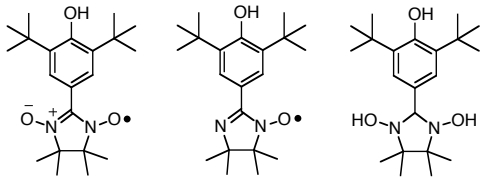
Supporting Material for

Crystallography and magnetism of radicals with hindered hydroxyl groups: 2-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4,4,5,5-tetramethyl-4,5-dihydro-*1H*-imidazole-3-oxide-1-oxyl and 2-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4,4,5,5-tetramethyl-4,5-dihydro-*1H*-imidazole-1-oxyl

Patrick Taylor and Paul M. Lahti*

Department of Chemistry, University of Massachusetts, Amherst MA 01003, USA.
E-mail: lahti@chem.umass.edu

(1) Synthetic Details for 1-2.



1 2 4

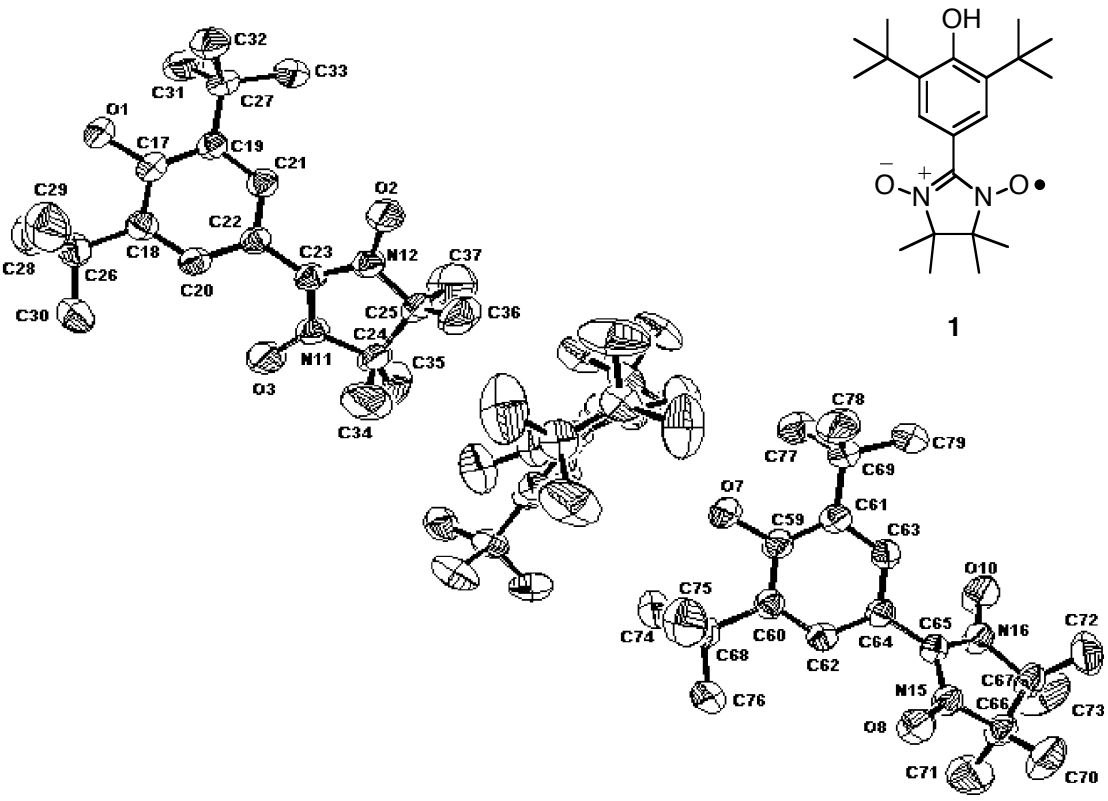
2-(3',5'-Di-tert-butyl-4-hydroxyphenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1,3-dihydoxy-1H-imidazole (**4**). 2,3-Bis(hydroxylamino)-2,3-dimethylbutane hydrogen sulfate monohydrate (0.246 g, 1 mmol) was suspended in 15 ml of absolute methanol in an oven-dried flask purged with argon. Triethyl amine (0.56 mL, 4 mmol) was added, followed by 3,5-di-*tert*-butyl-4-hydroxybenzaldehyde (0.500 g, 2.11 mmol). A West condenser was attached and the system heated gently under reflux for 4 days. The reaction was cooled and the resultant precipitate filtered to give **4** as a shiny white powder (0.155 g, 42%, mp 186-188 ºC). Additional product could be obtained by chromatography of the evaporated filtrate (silica, dichloromethane). This material was used without further purification in the subsequent reaction step. ^{1}H-NMR (DMSO-d_6): □ 7.67 (s, 2H), 7.19 (s, 2H), 6.79 (s, 1H), 4.35 (s, 1H), 1.37 (s, 18H), 1.05 (s, 12H)

2-(3',5'-Di-tert-butyl-4-hydroxyphenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazole-3-oxide-1-oxyl (**1**). Diol **4** (0.031 g, 0.085 mmol) was dissolved in 5 mL of dichloromethane under argon. Sodium periodate (0.041 g, 0.192 mmol) was dissolved in 5 mL of distilled water and added to the reaction. The two-phase mixture was stirred vigorously for 25 min. The organic phase was collected, and the aqueous layer was back-extracted with dichloromethane. The combined organic layers were dried over anhydrous sodium carbonate and filtered. The solvent was removed from the filtrate under reduced pressure to give a dark blue solid that was purified by column chromatography (silica, 7:3 hexanes:ethylacetate) to yield **1** as deep blue solid (0.026 g, 84%, mp 184-185 ºC [d]). FTIR (KBr, cm^{-1}): 3443 (br), 2968, 2361, 1733. ESR (toluene, 298 K, 9.650 GHz): pentet, a_N = 7.56 G. Analysis calc'd for $C_{21}H_{33}N_2O_3$; C 69.77, H 9.20, N 7.75: found C 69.83; H 9.16; N 20.49. MS(ESI, m/z): 252 (parent + H). Crystals suitable for X-ray analysis were obtained by slow evaporation under argon from a dichloromethane solution.

2-(3',5'-Di-tert-butyl-4-hydroxyphenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazole-1-oxyl (**2**). Radical **1** (9 mg, 0.025 mmol) was dissolved in 5 mL of dichloromethane under argon. Solid sodium nitrite (68 mg, 0.986 mmol) and 0.2 mL of a 0.1 M HCl solution were added to the dark blue solution, and the reaction allowed to stir until the reaction turned red (~30 min). The organic phase was collected, dried over anhydrous sodium carbonate, and evaporated under reduced pressure to give a brown/red solid. The crude product was purified by column chromatography (alumina, 7:3 hexanes:ethylacetate) to yield **2** as a red solid (3 mg, 35%, mp 190-192 ºC). FTIR (KBr, cm^{-1}): 3474 (br), 2969, 2367, 2341. ESR (toluene, 298 K, 9.652 GHz): seven lines, a_N = 9.33, 4.14 G. Analysis calc'd for $C_{21}H_{33}N_2O_2$; C 73.00, H 9.63, N 8.11: found C 72.92; H 9.55; N 7.83. Crystals suitable for X-ray analysis were obtained from a 1:1 ethylacetate:hexane solution.

