Supporting Material

Toward Multifunctional Biradicals: Anthracene and Anthraquinone Linkage of Nitronyl and Iminoyl Nitroxides

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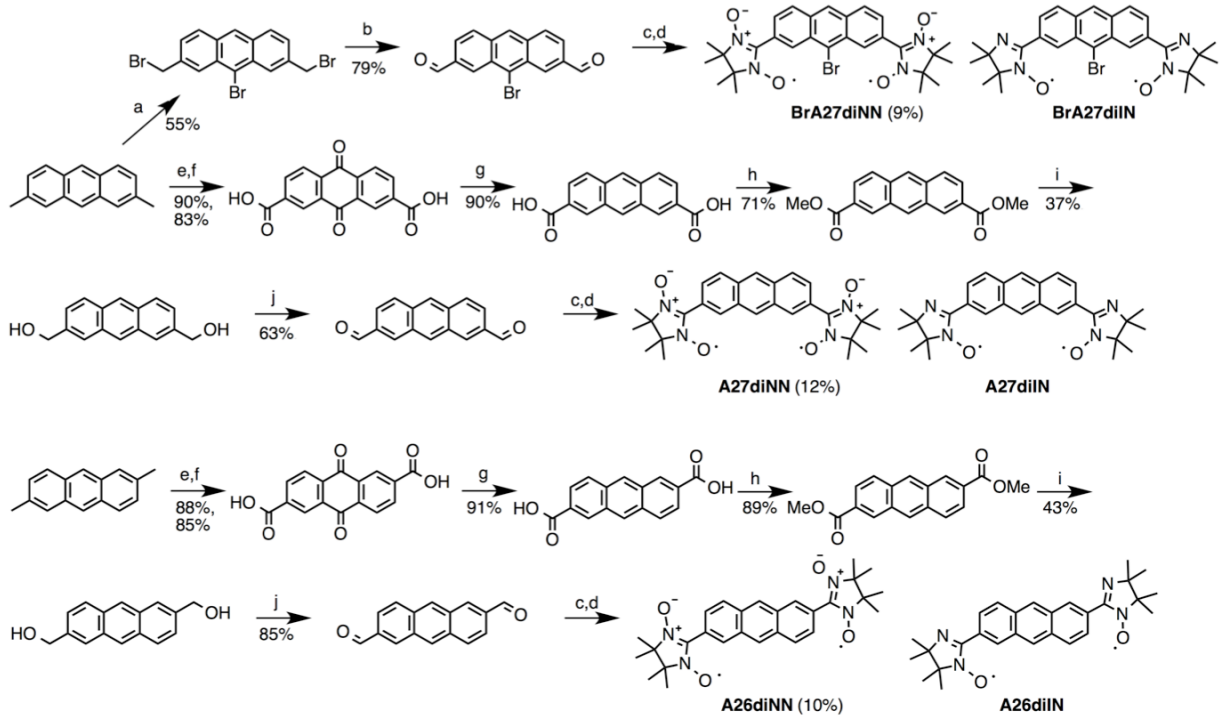
Experimental Details for Synthesis and Characterization of Biradicals.

General: All chemicals and solvents were obtained from commercial suppliers and were used as received unless otherwise stated. Infrared spectra were recorded on a Bruker Alpha FTIR spectrometer with attenuated total reflectance sample attachment. 1H-NMR spectra were recorded on a Bruker AVANCE-400 spectrometer in deuterated solvents, and are reported in ppm down-field of tetramethylsilane. Electron spin resonance (ESR) spectra were recorded on a Bruker Elexsys E-500 in X-band mode. Dr. S. Eyles collected Mass spectrometry data at the UMass-Amherst Mass Spectrometry Facility. Some magnetic measurements were carried out at the UMass Amherst Nanomagnetic Characterization Facility. Some X-ray crystallographic data were carried out at the UMass Amherst X-ray Structural Characterization Lab with assistance from Dr. A. Chandrasekaran.



2,4,4'-Trimethylbenzophenone: Equivalent weights of *p*-toluoyl chloride (10 g, 64.7 mmol) and *m*-xylene (6.87 g, 64.7 mmol) were mixed and dissolved in dry carbon disulfide (~20 mL). The solution was gradually added to a rapidly stirred suspension of powdered anhydrous aluminum trichloride (10 g) covered with carbon disulfide in a reflux apparatus and cooled with an ice bath. Heat was generated as the aluminum trichloride dissolved to give an orange then dark brown-green solution, and a vapor (hydrogen chloride) was evolved. When addition was complete, the solution was boiled in a hot water bath for 2 h. Water was added cautiously to the reaction mixture, then *m*-xylene and carbon disulfide were distilled away in steam. The residue was extracted with ether, and the combined ether layers were washed multiple times with 10 % NaOH solution then dried over anhydrous magnesium sulfate. After removal of the ether, 2,4,4'-trimethylbenzophenone was obtained as an oily liquid that was sufficiently pure for further use (11.6 g 80%). ^{1}H NMR (400 MHz, DMSO-d_6): δ 7.63-7.61 (d, 2H, J = 8.08 Hz), 7.38-7.36 (d, 2H, J = 8.08 Hz), 7.22-7.13 (m, 3H), 2.42 (s, 3H), 2.38 (s, 3H), 2.23 (s, 3H).

2,7-Dimethylanthracene: 2,4,4'-Trimethylbenzophenone (11.0 g, 49.0 mmol) was vigorously boiled for ~18 h using a sand bath set at ~560 °C. The resulting deep brown liquid solidified on cooling,then was partially purified by sublimation at 2 mm Hg and about 160 °C. Then, further purification was carried out by re-crystallization from glacial acetic acid to give 2,7-

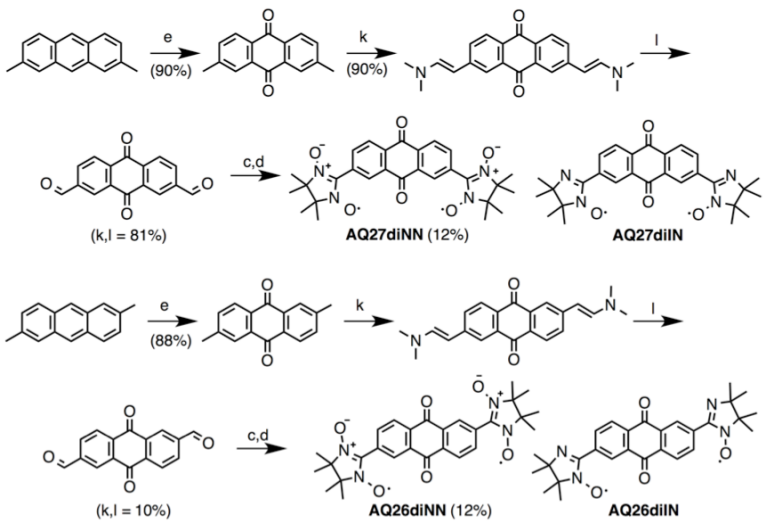
dimethylanthracene as light yellow colored crystals (4.04 g, 40%), mp240-244 °C, lit mp 241 °C[R1].^{1}H NMR (400 MHz, DMSO-d_6): δ 8.49 (s, 1H), 8.35 (s, 1H), 8.00 (d, 2H, *J* = 8.6 Hz), 7.83 (s, 2H), 7.36 (dd, 2H, J = 8.6 Hz, J' ~ 1 Hz), 2.54 (s, 6H).

9-Bromo-2,7-bis(bromomethyl)anthracene: 2,7-Dimethylanthracene (0.500 g, 2.42 mmol) and *N*-bromosuccinimide (1.294 g, 7.27 mmol) were placed in 20 mL of CCl_4 and heated under reflux until a flocculent solid floated. After hot filtration, the filtrate was evaporated and the resultant material recrystallized from CCl_4 to yield the product (0.594 g, 55%) as yellow needles with mp 213-215 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (br s, 2H), 8.39 (s, 1H), 8.00-7.98 (d, 2H, J = 8.6 Hz), 7.5-7.53 (dd, 2H, J = 8.6 Hz, J' = 1.6 Hz), 4.75 (s, 4H). MS (FAB): found *m/z* [intensities normalized to base peak]= 439.8 (34%), 441.8 (100%), 443.8 (96%), 445.8 (33%); calculated for $C_{16}H_{11}Br_3$ *m/z* = 439.841 (35%), 441.8391 (100%), 443.837 (97%), 445.8353 (32%).

