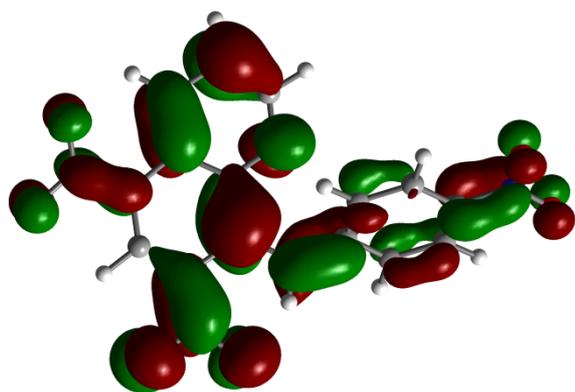
Figure S1. Molecular orbitals of N-(5,7-dinitro-8-quinolinyl)-N-(4-nitrophenyl)amine computed at the B3PW91/6-31G(d,p) level.



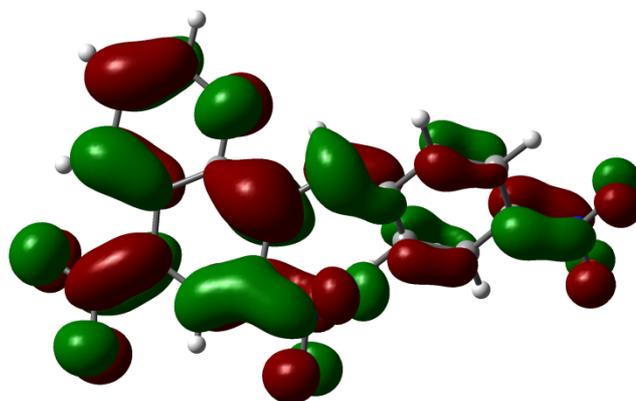
A, HOMO



B, HOMO



A, LUMO



B, LUMO