(2) Crystallography for 1

For **1**; mp 184-185 °C. *Crystal data*: deep blue needle from dichloromethane, 0.35 × 0.35 × 0.20 mm, formula = $C_{21}H_{33}N_2O_3$, M = 361.49, monoclinic, space group $P2_1/c$, T = 293 K, Z = 12, a = 17.3092(2), b = 30.9285(3), c = 12.1652(1) Å, β = 90.8163(5)°, V = 6511.95(11) Å^3, D_{calc} = 1.106 g cm^{-3}, λ(Mo-Kα) = 0.7107 Å, μ = 0.073 mm^{-1}, $F(000)$ = 2364. 21763 reflections were recorded at a threshold intensity of 2σ(I). 11406 independent reflections (R_{int} = 0.0406) were analyzed with 705 parameters using SHELXL-97. For 6818 reflections with I > 2σ(I)) $R(I>2\sigma)$ = 0.0779, $wR(I>2\sigma)$ = 0.2039; $R(all)$ = 0.1279, $wR(all)$ = 0.2281, goodness of fit on F^2 = 1.358. This structure has been submitted to the Cambridge Crystallographic Data Centre as CCDC Deposition #243200.



1

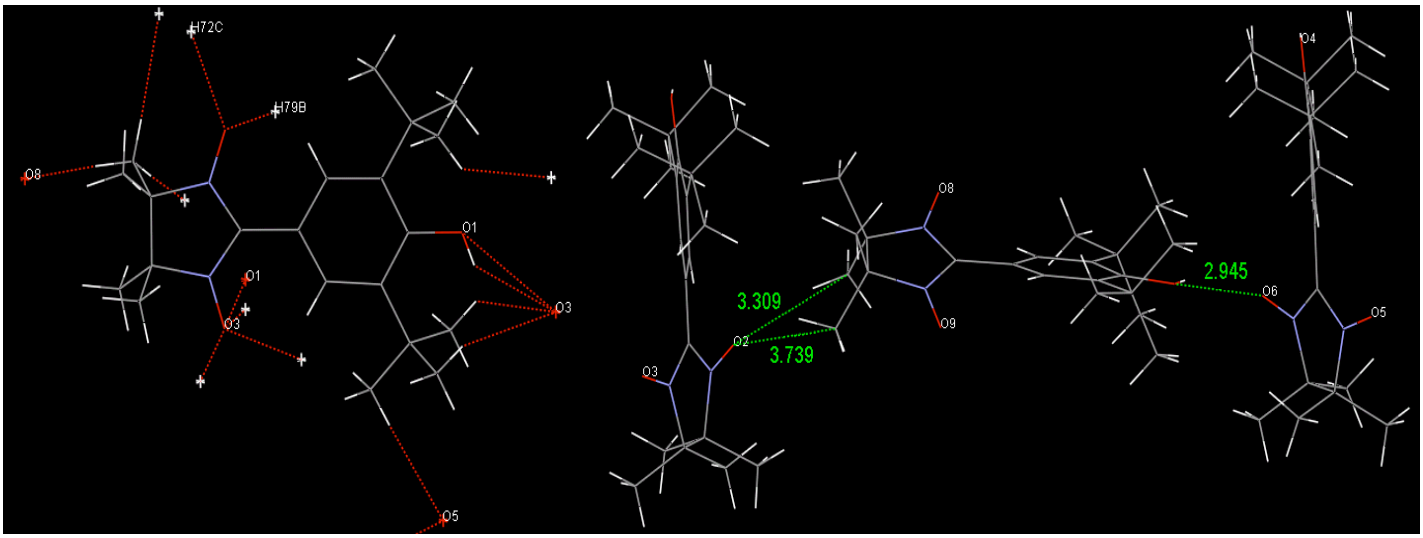
Notes: There are three different molecules in the unit cell, forming two slighly different H-bonding chains as shown in the main manuscript. The differences in the molecular geometries of the three molecules are very small.

Selected Bonding Parameters for Compound 1 in angstroms (see numbering diagram on page S3).

Nitronylnitroxide ONCNO units	
O(2)-N(12)	1.291(2)
O(3)-N(11)	1.275(3)
N(11)-C(23)	1.350(3)
N(12)-C(23)	1.333(3)
O(5)-N(14)	1.298(3)
O(6)-N(13)	1.275(3)
N(13)-C(44)	1.352(3)
N(14)-C(44)	1.327(3)
O(8)-N(15)	1.291(2)
O(10)-N(16)	1.276(2)
N(15)-C(65)	1.346(3)
N(16)-C(65)	1.340(3)
Phenolic Rings	
O(1)-C(17)	1.361(3)
C(17)-C(19)	1.407(3)
C(17)-C(18)	1.419(3)
C(18)-C(20)	1.378(3)
C(19)-C(21)	1.381(3)
C(20)-C(22)	1.392(3)
C(21)-C(22)	1.391(3)
O(4)-C(38)	1.357(3)
C(38)-C(40)	1.410(3)
C(38)-C(39)	1.417(3)
C(39)-C(41)	1.384(3)
C(40)-C(42)	1.380(3)
C(41)-C(43)	1.389(3)
C(42)-C(43)	1.403(3)
O(7)-C(59)	1.359(3)
C(59)-C(61)	1.412(3)
C(59)-C(60)	1.415(3)
C(60)-C(62)	1.384(3)
C(61)-C(63)	1.384(3)
C(62)-C(64)	1.386(3)
C(63)-C(64)	1.399(3)