9-Bromoanthracene-2,7-dicarbaldehyde: 9-Bromo-2,7-bis(bromomethyl)anthracene (0.200 g, 0.45 mmol)was added toa solution of 2-nitropropane (0.110 g, 1.22 mmol) in 2.5 ml of 0.5 M NaOEt and 5 mL of absolute ethanol. The yellow suspension was stirred at 50 °C for 30 h, after which the mixture was filtered; the solid was washed with 10% aqueous NaOH then with water, and then was air-dried to give the product (0.112 g, 79%) as a yellow solid, mp 254-256 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.29 (s, 2H), 9.06 (s, 2H), 8.53 (s, 1H), 8.14-8.12 (d, 2H,J = 8.6 Hz), 8.06-8.04 (d, 2H,J= 8.6 Hz). IR (KBr, cm-1): 1690 (strong, C=O). MS (FAB): found *m/z* = 311.9781; calculated for $C_{16}H_9O_2{}^{79}Br$ *m/z* = 311.97859.

2,7-Bis(1-oxyl-3-oxo-4,4,5,5-tetramethylimidazolin-2-yl)-9-bromoanthracene (BrA27diNN) and 2,7-Bis(1-oxyl-4,4,5,5-tetramethylimidazolin-2-yl)-9-bromoanthracene (BrA27diIN): 2,3-Bis(*N*-hydroxylamino)-2,3-dimethylbutane hydrogen sulfate[R2](0.630 g, 2.56 mmol) and 9-bromoanthracene-2,7-dicarbaldehyde (0.400 g, 1.28 mmol) were dissolved in a mixture of 60 mL of methanol and 40 mL of chloroform. Triethylamine (0.258 g, 2.56 mmol) was added, and the mixture was heated at reflux for 48 h under nitrogen at 75-80 °C. The reaction was then allowed to cool. After evaporation under reduced pressure, the resulting yellow crude product **(**radical precursorbis(*N*-hydroxyl)imidazoline**)** was dissolved in 150 mL of dichloromethane. The mixture was then stirred under nitrogen at 0-3 °C in an ice-bath for 15 min and 0.2 M aqueous $NaIO_4$ (0.547 g, 2.56 mmol in 12.8 mL of H_2O)was added. A green color formed at once, after which the mixture was stirred for 10 min. Next, 150 mL of cold water was added to the mixture, and the organic layer rapidly extracted with dichloromethane. The combined organic layers were dried over anhydrous magnesium sulfate and evaporated to dryness by rotary evaporation. Chromatography on silica gel with ethyl acetate yielded the product **BrA27diNN** (0.067 g, 9%), which crystallizedas dark green needles or prisms from dichloromethane/acetonitrile, mp >300 °C. MS (FAB): found *m/z* = 568.1714; calculated for ($C_{28}H_{31}{}^{79}BrN_4O_4$ + 2 H) *m/z* = 566.16852. A small amount of **BrA27diIN** was isolated as a red solid from the chromatography. MS (FAB): found *m/z* = 536.1785, calculated for ($C_{28}H_{31}{}^{79}BrN_4O_2$+ 2H) *m/z* = 536.16304.

2,7-Dimethylanthra-9,10-quinone: CrO_3 (0.267 g, 2.67 mmol) dissolved in a minimum amount of water was slowly added to a solution of 2,7-dimethylanthracene (0.20 g, 0.97 mmol) in boiling glacial acetic acid (20 mL). The resulting solution was then boiled until chromic acid reduced to give a green color (30-45 min); the solution was then allowed to cool and poured into water, giving a precipitate. This solid product was collected by filtration and air-dried to give 2,7-dimethylanthracene-9,10-dione as a white solid (0.206 g, 90%), mp 163-166 °C, lit mp 170 °C[R1]. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.22-8.20 (d, 2H, *J* = 7.9 Hz), 8.10 (s, 2H), 7.60-7.58 (d, 2H, *J* =7. 9 Hz), 2.18 (s, 6H).



Anthra-9,10-quinone-2,7-dicarbaldehyde*:N,N*-Dimethylformamide dimethyl acetal (0.263 g, 2.2 mmol) was added to a solution of 2,7-dimethylanthra-9,10-quinone(0.200 g, 0.85 mmol) in dry *N,N*-dimethylformamide (10 ml). This mixture was heated at reflux for 24 h at 140 °C to form a bis-enamine. The reaction was allowed to cool, the solvent removed under vacuum, and the residual crude bis-enamine (0.294 g, 0.85 mmol) was stirred with $NaIO_4$ (1.28 g, 5.1 mmol) in 12 mL of 50% aqueous THF for 1 h at room temperature. The resulting insoluble material was filtered away and washed with ethyl acetate. The organic filtrate and the ethyl acetate washings were combined, washed with saturated aqueous $NaHCO_3$ (3 × 20 mL), separated, dried over anhydrous magnesium sulfate, filtered and subjected to rotary evaporation. Chromatography of the resulting solid on silica gel with 50% ethyl acetate: hexane yielded the product (0. 183 g, 81%) as a light yellow colored solid, mp 257-260 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.31 (s, 2H), 8.79 (br s, 2H), 8.46-8.45 (m, 4H).MS (FAB): found *m/z* = 264.0415, calculated for $C_{16}H_8O_4$ *m/z* = 264.04171.

2,7-Bis(1'-oxyl-3'-oxo-4',4',5',5'-tetramethylimidazolin-2'-yl)-9,10-anthraquinone (AQ27diNN): 2,3-Bis(*N*-hydroxylamino)-2,3-dimethylbutane hydrogen sulfate[R2] (0.573 g, 2.33 mmol) and anthraquinone-2,7-dicarbaldehyde(0.205 g, 0.77 mmol) were dissolved in a mixture of 55 mL of methanol and 30 mL of chloroform. Triethylamine (0.235 g, 2.33 mmol) was added, and the mixture was heated at reflux for 48 h under nitrogen at 75-80 °C. The reaction was then allowed to cool. After evaporation under reduced pressure, the resulting yellow crude product **(**radical precursorbis(*N*-hydroxyl)imidazoline**)** was dissolved in 140 mL of dichloromethane. The mixture was stirred under nitrogen at 0-3 °C in an ice-bath for 15 min. Next, 0.2 M aqueous $NaIO_4$ (0.329 g, 1.54 mmol in 7.70 mL of H_2O)was added to the mixture. A green color formed at once, after which the mixture was stirred for 10 min. Next, 80 mL of cold water was added to the mixture, and the organic layer rapidly extracted with dichloromethane. The combined organic layers were dried over anhydrous magnesium sulfate and evaporated to dryness by rotary evaporation. Chromatography on silica gel with ethyl acetate yielded the product **AQ27diNN** (0.048 g, 12%), as a brown powder, mp 260-270 °C. In solution, its color is green, but after a few days stored solutions turn brown from biradical decomposition. MS (FAB): found *m/z* = 519.2230, calculated for ($C_{28}H_{30}N_4O_6$+H) *m/z* = 519.2244; found *m/z* = 518.2165, calculated for $C_{28}H_{30}N_4O_6$ *m/z* = 518.2165. IR (neat, cm^{-1}; C=O stretch): 1727 (wk), 1684 (str). A small amount of **AQ27diIN** was isolated as a red solid from the chromatography. MS (FAB): found *m/z* = 487.2338, calculated for ($C_{28}H_{30}N_4O_4$ + H) *m/z* = 487.23453; found *m/z* = 486.1858, calculated for $C_{28}H_{30}N_4O_4$ *m/z* = 486.22745. IR (neat, cm^{-1}; C=O stretch): 1725 (wk), 1680 (str).

Anthra-9,10-quinone-2,7-dicarboxylic acid. CrO_3 (5.94 g, 59.4 mmol) was added to a solution of conc sulfuric acid (0.2 ml), acetic anhydride (1.5 ml, 16 mmol) and glacial acetic acid (35 ml) cooled at 20 °C in a water-ice bath. 2,7-Dimethylanthracene-9,10-dione (1.16 g, 4.9 mmol) was added in small portions with stirring, while the reaction temperature was kept below 35 °C using the ice-water bath. After the addition was complete, the reaction was heated to 120 °C and stirred at this temperature for 4 h. The mixture was then cooled to room temperature and poured into water (400 mL), and the resulting precipitate collected by filtration. The white solid was washed with water and air-dried to give anthracene-9,10-dione-2,7-dicarboxylic acid as a white solid (1.20 g, 83%), mp >300 °C, lit mp >360 °C[R1]. ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.8 (br s, 2H), 8.74-8.73 (d, 2H, J = 1.5 Hz), 8.47-8.45 (dd, 2H, J= 8.0 Hz, J' = 1.5 Hz), 8.38-8.36 (d, 2H, J = 8.0 Hz).