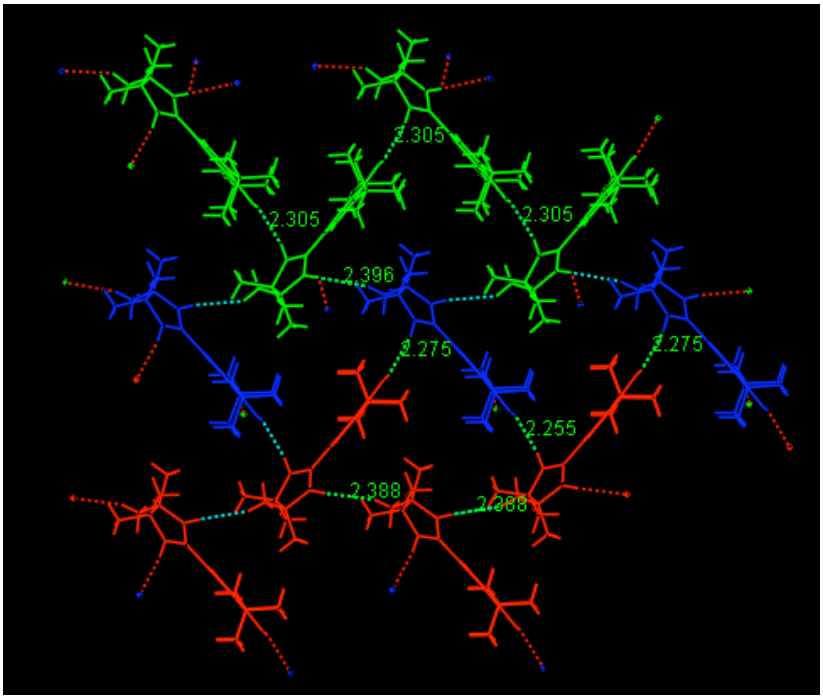
Transannular Linkages	
C(22)-C(23)	1.453(3)
C(43)-C(44)	1.453(3)
C(64)-C(65)	1.450(3)
Transannular Torsions	
N(11)-C(22)-C(21)C(19)	-33.45°
N(13)-C(44)-C(43)C(42)	-33.85°
N(15)-C(65)-C(64)C(62)	-30.81°
OH to ON contacts	
Phenol O(1) to nitroxide O(3)	2.945
Phenol O(4) to nitroxide O(9)	2.901
Phenol O(6) to nitroxide O(7)	2.880
Phenol H(?) to nitroxide O(3)	2.880
Phenol H(4) to nitroxide O(9)	2.901
Phenol H(6) to nitroxide O(7)	2.880
Nitronylnitroxide CH_3 to ON contacts	
Methyl C(72) to nitroxide O(2)	3.393
Methyl C(79) to nitroxide O(2)	3.309
Methyl C(31) to nitroxide O(5)	3.429
Methyl C(58) to nitroxide O(5)	3.271

Contacts for molecules in the unit cell of 1



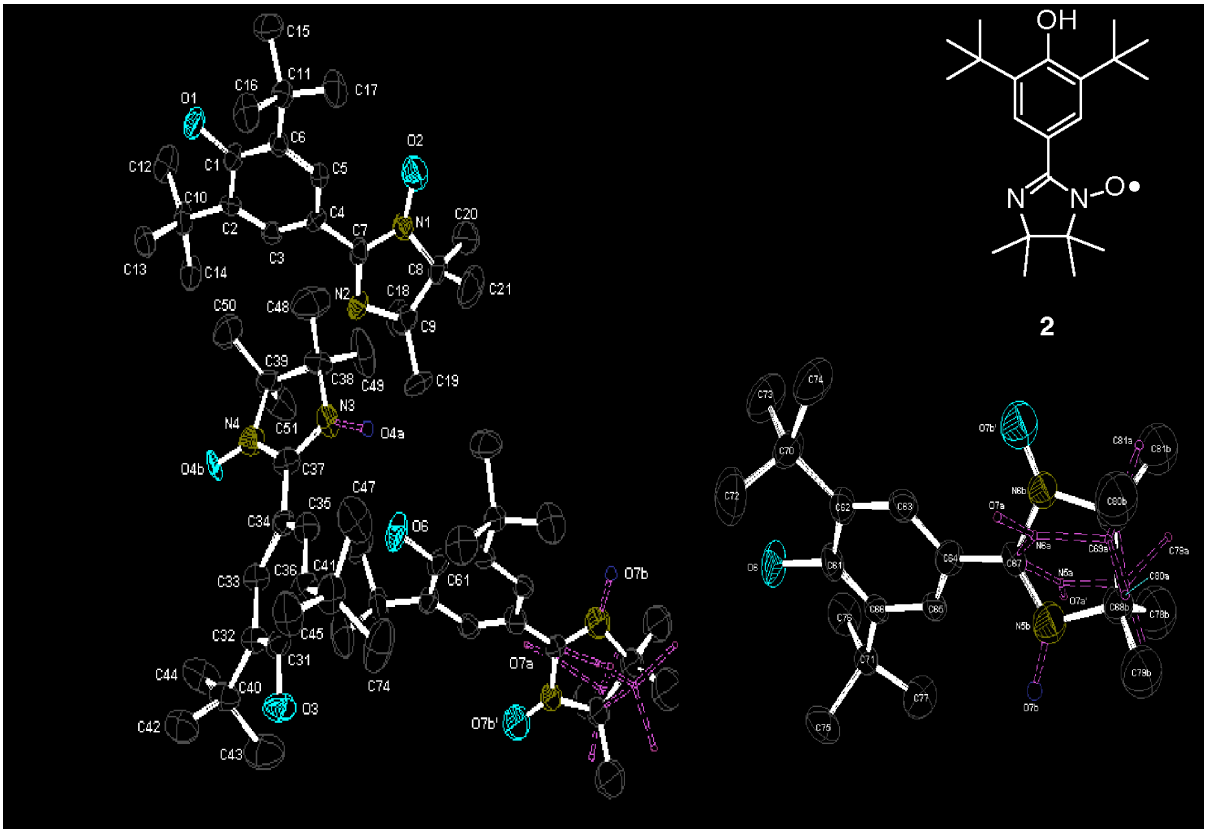
The exapansion above shows one of the three distinct molecules in the unit cell. Note the O(3)•••H-O(1) contact, nitroxide to phenolic OH. O(8) and O(5) (which show methyl CH to nitroxide ON close contacts) are nitroxide oxygens from the other two molecules of the units cell. The methyl CH to nitroxide ON contacts form their own CH to ON chains (blue to green contacts between molecules shown below, and red to red contacts, running almost exactly horizontal as shown). The distances shown below are based on the crystallographic assignments for the hydrogen atoms in the methyl units.

One phenolic OH to nitroxide ON chain is comprised of molecules containing the O(3)•••H-O(1) contacts shown above (green molecules below), the other chain is formed by the same motif, but with the other two molecules of the unit cell (blue and red molecules). The zig-zag chains are almost identical in geometry, as shown below, hence our treatment of the magnetic behavior by a single chain model. The distances shown below are based on the crystallographic assignments for the hydrogen atoms in the phenolic units. Both of these figures were made using the CCDC program Mercury version 1.2.



(3) Crystallography for 2

For **2**, mp 190-192 °C. *Crystal data*: red needle from hexanes/ethyl aceteate, 0.70 × 0.50 × 0.15 mm, formula = $C_{21}H_{33}N_2O_2$, M = 345.49, orthorhombic, space group $P2_12_12_1$, T = 173 K, Z = 12, a = 111.8548(1), b = 17.1035(2), c = 30.8698(4) Å, V = 625912(12) Å^3, D_{calc} = 1.100 g cm^{-3}, λ(Mo-Kα) = 0.7107 Å, μ = 0.070 mm^{-1}, $F(000)$ = 2268. 10723 reflections were recorded at a threshold intensity of 2σ(I). 10723 independent reflections (R_{int} = 0.000) were analyzed with 705 parameters using SHELXL-97. For 7222 reflections with I > 2σ(I)) $R(I>2\sigma)$ = 0.0680, $wR(I>2\sigma)$ = 0.1579; $R(all)$ = 0.1122, $wR(all)$ = 0.1834, goodness of fit on F^2 = 1.032. An absolute structure parameter of 0(3) was used. This structure has been submitted to the Cambridge Crystallographic Data Centre as CCDC Deposition #243201.