Anthracene-2,7-dicarboxylic acid. This compound was prepared by adapting a procedure by Jones et al.[R3]A mixture of anthracene-9,10-dione-2,7-dicarboxylic acid (1.00 g, 3.38 mmol), Zn powder (3.51 g, 53.7 mmol) and concentrated aqueous ammonia (25 ml) was heated at reflux for 4 h. Additional ammonia (25 mL) was added dropwise throughout the heating. The mixture was then cooled and vacuum filtered, and the filtrate was acidified by dropwise addition of 12 M HCl to give a yellow precipitate. The precipitate was collected by vacuum filtration and air-dried to give anthracene-2,7-dicarboxylic acid as a yellow solid (0.81 g, 90%), mp >300 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.5 (br s, 2H), 9.10 (s, 1H), 8.87 (s, 2H), 8.77 (s, 1H), 8.25-8.23 (d, 2H, J = 8.8 Hz), 8.05-8.02 (dd, 2H,J= 8.8 Hz, J' = 1.2 Hz).

Dimethyl anthracene-2,7-dicarboxylate: A suspension of anthracene-2,7-dicarboxylic acid (1.10 g, 4.13 mmol), methyl iodide (5.86 g, 41.30 mmol), and lithium carbonate (3.02 g, 41.3 mmol) in dry *N*,*N*-dimethylformamide (55 mL) was stirred overnight at room temperature. The mixture was added to 1 M aq HCl (204 mL); the resulting yellow precipitate was collected by vacuum filtration and air-dried to give dimethyl anthracene-2,7-dicarboxylate **(**0.86 g, 71%), mp 226-228 °C, lit mp 222-223 °C[R5]. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.16 (s, 1H), 8.91 (s, 2H), 8.80 (s, 1H), 8.30-8.28 (d, 2H, *J* = 8.8 Hz), 8.06-8.04 (dd, 2H,J = 8.8 Hz, J'= 1.5 Hz), 4.00 (s, 6H).

2,7-Dihydroxymethylanthracene*:*Dimethyl anthracene-2,7-dicarboxylate (0.82 g, 2.79 mmol) was added in small proportions into a suspension of lithium aluminum hydride (0.32 g, 8.36 mmol) in 15 mL of dry diethyl ether cooled with an ice bath. After the addition was complete the reaction mixture was stirred while warming to room temperature overnight. The mixture was then poured into ice and extracted with ethyl acetate. The combined organic layers were washed with brine, dried over anhydrous magnesium sulfate, and evaporated to dryness by rotary evaporation to yield the product as a yellow powder (0. 25 g, 37%), mp 236-240 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.54 (s, 1H), 8.52 (s, 1H), 8.07-8.05 (d, 2H, *J* = 8.8 Hz), 7.99 (br s, 2H), 7.49-7.46 (d, 2H, J = 8.8 Hz), 5.40 (t, 2H, J = 5.6 Hz), 4.73 (d, 4H, J = 5.6 Hz).

Anthracene-2,7-dicarbaldehyde*:*2,7-Dihydroxymethylanthracene (0.500 g, 2.1 mmol) was dissolved in 150 mL of dichloromethane. Manganese(IV) oxide (2.180 g, 25.2 mmol) was added to the solution and the reaction mixture stirred for 2 days at room temperature. The mixture was filtered through Celite, and the filtrate evaporated under vacuum to give the product as a yellow powder (0.312 g, 63%), mp 170-175 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.26 (s, 2H), 9.22 (s, 1H), 8.94 (s, 2H), 8.84 (s, 1H), 8.33-8.31 (d, 2H, J = 8.8 Hz), 7.99-7.97 (d, 2H, J = 8.8 Hz).MS (FAB): found *m/z* = 264.0677, calculated for $C_{16}H_{10}O_2$ *m/z* = 234.06808.

2,7-Bis(1-oxyl-3-oxo-4,4,5,5-tetramethylimidazolin-2-yl)anthracene (A27diNN) and 2,7-Bis(1-oxyl-4,4,5,5-tetramethylimidazolin-2-yl)anthracene (A27diIN)*:*2,3-Bis(*N*-hydroxylamino)-2,3-dimethylbutane hydrogen sulfate[R2] (0.631 g, 2.56 mmol) and anthracene-2,7-dicarbaldehyde(0.200 g, 0.85 mmol) were dissolved in a mixture of 60 mL of methanol and 40

mL of chloroform. Triethylamine (0.259 g, 2.56 mmol) was added, and the mixture was heated at reflux for 48 h under nitrogen at 75-80 °C. The reaction was then allowed to cool. After evaporation under reduced pressure, the resulting yellow crude product **(**radical precursorbis(*N*-hydroxyl)imidazoline**)** was dissolved in 150 mL of dichloromethane. The mixture was then stirred under nitrogen at 0-3 °C in an ice-bath for 15 min. Next, 0.2 M aqueous $NaIO_4$ (0.363 g, 1.70 mmol in 8.50 mL of H_2O)was added to themixture. A green color formed at once, after which the mixture was stirred for 10 min. Next 100 mL of cold water was added to the mixture, and the organic layer rapidly extracted with dichloromethane. The combined organic layers were dried over anhydrous magnesium sulfate and evaporated to dryness by rotary evaporation. Chromatography on silica gel with ethyl acetate yielded the product **A27diNN** (0.048 g, 12%), which forms very dark green, delicate needles from dichloromethane/acetonitrile, mp 244-246 °C. MS (FAB): found *m/z* = 488.2427, calculated for $C_{28}H_{32}N_4O_4$ *m/z* = 488.2424. A small amount of **A27diIN** was isolated as a red solid from the chromatography. MS (FAB): found *m/z* = 456.25161, calculated for $C_{28}H_{32}N_4O_2$ *m/z* = 456.25252.

2,4,3'-Trimethylbenzophenone: This compound was prepared using the procedure of Morgan and Coulson[R1].Equivalent weights of *p*-toluoyl chloride (10 g, 64.7 mmol) and *p*-xylene (6.9 g, 64.7 mmol) were mixed and dissolved in carbon disulfide (~20 mL). The solution was gradually added to a powdered anhydrous aluminum trichloride (10 g) covered with carbon disulfide in a reflux apparatus and cooled with an ice bath. Heat was generated as the aluminum trichloride dissolved to give an orange then dark brown-green solution, and a vapor (hydrogen chloride) was evolved. When addition was complete, the solution was boiled in a hot water bath for 2 h. Water was added cautiously to the reaction mixture, then *m*-xylene and carbon disulfide were distilled away in steam. The residue was extracted with ether, and the combined ether layers were washed multiple times with 10% aqueous NaOH solution then dried over anhydrous magnesium sulfate. After filtration and removal of organic volatiles under vacuum, 2,4,3'-trimethylbenzophenone was obtained as oily liquid that was sufficiently pure for further use (11.3 g, 78%). ^{1}H NMR (400 MHz, DMSO-d_6): δ 7.65-7.63 (d, 2H, *J* = 8.08 Hz), 7.39-7.37 (d, 2H, *J* = 8.08 Hz), 7.28-7.27 (d, 2H, *J* = 3.28 Hz), 7.11 (s, 1H), 2.43 (s, 3H), 2.33 (s, 3H), 2.18 (s, 3H).

2,6-Dimethylanthracene: 2,4,3'-Trimethylbenzophenone (11.0 g, 49.0 mmol) was vigorously boiled for ~18 h using a sand bath set at ~ 560 °C. The resulting deep brown liquid solidified on cooling, and was partially purified by sublimation. Then, further purification was carried out by re-crystallization from glacial acetic acid. 2,6-Dimethylanthracene was obtained as light yellow colored crystals (4.2 g, 42 %), mp 249-252 °C, lit mp 250 °C[R1]. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.42 (s, 2H), 8.01-7.99 (d, 2H, *J* = 8.7 Hz), 7.84 (s, 2H), 7.39-7.37 (dd, 2H,J = 8.7 Hz, J' = 1.5 Hz), 2.54 (s, 6H).