Notes: No hydrogen atoms are shown, for ease of viewing. See the CIF file deposited with the CCDC, and submitted as supporting material with this manuscript, for further details. (a) the proton attached to O1 was not located. (b) All positions shown in green are alternate positions due to disorder, even at –100 ºC [disorder was worse at room temperature]. (c) the N-O positions are substantially disordered: the occupancies are

- C68a = 50%, C68b = 50%;
- N5a = 50 %, N6a = 50%;
- O4a = 65%/ O4b = 35%;
- O7a = 40%, O7a' = 10% (not labeled above), O7b = 30%, O7b' = 20%.

There are three different molecules in the cell – the most disordered is shown to the right.

Selected Bonding Parameters for Compound 2 in angstroms (see numbering diagram on page S6).

Iminoylnitroxide ONCN units	
O(1)-C(1)	1.363(5)
O(2)-N(1)	1.275(4)
N(1)-C(7)	1.360(5)
N(1)-C(8)	1.474(5)
N(2)-C(7)	1.308(5)
N(2)-C(9)	1.478(5)
O(4A)-N(3)	1.201(4)
O(4B)-N(4)*	1.160(6)
N(3)-C(37)	1.366(5)
N(3)-C(38)	1.480(5)
N(4)-C(37)	1.309(5)
N(4)-C(39)	1.487(5)
O(7A)-N(6A)	1.226(8)
O(7B')-N(6B)*	1.162(15)
O(7A')-N(5A)**	1.06(3)
O(7B)-N(5B)***	1.206(12)
N(5A)-C(67)	1.365(7)
N(5A)-C(68A)	1.539(10)
N(6A)-C(67)	1.310(7)
N(6A)-C(69A)	1.500(11)
N(5B)-C(67)	1.278(8)
N(5B)-C(68B)	1.508(10)
N(6B)-C(67)	1.390(7)
N(6B)-C(69B)	1.516(11)
Phenolic Rings	
O(1)-C(1)	1.363(5)
C(1)-C(6)	1.406(5)
C(1)-C(2)	1.445(5)
C(2)-C(3)	1.366(5)
C(3)-C(4)	1.389(5)
C(4)-C(5)	1.402(5)
C(5)-C(6)	1.381(5)
O(3)-C(31)	1.378(5)
C(31)-C(32)	1.381(6)
C(31)-C(36)	1.415(6)
C(32)-C(33)	1.403(5)
C(33)-C(34)	1.391(5)
C(34)-C(35)	1.396(5)
C(35)-C(36)	1.385(6)
O(6)-C(61)	1.391(5)
C(61)-C(66)	1.370(6)
C(61)-C(62)	1.416(6)
C(62)-C(63)	1.393(5)
C(63)-C(64)	1.384(6)
C(64)-C(65)	1.382(5)
C(65)-C(66)	1.404(5)

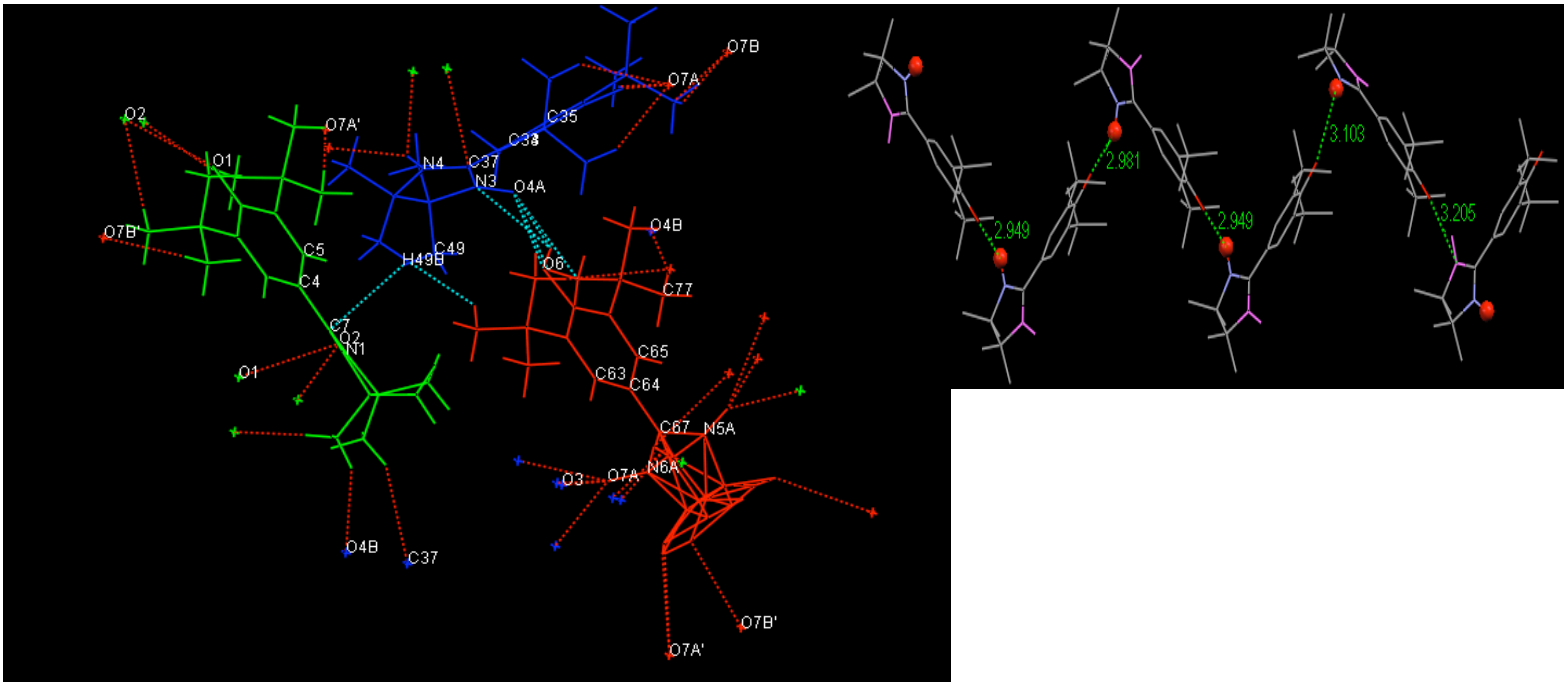
Transannular Linkages	
C(4)-C(7)	1.489(5)
C(34)-C(37)	1.482(5)
C(64)-C(67)	1.447(6)
Transannular Torsions	
N(4)-C(37)-C(34)C(33)	-32.40°
N(1)-C(7)-C(4)C(5)	-29.03°
N(6A)-C(67)-C(64)C(63)	-24.87°
N(5B)-C(67)-C(64)C(65)***	-30.81°
OH to ON contacts	
Phenol O(1) to nitroxide O(2)	2.936
Phenol O(3) to nitroxide O(7A)	2.981
Phenol O(6) to nitroxide O(4A)	2.949
Phenol H(1C) to nitroxide O(4A)	2.191
Phenol H(1B) to nitroxide O(7A)	2.186
(the hydrogen on O(1) was not located)	
Iminoylnitroxide CH_3 to ON contacts	
Methyl C(18) to nitroxide O(4B)	3.285
Methyl C(20) to nitroxide O(4B)	3.774
Methyl C(80A) to nitroxide O(7A)	2.930
Methyl C(80B) to nitroxide O(7A)	3.153
Methyl C(45) to nitroxide O(7B)	3.383
Methyl C(46) to nitroxide O(7B)	2.933

* Disordered position relative to N(6A).