2,6-Dimethylanthra-9,10-quinone: CrO_3 (4.00 g, 40 mmol) dissolved in a minimum amount of water was slowly added to a solution of 2,6-dimethylanthracene (3.00 g, 14.5 mmol) in boiling glacial acetic acid (550 mL). The resulting solution was then boiled until chromic acid reduced to give a green color (30-45 min); the solution was then allowed to cool and poured into water, which precipitated the quinone. This solid product was collected by filtration and air-dried to give 2,6-dimethylanthracene-9,10-dione as a white solid (3.012 g, 88%), mp 234-235 °C, lit mp 230 °C (mp 242 °C from acetic acid)[R1]. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.16-8.14 (d, 2H, *J* = 7.8 Hz), 8.05 (s, 2H), 7.78-7.76 (d, 2H, J =7. 8 Hz), 2.55 (s, 6H). IR (neat, cm^{-1}): 1710 (s), 1690 (s), 1675(shoulder).

Anthra-9,10-quinone-2,6-dicarboxylic acid. CrO_3 (6.550 g, 65.5 mmol) was added to a solution of conc. sulfuric acid (0.22 ml), acetic anhydride (1.7 ml, 18.1 mmol) and glacial acetic acid (40 ml) cooled at 20 °C in a water-ice bath. 2,6-Dimethylanthracene-9,10-dione (1.28 g, 5.4 mmol) was added in small proportions with stirring, while the reaction temperature was kept below 35 °C in the ice-water bath. After the addition was complete, the reaction was heated to 120 °C and stirred at this

temperature for 4 h. The mixture was then cooled to room temperature and poured into water (400 mL), and the resulting precipitate collected by filtration. The white solid was washed with water and air-dried to give anthracene-9,10-dione-2,6-dicarboxylic acid as a white solid (1.36 g, 85%) (lit mp > 300 °C[R3].^{1}H NMR (400 MHz, DMSO-d_6): δ 13.79 (s, 2H), 8.73 (d, 2H, J = 1.5 Hz), 8.48-8.46 (dd, 2H, J= 7.8 Hz, J'= 1.5 Hz), 8.40-8.38 (d, 2H, J = 7.8 Hz).

Anthracene-2,6-dicarboxylic acid: A mixture of anthracene-9,10-dione-2,6-dicarboxylic acid (1.52 g, 5.13 mmol), Zn powder (4.74 g, 72.4 mmol) and concentrated aqueous ammonia (40 ml) was heated at reflux for 4 h. Additional ammonia (40 mL) was added dropwise throughout the heating. The mixture was then cooled and vacuum filtered, and the filtrate was acidified by dropwise addition of 12 M HCl to give a yellow precipitate. The precipitate was collected by vacuum filtration and air-dried to give anthracene-2,6-dicarboxylic acid as yellow solid (1.240 g, 91%), mp >300 °C.^{1}H NMR (400 MHz, DMSO-d_6): δ 13.2 (br s, 2H), 8.94 (s, 2H), 8.87 (br s, 2H), 8.26-8.24 (d, 2H, *J* = 8.8 Hz), 8.03-8.00 (dd, 2H, J= 8.8 Hz, J= 1.5 Hz).

Dimethyl anthracene-2,6-dicarboxylate: A suspension of anthracene-2,6-dicarboxylic acid (1.40 g, 5.26 mmol), methyl iodide (7.46 g, 52.6 mmol), and lithium carbonate (3.89 g, 52.6 mmol) in dry *N*,*N*-dimethylformamide (70 mL) was stirred overnight at room temperature. The mixture was added to 1 M aq HCl (259 ml); the resulting yellow precipitate was collected by vacuum filtration and air-dried to give dimethyl anthracene-2,6-dicarboxylate **(**1.380 g, 89%), mp 265-270 °C (lit mp 274-276 °C[R3]). ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.98 (s, 2H), 8.92 (br s, 2H), 8.30-8.27 (d, 2H, J= 8.8 Hz), 8.07-8.02 (dd, 2H, J = 8.8 Hz, J' = 1.8 Hz), 4.00 (s, 6H).

2,6-Dihydroxymethylanthracene: Dimethyl anthracene-2,6-dicarboxylate (0.613 g, 2.08 mmol) was added in small proportions into a suspension of lithium aluminum hydride (0.237 g, 6.24 mmol) in 12 ml of dry diethyl ether cooled with an ice bath. After the addition was complete the reaction mixture was stirred while warming to room temperature overnight. The mixture was then poured into ice and extracted with ethyl acetate. The combined organic layers were washed with brine and dried over anhydrous magnesium sulfate, and dried by rotary evaporation to yield 2,6-dihydroxymethylanthracene as a yellow powder (0. 213 g, 43%), mp 240-250 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.53 (s, 2H), 8.08-8.06 (d, 2H, J = 8.8 Hz), 7.99 (s, 2H), 7.49-7.47 (dd, 2H, J = 8.9 Hz, J' ~ 1 Hz), 5.40 (t, 2H, J = 5.8 Hz), 4.73 (d, 4H, J = 5.5 Hz).

Anthracene-2,6-dicarbaldehyde: 2,6-Dihydroxymethylanthracene (0.152 g, 0.64 mmol) was dissolved in 80 mL of dichloromethane. Manganese(IV) oxide (0.666 g, 7.7 mmol) was added to the solution and the reaction mixture stirred for 2 days at room temperature. The mixture was filtered through Celite, and the filtrate evaporated under vacuum to give anthracene-2,6-dicarbaldehydeas yellow powder (0.127 g, 85%), mp 260-265 °C[R4]. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.27 (s, 2H), 9.03 (s, 2H), 8.89 (br s, 1H), 8.37-8.27 (d, 2H, J= 8.0 Hz), 8.05-7.95 (dd, 2H, J= 8.0 Hz, J'= 1.3 Hz). MS (FAB): calculated for $C_{16}H_{10}O_2$ *m/z* = 234.0681; found *m/z* = 207 (M+2H, loss of –CH=O), *m/z* = 221 (M-CH),no parent ion.

2,6-Bis(1-oxyl-3-oxo-4,4,5,5-tetramethylimidazolin-2-yl)anthracene (A26diNN) and 2,6-Bis(1-oxyl-4,4,5,5-tetramethylimidazolin-2-yl)anthracene (A26diIN)*:*2,3-Bis(*N*-hydroxylamino)-2,3-dimethylbutane hydrogen sulfate[R2] (0.631 g, 2.56 mmol) and anthracene-2,6-dicarbaldehyde(0.200 g, 0.85 mmol) were dissolved in 60 mL of methanol and 40 mL of chloroform. Triethylamine (0.259 g, 2.56 mmol) was added, and the mixture was heated at reflux for 48 h under nitrogen at 75-80 °C. The reaction was then allowed to cool. After evaporation under reduced pressure, the resulting yellow crude product **(**radical precursorbis(*N*-hydroxyl)imidazoline**)** was dissolved in 150 mL of dichloromethane. The mixture was stirred under nitrogen at 0-3 °C in an ice-bath for 15 min. Next, 0.2 M aqueous $NaIO_4$ (0.363 g, 1.70 mmol in 8.50 mL of H_2O)was added to the mixture. A green color formed at once, after which the mixture was stirred for 10 min. Next, 100 mL of cold water was added to the mixture,

and the organic layer rapidly extracted with dichloromethane. The combined organic layers were dried over anhydrous magnesium sulfate and evaporated to dryness by rotary evaporation. Chromatography on silica gel with ethyl acetate yielded the product **A26diNN** (0.041 g, 10%), which forms delicate dark green needles from dichloromethane/acetonitrile, mp 238-240 °C. MS (FAB): found *m/z* = 488.2416, calculated for $C_{28}H_{32}N_4O_4$ *m/z* = 488.24236. A small amount of **A26diIN** side product was isolated as a red solid from the chromatography. MS (FAB): found *m/z* = 456.2634, calculated for $C_{28}H_{32}N_4O_2$ *m/z* = 456.25253.

Anthra-9,10-quinone-2,6-dicarbaldehyde*:N,N*-Dimethylformamide dimethyl acetal (1.315 g, 11 mmol) was added to a solution of 2,6-dimethylanthra-9,10-quinone (1.00 g, 4.25 mmol) in dry *N,N*-dimethylformamide (80 mL). This mixture was heated at reflux for 24 h at 140 °C to form a bis-enamine. The reaction was allowed to cool, the solvent removed under vacuum, and the residual crude bis-enamine was stirred with a solution of $NaIO_4$ (6.415 g, 25.5 mmol) in 60 mL of 50% aqueous THF for 1 h at room temperature. The resulting insoluble material was filtered away and washed with ethyl acetate. The organic filtrate and the ethyl acetate washings were combined, washed with saturated aqueous $NaHCO_3$ (3 × 100 mL), separated, dried over anhydrous magnesium sulfate, filtered, and subjected to rotary evaporation. Chromatography of the resulting solid on silica gel with 50% ethyl acetate:hexane yielded the product (0. 113 g, 10%) as yellow solid, mp 245-255 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.31 (s, 2H), 8.77 (d, 2H, J = 1.3 Hz), 8.50-8.43 (AA'BB' q, 4H, J = 8 Hz, J' ~ 1 Hz). MS (FAB): found *m/z* = 264.0423, calculated for $C_{16}H_8O_4$ *m/z* = 264.04171.