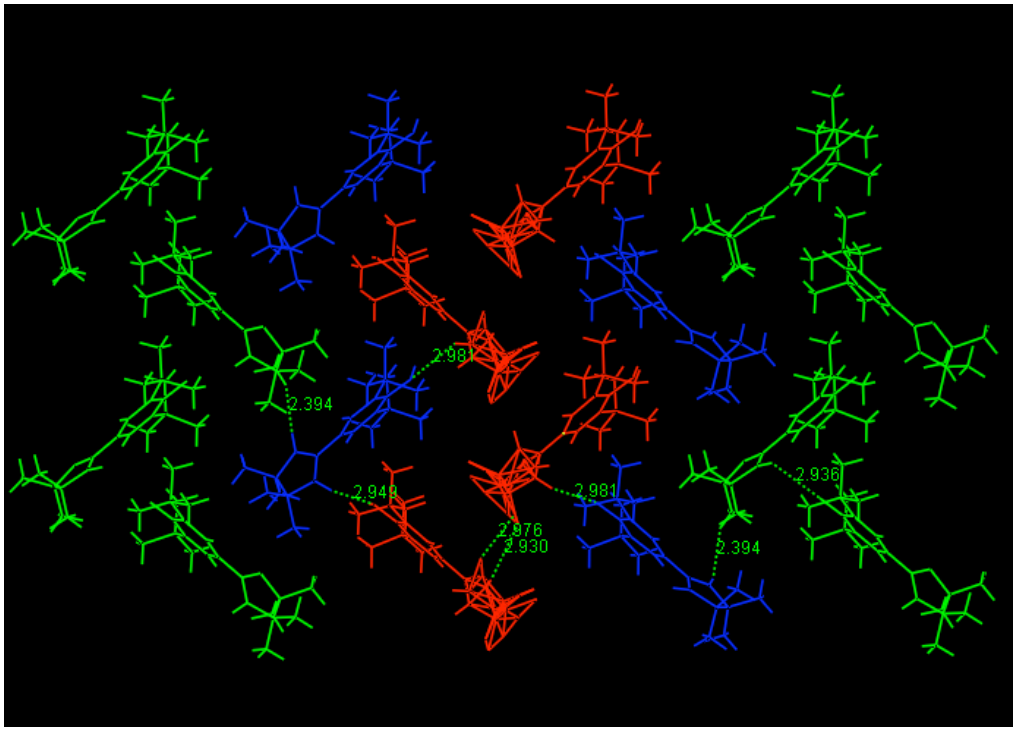
**Alternate position (torsional disordered site)

***Alternate position (torsional disordered site).

Contacts for molecules in the unit cell of 2.

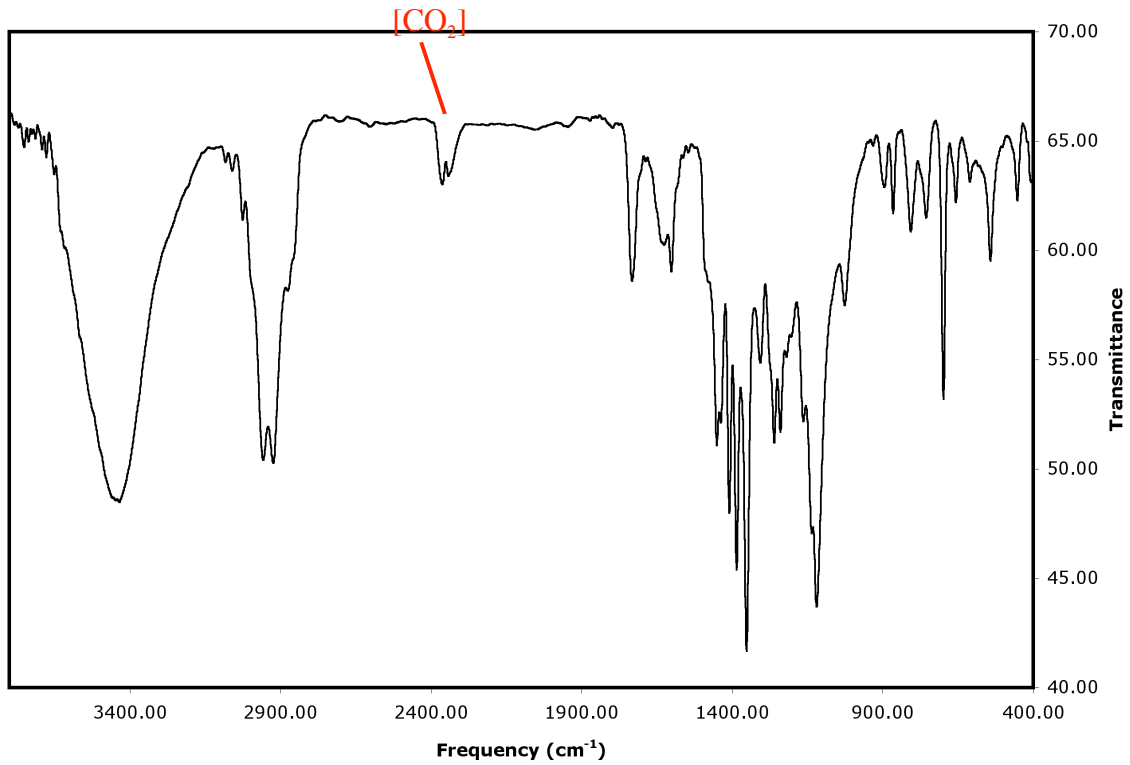


The exapansion above shows the three distinct molecules in the unit cell, and various close contacts from the nitroxide NO groups to nitroxide methyl CH and phenolic OH groups. One OH proton was not located crystallographically, so only the oxygen is shown, O(1). The figure below shows the close contact CH to ON and OH to NO for the "chains" in this system, showing both of the disordered NO group positions in cases where there is nitroxide disorder in the iminoylnitroxide group. Thus, *the reader should keep in mind that the actual "chains" are incomplete (frustrated)*, due to a lack of sufficient N-O bonds to form extended chains. If each chain were essentially complete, with disorder in the directionality of one chain versus another, we would have expected that the magnetic behavior of **2** would fit a relatively simple AFM 1-D chain behavior (it does not). These figures were made using the CCDC program Mercury version 1.2.