2,7-Bis(1-oxyl-3-oxo-4,4,5,5-tetramethylimidazolin-2-yl)-9,10-anthraquinone (AQ26diNN) and 2,7-bis(1-oxyl-4,4,5,5-tetramethylimidazolin-2-yl)-9,10-anthraquinone (AQ26diIN): 2,3-Bis(*N*-hydroxylamino)-2,3-dimethylbutane hydrogen sulfate[R2] (0.280 g, 1.17 mmol) and 9,10-anthraquinone-2,7-dicarbaldehyde(0.100 g, 0.38 mmol) were dissolved in a mixture of 30 mL of methanol and 15 mL of chloroform. Triethylamine (0.112 g, 1.14 mmol) was added, and the mixture was heated at reflux for 48 h under nitrogen at 75-80 °C. The reaction was then allowed to cool. After evaporation under reduced pressure, the resulting yellow crude product **(**radical precursorbis(*N*-hydroxyl)imidazoline**)** was dissolved in 70 mL of dichloromethane. The mixture was then stirred under nitrogen at 0-3 °C in an ice-bath for 15 min. Next, 0.2 M aqueous $NaIO_4$ (0.16 g, 0.75 mmol in 3.80 mL of H_2O)was added to the mixture. A green color formed at once, after which the mixture was stirred for 10 min. Next, 40 mL of cold water was added to the mixture, and the organic layer rapidly extracted with dichloromethane. The combined organic layers were dried over anhydrous magnesium sulfate and evaporated to dryness by rotary evaporation. Chromatography on silica gel with ethyl acetate yielded the product**AQ26diNN** (0.012 g, 12%) as a brown powder, mp 215-220 °C. MS (FAB): found *m/z* = 518.2169, calculated for $C_{28}H_{30}N_4O_6$ *m/z* = 518.21653. IR (neat, cm^{-1}; C=O stretch): 1725 (str), 1676 (str). A small amount of **AQ26diIN** side product was isolated as a red solid from the chromatography. MS (FAB): found *m/z* = 488.2437, calculated for ($C_{28}H_{30}N_4O_4$ + 2H) *m/z* = 488.24236. IR (neat, cm^{-1}; C=O stretch): 1728 (str), 1677 (str).

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(R2) Ovcharenko, V.; Fokin S.; Rey, P. *Mol. Cryst. Liq. Cryst. Sect. A***1999**, *334*, 109-119.

(R3) Jones J. R.; Liotta, C. L.; Collard D. M.; Schiraldi D. A., *Macromolecules*, **1999**, *32*, 5786

(R4) Schwab, M. G.; Hamburger, M.; Feng, X.; Shu, J.; Spiess, H. W.; Wang, X.; Antonietti, M.; Müllen, K. *Chem. Commun*.**2010**, *46*, 8932-8934.

(R5) Staab, H. A.; Sauer, M. *Liebigs Ann. Chem*. **1984**, (*4*), 742-760.

Table S1. Expanded selection of crystallographic contacts intermolecular contacts for biradicals in this study

Compound	Contact	Value	Compound	Contact	Value
BrA27diNN			BrA27diIN		
	O2 ⋯ O2^{i}	3.655(5)*		O1A ⋯ C19^{xv}	3.865(11)**
	O2 ⋯ O2^{ii}	3.655(5)*		O1A ⋯ C20^{xv}	3.942(11)**
	O2 ⋯ N2^{ii}	3.390(5)*		O1A ⋯ C25^{xv}	3.587(14)**
	O2 ⋯ C9^{ii}	3.680(4)*		O1A ⋯ C26^{xv}	3.749(15)**
				O1A ⋯ C27^{xv}	3.955(15)**
	O2 ⋯ C13^{ii}	3.510(5)**		O1A ⋯ C28^{xv}	3.647(13)**
	O2 ⋯ C15^{ii}	3.312(4)**		O1B ⋯ N3^{iv}	3.895(19)*
	Br1 ⋯ C2^{vii}	2.848(2)		O1B ⋯ C18^{iv}	3.698(18)*
	Br1 ⋯ C3^{vii}	3.138(3)		O1B ⋯ C26^{iv}	3.74(2)**
	Br1 ⋯ C14^{viii}	3.861(3)		O1B ⋯ C22^{xiii}	3.36(2)**
	Br1 ⋯ C14^{ix}	3.861(3)		O1B ⋯ C21'^{xiii}	3.89(2)**
				O2A ⋯ C21'^{xvi}	3.726(15)**
A27diIN				O2A ⋯ C21^{xvi}	3.850(17)**
	O2 ⋯ N4^{iii}	4.593(4)*		O2A ⋯ C23^{xvii}	3.873(17)**
	O2⋯ C22^{iii}	4.230(5)*		O2A ⋯ C24'^{xvii}	3.47(2)**
	O2⋯ C18^{iii}	3.492(4)**			
	O2⋯ C19^{iii}	3.204(4)**		O2B ⋯ N3^{iv}	3.895(19)*
	O2⋯ C20^{iii}	4.230(5)**		O2B ⋯ C18^{iv}	3.698(18)*
	O2 ⋯ C25^{x}	3.565(6)**		O2B ⋯ C21'^{xviii}	3.36(2)**
	O2⋯ C26^{x}	3.688(7)**		O2B ⋯ C22^{xiii}	3.36(2)**
	O2 ⋯ C27^{x}	3.598(6)**		O2B ⋯ C26^{iv}	3.74(2)**
	O1⋯ C5^{xi}	3.70(3)**		Br1 ⋯ C5^{iv}	3.960(4)
	O1⋯ C9^{iii}	3.71(2)			
	O1⋯ C10^{iii}	3.77(2)			
	O1A⋯ C4A^{xi}	3.56(3)**			
	O1A⋯ C6A^{xi}	3.63(3)**			
	O1A⋯ C9^{iii}	3.683(19)			
	O1A⋯ C10^{iii}	3.627(17)			
A26diNN			A26diIN		
	O2 ⋯ O2^{v}	3.6523(13)*		N2 ⋯ C12^{xii}	3.523(12)**
	O2 ⋯ N1^{v}	3.9338(14)*		O1 ⋯ C12^{xiv}	3.311(10)**
	O2 ⋯ N2^{v}	3.5189(13)*		O1 ⋯ C13^{xiv}	3.622(9)**
	O2 ⋯ C14^{v}	3.9501(14)*		O1 ⋯ C11^{xiv}	3.866(10)**
	O1 ⋯ N1^{vi}	3.9501(14)*			
	O1 ⋯ C12^{vi}	3.5429(17)**			
	O1 ⋯ C12^{xii}	3.6024(15)**			

Symmetry operations used to generate the molecule in close contact: *i = x,2-y,-1/2+z; ii= x,2-y,1/2+z; iii= x,y,1+z; iv = 1-x,-y,1-z; v=2-x,-y,-z; vi=1-x,-y,-z, vii= 1-x, y,1/2-z; viii=3/2-x,3/2-y,1/2-z; ix=-1/2+x,3/2-y,-z; x=3/2-x,-1/2+y,1/2+z; xi=1-y,1+x,1-z; xii=1-x,-1/2+y,-1/2-z; xiii=1+x, y, z; xiv=-1/2-x,-1/2+y,1/2-z; xv=1/2-x,1/2+y,3/2-z; xvi=1/2+x,1/2-y,1/2+z; xvii=-1/2+x,1/2-y,1/2+z; xviii=1-x, y, z;* *Direct contact between radical units, both sites of high spin density. **NO to methyl contact.