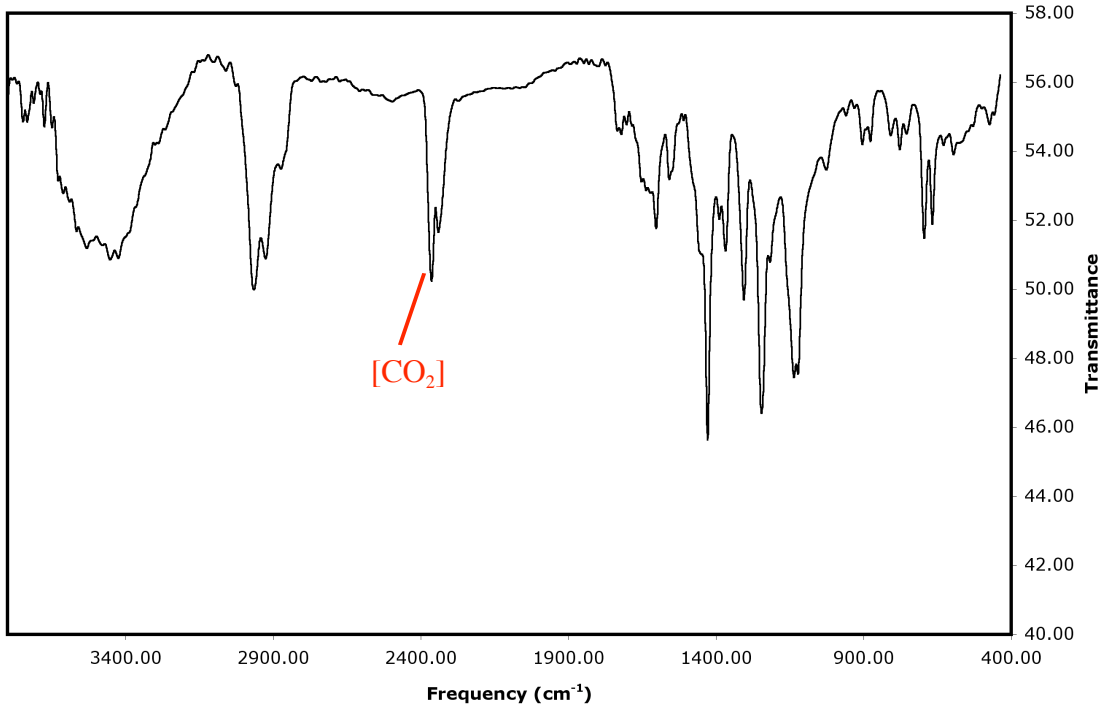


(4) FTIR spectra for 1-2

SPECTRUM Of **1**, KBr pellet, below.

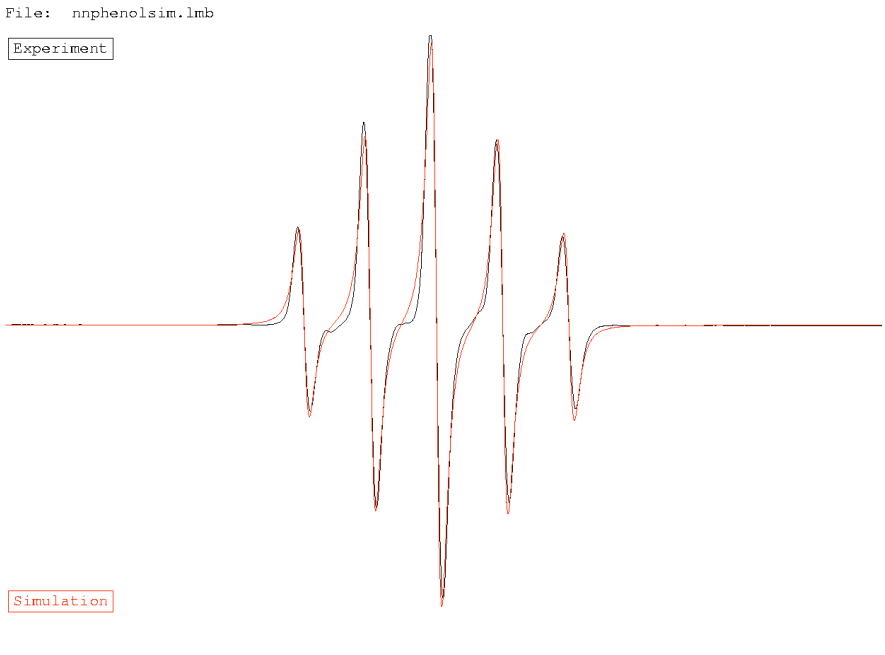


SPECTRUM Of **2**, KBr pellet, below.



(4) ESR spectra, room temperature.

SPECTRUM Of **1**, 9.650 GHz, toluene, below, black trace. Red trace from WINSIM simulator (D. R. Duling, *J. Magn. Res.*, 1994, **B104**, 105-110), a(N) = 7.55 G (2), correlation coefficient = 0.99.



SPECTRUM Of **2**, 9.652 GHz, toluene, below, black trace. Red trace from WINSIM simulator (D. R. Duling, *J. Magn. Res.*, 1994, **B104**, 105-110), a(N) = 9.33, 4.14 G, correlation coefficient = 0.98.

(4) Magnetic Analyses.

(1) Bonner-Fisher 1-D Heisenberg Chain Model (J. C. Bonner and M. E. Fisher, *Phys. Rev. A*, 1964, **135**, 650. J. C. Bonner, Ph. D. Dissertation, University of London, UK, 1968.

T = absolute temperature, J = exchange constant, S = spin quantum number, β_B = Bohr magneton, g = Landé constant, θ = mean field constant, P = fraction of isolated paramagnetic spins in sample.

$$\chi = (1-P)\left[\frac{4\cdot C_0}{[T-\theta]}\right]\left[\frac{A+Bx+Cx^2}{1+Dx+Ex^2+Fx^3}\right]+P\frac{0.375}{T}$$

$$x = |J/kT|; C_0 = Ng^2\beta_B{}^2 S(S+1)/3k$$

P=paramagnetic component

The fitted parameters were P, J, θ.

(2) Double Bleaney-Bowers fit (B. Bleaney and K. D. Bowers, *Proc. R. Soc. London, A*, 1952, 214.)

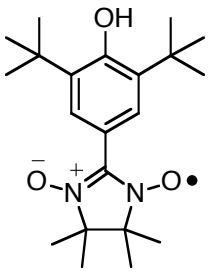
$$\chi = (1-P)\left[\frac{2\cdot C_0}{T}\right]\left[\frac{2e^x}{1+3e^x}\right]+P\left[\frac{2\cdot C_0}{T}\right]\left[\frac{2e^y}{1+3e^y}\right]$$

$$x = |J_1/kT|; y = |J_2/kT|; C_0 = 0.375g^2/4$$

Here, P = fraction of **2** with exchange coupling J_1, (1-P) = fraction with J_2.
The fitted parameters were P, J_1, J_2, g.

(4) Computational Modeling for Exchange Involving H-bonding contact

(Model for H-bond in molecule 1)



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Test job not archived.
 1\1\GINC-GROND\SP\UB3LYP\6-31G(d)\C8H10N4O5(3)\LAHTI\31-Mar-2004\0\\#P
  GFINPUT IOP(6/7=3) UB3LYP DIRECT 6-31G(D) TEST GUESS=(READ)\\Triplet
 state of 4-hydroxy-3,5-di-t-butylphenol nitronylnitroxide H-Bond conta
 ct interaction\\0,3\C,0,4.269,11.14,1.125\O,0,2.308,3.242,7.873\O,0,6.
 165,4.876,5.955\N,0,5.167,4.109,6.246\N,0,3.332,3.355,7.122\C,0,5.514,
 9.592,2.57\C,0,4.293,10.052,2.086\N,0,3.332,12.109,1.04\O,0,6.165,10.5
 89,-0.127\O,0,4.388,6.855,4.691\C,0,4.269,4.324,7.207\H,0,2.302,9.804,
 2.275\H,0,5.156,6.643,4.885\C,0,3.138,8.412,3.446\O,0,2.308,12.222,1.7
 91\C,0,4.407,7.944,3.876\N,0,5.167,11.355,0.163\C,0,5.61,8.558,3.481\H
 ,0,2.206446882,7.938014333,3.775791206\H,0,6.296,9.996,2.268\H,0,3.480
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 631\H,0,4.287109433,5.144960939,7.932886452\H,0,3.480175198,2.73185221
 8,6.338498248\H,0,6.590990572,8.231712471,3.844881517\H,0,5.032534828,
 3.232611382,5.758141409\C,0,3.121,9.47,2.562\\Version=SGI64-G03RevB.03
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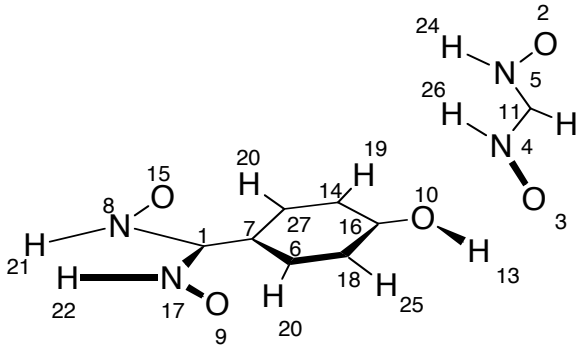
Mulliken atomic spin densities:



		1
1	C	-0.222481
2	O	0.431661
3	O	0.341915
4	N	0.256242
5	N	0.245144
6	C	-0.032557
7	C	0.038788
8	N	0.258686
9	O	0.375821
10	O	-0.005106
11	C	-0.264612
12	H	0.001399
13	H	0.002838
14	C	0.014813
15	O	0.396878
16	C	-0.028503
17	N	0.244426
18	C	0.014459
19	H	-0.000552
20	H	0.001409
21	H	-0.013723
22	H	-0.012988
23	H	0.012451
24	H	-0.012912
25	H	-0.000674
26	H	-0.013013
27	C	-0.029807

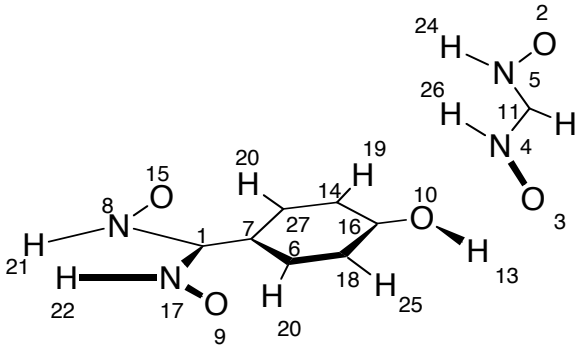
Sum of Mulliken spin densities= 2.00000

Heavy atom positions taken from crystal structure of **1** in this work.

Test job not archived.
1\1\GINC-GROND\SP\UB3LYP\6-31G(d)\C8H10N4O5\LAHTI\30-Mar-2004\0\\# UB3
LYP DIRECT 6-31G(D) TEST GUESS=(READ,MIX)\\Singlet state of 4-hydroxy-
3,5-di-t-butylphenol nitronylnitroxide\\0,1\C,0,4.269,11.14,1.125\O,0,
2.308,3.242,7.873\O,0,6.165,4.876,5.955\N,0,5.167,4.109,6.246\N,0,3.33
2,3.355,7.122\C,0,5.514,9.592,2.57\C,0,4.293,10.052,2.086\N,0,3.332,12
.109,1.04\O,0,6.165,10.589,-0.127\O,0,4.388,6.855,4.691\C,0,4.269,4.32
4,7.207\H,0,2.302,9.804,2.275\H,0,5.156,6.643,4.885\C,0,3.138,8.412,3.
446\O,0,2.308,12.222,1.791\C,0,4.407,7.944,3.876\N,0,5.167,11.355,0.16
3\C,0,5.61,8.558,3.481\H,0,2.206446882,7.938014333,3.775791206\H,0,6.2
96,9.996,2.268\H,0,3.480098532,12.731825321,0.256227451\H,0,5.03261253
8,12.231557432,-0.324576631\H,0,4.287109433,5.144960939,7.932886452\H,
0,3.480175198,2.731852218,6.338498248\H,0,6.590990572,8.231712471,3.84
4881517\H,0,5.032534828,3.232611382,5.758141409\C,0,3.121,9.47,2.562\\
Version=SGI64-G03RevB.03\State=1-A\HF=-905.5785338\S2=1.127808\S2-1=0.
\S2A=1.001808\RMSD=1.376e-05\Dipole=0.4070793,-0.6831437,-0.1788483\PG
=C01 [X(C8H10N4O5)]\\@

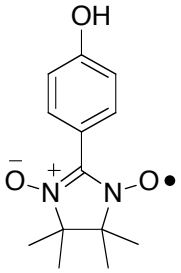
Mulliken atomic spin densities:

		1
1	C	0.223535
2	O	0.430706
3	O	0.343753
4	N	0.255787
5	N	0.246345
6	C	0.032447
7	C	-0.039005
8	N	-0.259203
9	O	-0.376868
10	O	0.006148
11	C	-0.266513
12	H	-0.001379
13	H	0.002558
14	C	-0.014434
15	O	-0.396230
16	C	0.028042
17	N	-0.244432
18	C	-0.014149
19	H	0.000517
20	H	-0.001413
21	H	0.013725
22	H	0.013008
23	H	0.012711
24	H	-0.012963
25	H	0.000587
26	H	-0.013010
27	C	0.029730



Heavy atom positions taken from crystal structure of **1** in this work.