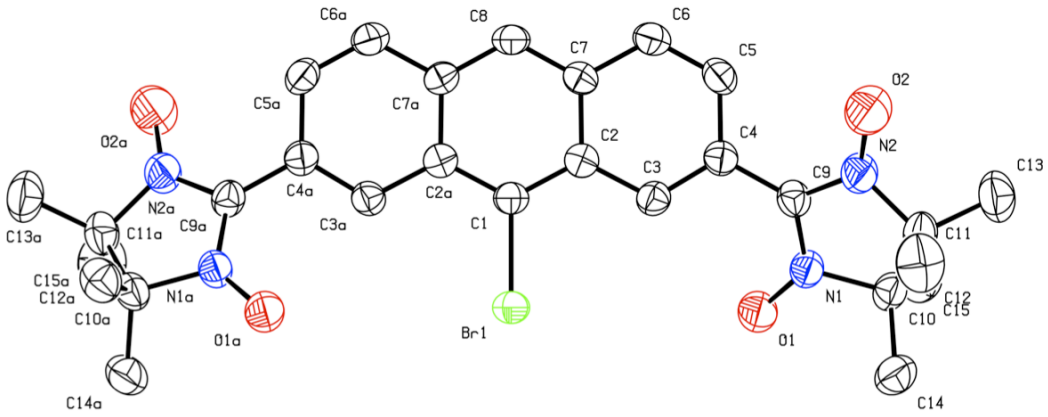


Figure S1. ORTEP diagram for **BrA27diNN**. Structure acquired at 293 K. Thermal ellipsoids shown at 50% probability. H-atoms omitted for ease of viewing.

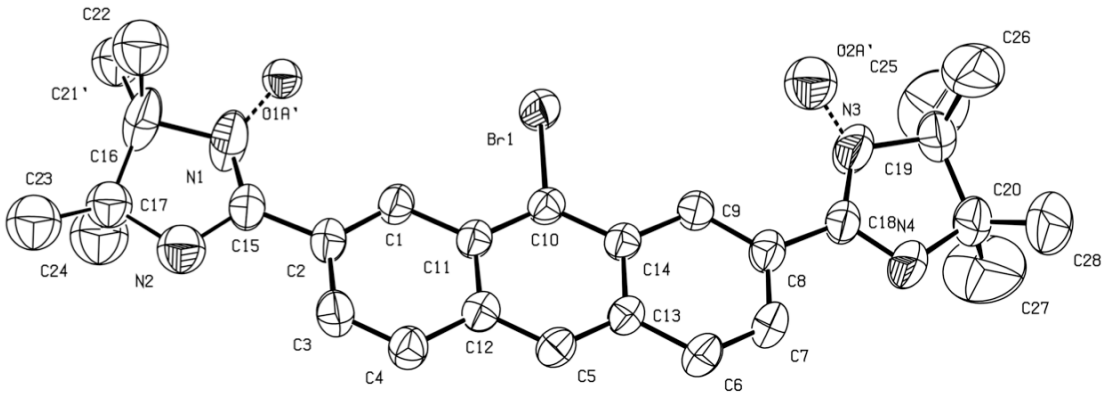


Figure S2. ORTEP diagram for **BrA27diIN**. Structure acquired at 293 K. Thermal ellipsoids shown at 50% probability. H-atoms and disordered positions of the iminoyl nitroxide groups are omitted for ease of viewing.

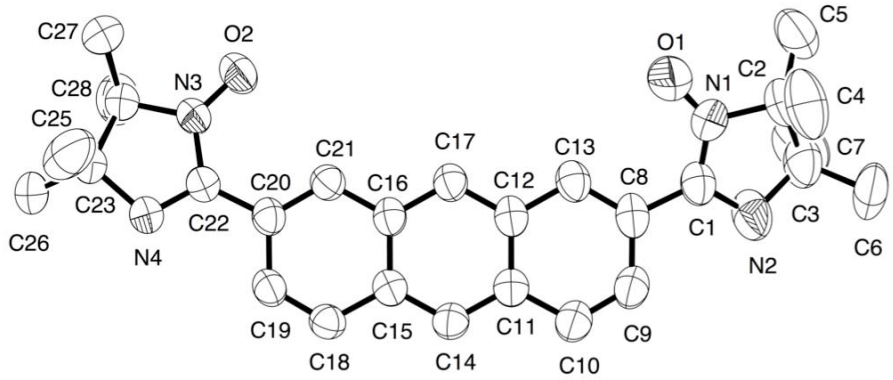


Figure S3. ORTEP diagram for **A27diIN**. Structure acquired at 293 K. Thermal ellipsoids shown at 50% probability. H-atoms and disordered positions of the iminoyl nitroxide groups are omitted for ease of viewing.

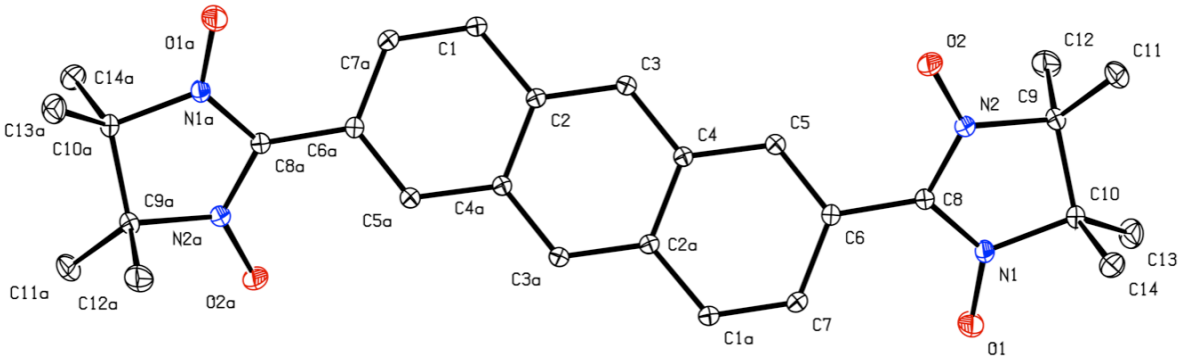
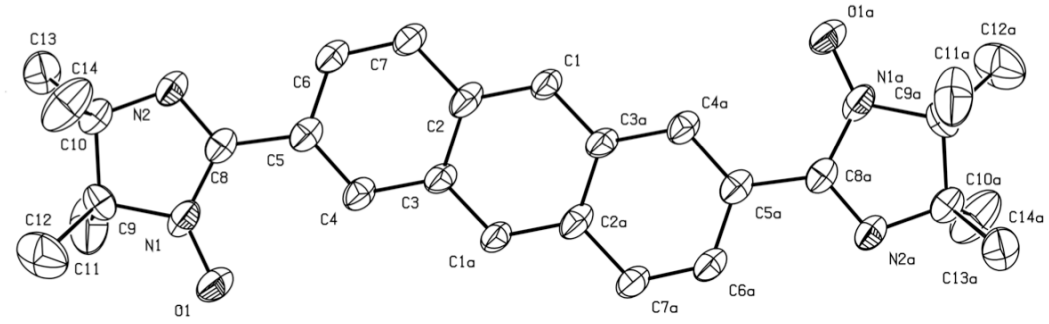
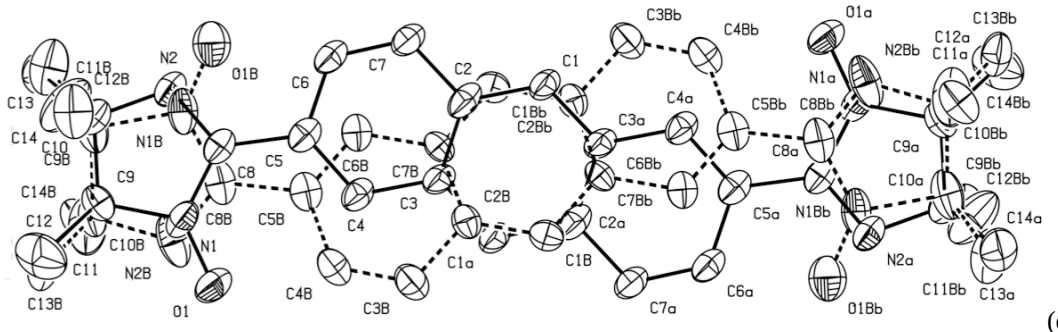


Figure S4. ORTEP diagram for **A26diNN**. Structure acquired at 95 K. Thermal ellipsoids shown at 50% probability.



(disorder not shown)



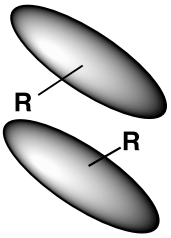
(disorder shown)

Figure S5. ORTEP diagram for **A26diIN**. Structure acquired at 296 K. Thermal ellipsoids shown at 50% probability. Rotational disorder of the structure is shown in the lower representation.

Crystal Search S1. 9-Substituted anthracenes with alternating 9-substituent placement in stack/dyad.