(Model for H-bond in molecule 3)



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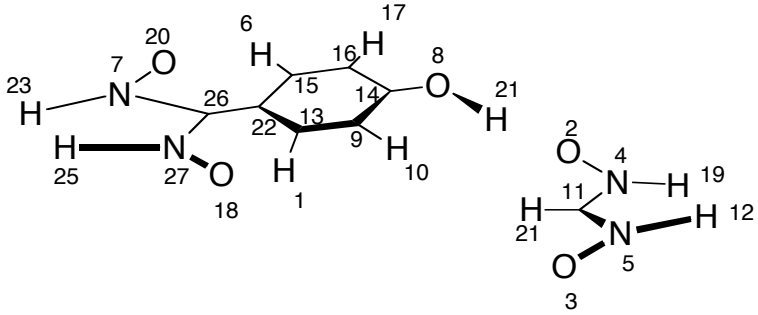
Test job not archived.
 1\1\GINC-GROND\SP\UB3LYP\6-31G(d)\C8H10N4O5(3)\LAHTI\31-Mar-2004\0\\#P
  GFINPUT IOP(6/7=3) UB3LYP DIRECT 6-31G(D) TEST GUESS=(READ)\\Veciana
 4OHPh-NN h-bond contact, triplet state\\0,3\H,0,6.612,5.256,16.615\O,0
 ,10.274,8.29,15.691\O,0,12.864,12.076,16.172\N,0,10.654,9.513,15.839\N
 ,0,11.865,11.296,16.031\H,0,8.294,2.113,14.75\N,0,5.983,1.43,16.031\O,
 0,10.698,5.731,14.98\C,0,8.476,5.616,15.913\H,0,8.518,6.541,16.263\C,0
 ,11.912,9.947,15.855\H,0,10.934340466,11.674562036,15.909726141\C,0,7.
 332,4.874,16.145\C,0,9.544,5.05,15.257\C,0,8.339,3.012,15.051\C,0,9.47
 9,3.726,14.836\H,0,10.271,3.398,14.433\O,0,4.392,4.436,15.691\H,0,9.96
 610969,10.229215157,16.033902252\O,0,6.981,0.65,16.172\H,0,12.83067355
 ,9.362872316,15.728312558\C,0,7.24,3.549,15.688\H,0,5.052237099,1.0516
 68307,15.909799939\H,0,10.612442341,6.638091523,15.27602132\H,0,4.0841
 0969,2.496784843,16.033902252\C,0,6.03,2.779,15.855\N,0,4.772,3.213,15
 .839\\Version=SGI64-G03RevB.03\State=3-A\HF=-905.5941257\S2=2.129074\S
 2-1=0.\S2A=2.007094\RMSD=7.126e-06\Dipole=0.1926881,1.7879341,0.1715823
 \PG=C01 [X(C8H10N4O5)]\\@
```

Mulliken atomic spin densities:

		1
1	H	0.001623
2	O	0.321609
3	O	0.457095
4	N	0.254599
5	N	0.247466
6	H	0.001468
7	N	0.271016
8	O	-0.006878
9	C	0.014396
10	H	-0.000829
11	C	-0.265583
12	H	-0.012944
13	C	-0.035385
14	C	-0.028043
15	C	-0.031255
16	C	0.015532
17	H	-0.000611
18	O	0.363023
19	H	-0.012217
20	O	0.408366
21	H	0.012659
22	C	0.040306
23	H	-0.013962
24	H	-0.002442
25	H	-0.012259
26	C	-0.222454
27	N	0.235702



```
 Sum of Mulliken spin densities=   2.00000
```

Heavy atom positions taken from CCDC ref # 624500 (HAFXOB); E. Hernandez, M. Mas, E. Molins, C. Rovira, J. Veciana, *Angew. Chem. Int. Ed. Engl*, **32**, 882 (1993).

```
Test job not archived.
 1\1\GINC-GROND\SP\UB3LYP\6-31G(d)\C8H10N4O5\LAHTI\31-Mar-2004\0\\#P GF
 INPUT IOP(6/7=3) UB3LYP DIRECT 6-31G(D) TEST GUESS=(READ,MIX)\\Veciana
  4OHPh-NN h-bond contact, singlet state\\0,1\H,0,6.612,5.256,16.615\O,
 0,10.274,8.29,15.691\O,0,12.864,12.076,16.172\N,0,10.654,9.513,15.839\
 N,0,11.865,11.296,16.031\H,0,8.294,2.113,14.75\N,0,5.983,1.43,16.031\O
 ,0,10.698,5.731,14.98\C,0,8.476,5.616,15.913\H,0,8.518,6.541,16.263\C,
 0,11.912,9.947,15.855\H,0,10.934340466,11.674562036,15.909726141\C,0,7
 .332,4.874,16.145\C,0,9.544,5.05,15.257\C,0,8.339,3.012,15.051\C,0,9.4
 79,3.726,14.836\H,0,10.271,3.398,14.433\O,0,4.392,4.436,15.691\H,0,9.9
 6610969,10.229215157,16.033902252\O,0,6.981,0.65,16.172\H,0,12.8306735
 5,9.362872316,15.728312558\C,0,7.24,3.549,15.688\H,0,5.052237099,1.051
 668307,15.909799939\H,0,10.612442341,6.638091523,15.27602132\H,0,4.084
 10969,2.496784843,16.033902252\C,0,6.03,2.779,15.855\N,0,4.772,3.213,1
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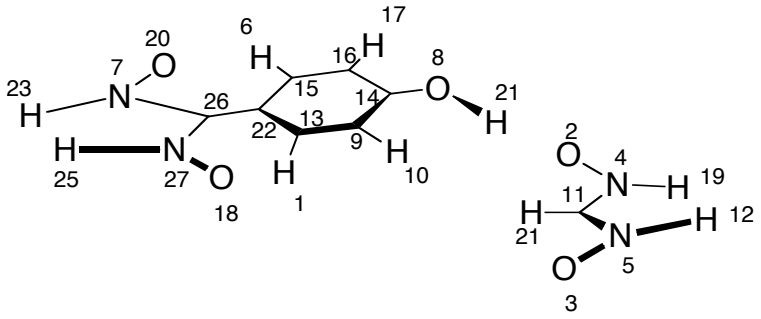
 S2-1=0.\S2A=1.004133\RMSD=2.592e-05\Dipole=-0.1902365,1.7878256,0.1739
 83\PG=C01 [X(C8H10N4O5)]\\@
```

Mulliken atomic spin densities:

		1
1	H	-0.001510
2	O	0.321108
3	O	0.457399
4	N	0.254781
5	N	0.247746
6	H	-0.001355
7	N	-0.271686
8	O	0.006466
9	C	-0.012493
10	H	0.000124
11	C	-0.265965
12	H	-0.012986
13	C	0.033522
14	C	0.026808
15	C	0.029499
16	C	-0.013804
17	H	0.000498
18	O	-0.360491
19	H	-0.012188
20	O	-0.409735
21	H	0.012824
22	C	-0.038353
23	H	0.014099
24	H	-0.002865
25	H	0.012020
26	C	0.220949
27	N	-0.234411



Heavy atom positions taken from CCDC ref # 624500 (HAFXOB); E. Hernandez, M. Mas, E. Molins, C. Rovira, J. Veciana, *Angew. Chem. Int. Ed. Engl*, **32**, 882 (1993).