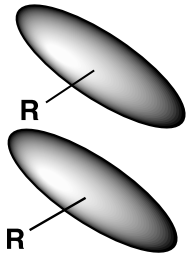
Search was made of the Cambridge Structure Database using ConQuest (version 1.18, build RC2, © Cambridge Crystallographic Data Centre 20145 CSD version 5.37 November 2015 version) for anthracenes with H in positions 1, 4, 5, 8 and non-H in position 9, no co-crystals, no organometallics, no macrocycles, no compounds with OH, NH, SH hydrogen bonding units, no double-inclusion of anthracene in the structure, no additional attachment of other PAHs like naphthalene, text inclusion for "anthracene". Core stacking was sought as near planarity between anthracene units, at a core-to-core plane-to-plane distance of < 4 ångstroms. The following listing is not intended to be exhaustive within these criteria, but to demonstrate that the alternating side 9-substituent stack is well-known for anthracenes.

The following structures show *opposing side* dyad or 1-D stack placement of substituents in the 9-position.



ANNIZUT, ANOBAH, ANOBEL, ANOBOV, ANOCIQ, ANOCUC, AYOTEO (offset, slip-stack), ANOCOW, DEZCAM, FEKVEY, FOGKAO, GASWIG (same and opposite side substitution placement motifs), HIXQOV, JAPYUV, JEYVOZ, JUDXEN, KANMOB, KANMUH, LOGQAA (also slipped along long axis), LOGQEE (slip stack), LOGQII, MANTHR01, MOCANT, NTRANT, NUKMAH (also slipped along long axis), NUKMEL, NUKMIP, NUKMUB, NUKNAI, NUKNOW, OGEDAG, PAXCOI, PECQIZ (also slipped along long axis), PIFJIY, QUESOY, TIVBOQ, WEFDIV, WUPZUD, XAYFOS, YAFPOL

The following structures show *same-side* placement of substituents in the 9-position, often with staircase offset of the anthracene unit along the short molecular axis, occasionally with offset along the long axis.



ANOBIP, AYOCIA (slip stack), AYOTEO, CEKNAI, CETMAN (staircase), CNANTH, DASTOG (staircase), DASTUM, ECUMEV, FEKTAS, GASWIG (staircase), HIXQOV, KUBWEJ (staircase), LOGQAA (slip stack) QQQFDS02, UNASIM (also slipped along long axis), WEFDER(staircase), XASMUB (same side)

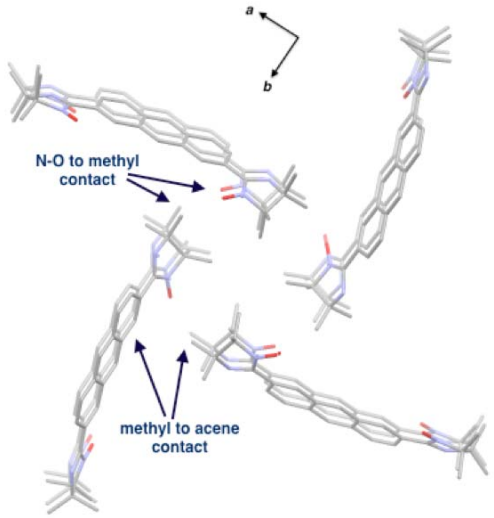


Figure S6. A27diIN crystallographic contacts between staircase stacks.

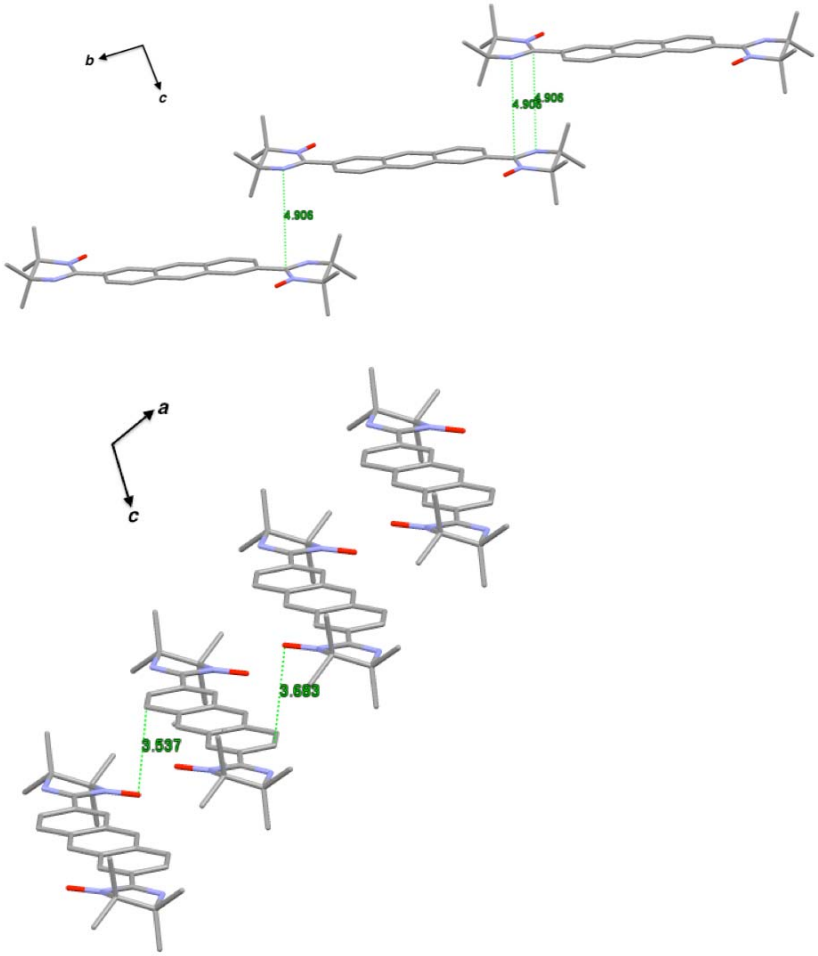


Figure S7. A26diIN crystallographic packing; slipstack (above) and staircase stack (below). Distances in angstroms.

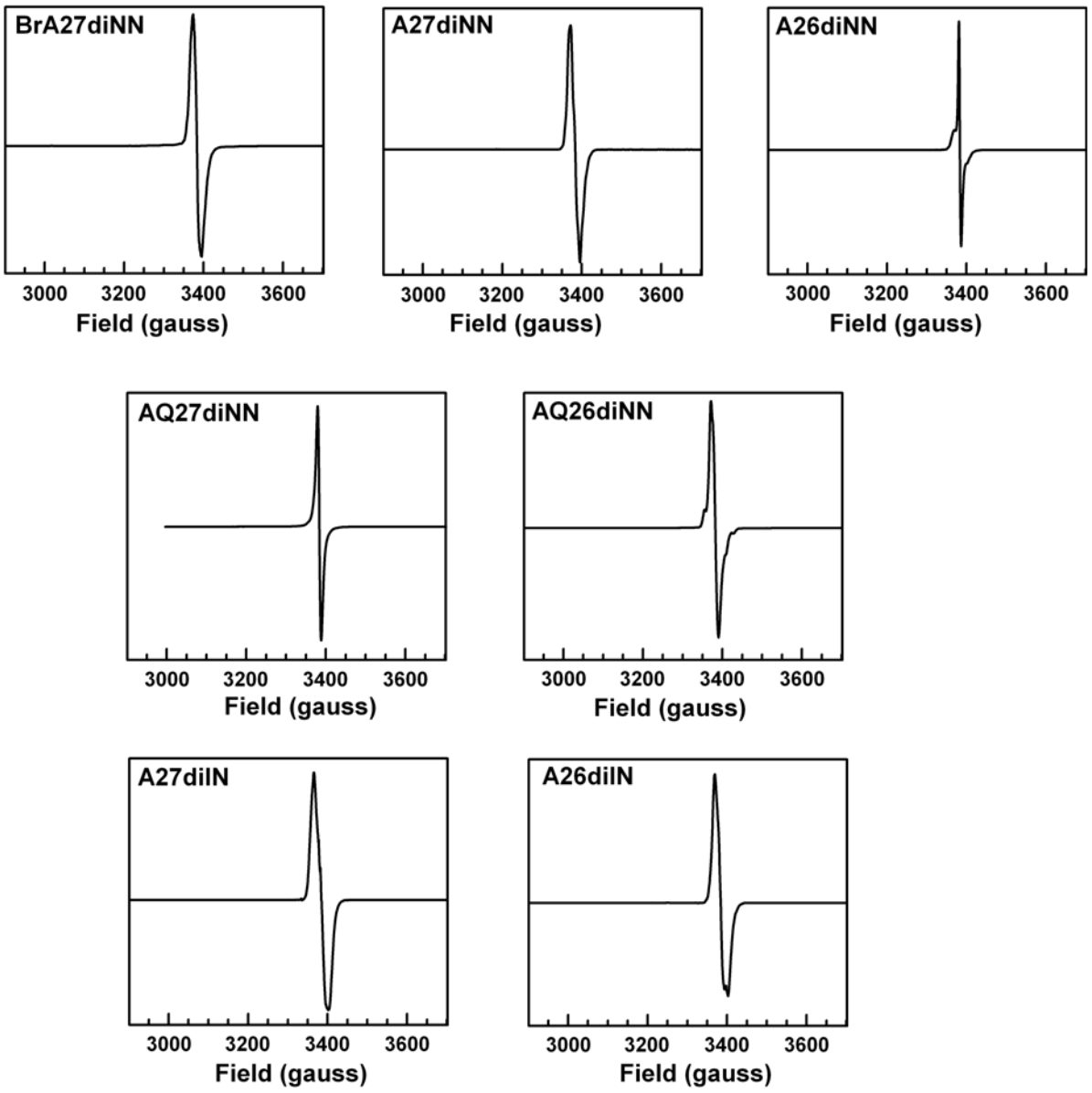


Figure S8. Frozen solution ESR spectra (dichloromethane, toluene) for biradicals at 77 K, at ν_0 = 9.37-9.50 GHz. No peaks were detected in the half-field region, 1500-1800 G, for any spectra.

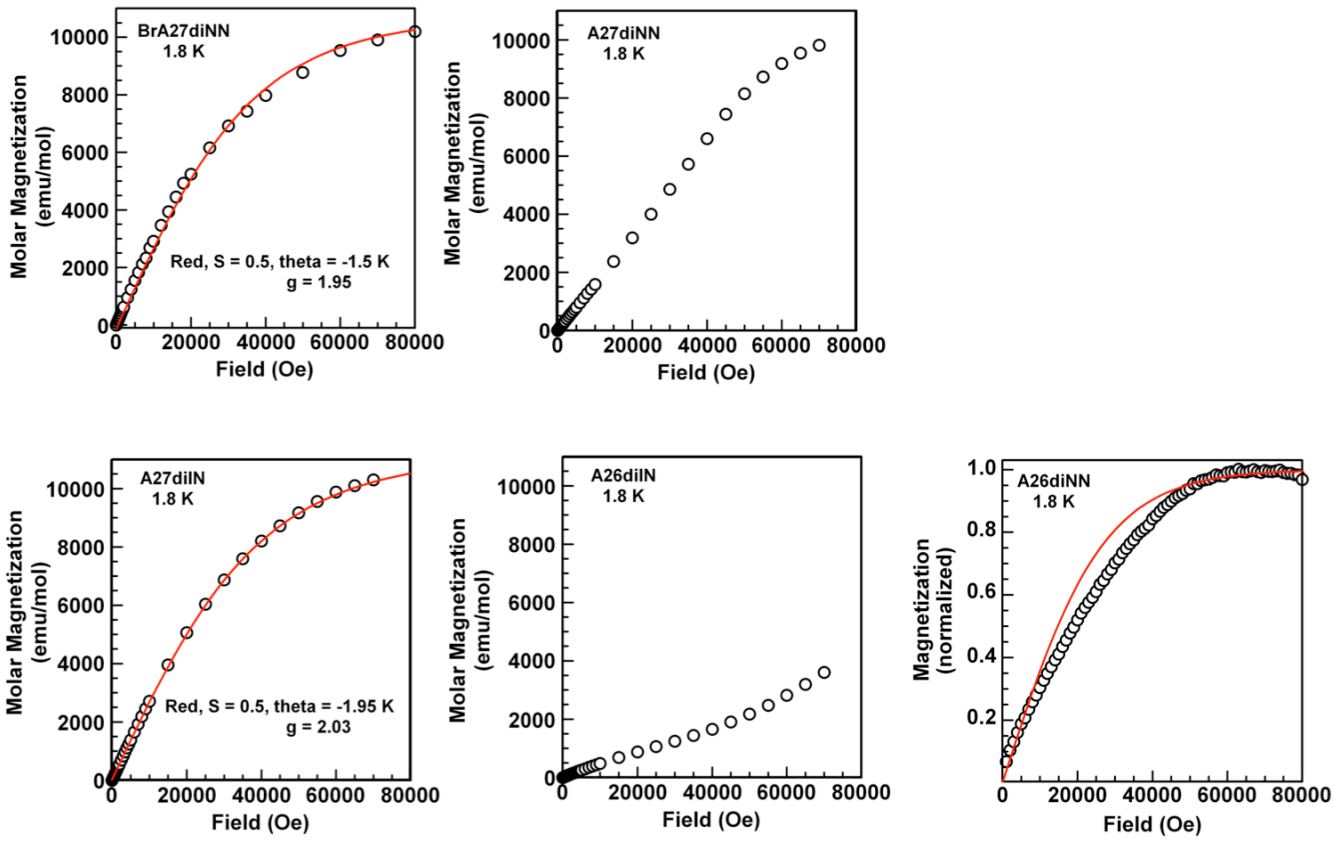


Figure S9. Magnetization versus field (*M* vs. *H*) plots for biradicals. All plots at 1.8 K using dc magnetometry. Solid lines on selected plots show Brillouin curves for $S = ½$ states (with a mean field correction "theta" applied, where shown), scaled on the ordinate to compare to the experimental magnetization data (which approach expected values of two $S = ½$ for BrA27diNN, A27diNN, A27diIN biradicals). Most data for A27diNN and all data for A26diIN are well below expected values for two $S = ½$ spins, indicative of antiferromagnetic exchange much stronger than a modest mean field correction. Experimental sample magnetization data (emu) for A26diNN with an $S = ½$ Brillouin curve (no mean field) are compared, both normalized to their highest values.

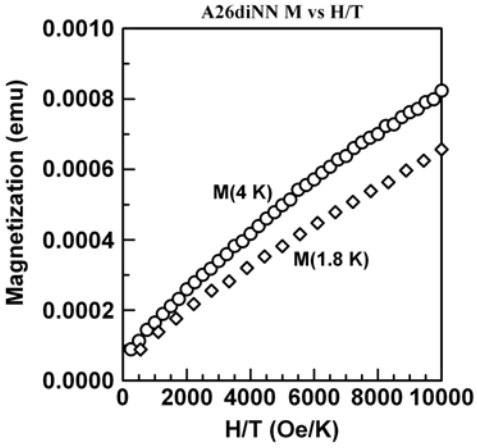


Figure S10. Raw magnetizationversus field/temperature (*M* vs. *H*/*T*) plots for one sample of A26diNN, measured at 4 K and 1.8 K.

Table S2. Computational intramolecular exchange energies for biradicals in this study.

Compound	Computational Method	Computed E_T ($<S^2>$)	Computed E_S ($<S^2>$)	Computed ΔE(T-S) (J_{intra}/k)
BrA27diNN	UB97D/6-31G(d)	–3862.781722[b] (2.039)	–3862.781696[c] (1.036)	69 J/mol[d] (8.3 K[e])
BrA27diNN	UB3LYP/6-31G(d)	–3862.524332 (2.161)	–3862.524044 (1.134)	735 (88.5)
A27diNN	UB97D/6-31G(d)	–1290.540739 (2.044)	–1290.540691 (1.040)	125 (15.0)
A27diNN	UB3LYP/6-31G(d)	–1291.422424 (2.155)	–1291.422156 (1.131)	685 (82.5)
A27diIN	UB97D/6-31G(d)	–1140.273823 (2.021)	–1140.273812 (1.019)	30 (3.7)
A27diIN	UB3LYP/6-31G(d)	–1141.087904 (2.042)	–1141.087860 (1.038)	114 (13.7)
A26diNN	UB97D/6-31G(d)	–1290.540724 (2.039)	–1290.540835 (1.046)	–294 (–35.4)
A26diNN	UB3LYP/6-31G(d)	–1291.422085 (2.127)	–1291.422521 (1.158)	–1178 (–142)
A26diIN	UB97D/6-31G(d)	–1140.273696 (2.019)	–1140.27372 (1.021)	–63 (–7.6)
A26diIN	UB3LYP/6-31G(d)	–1141.087793 (2.037)	–1141.087862 (1.042)	–184 (–22.1)
AQ27diNN	UB97D/6-31G(d)	–1439.701644 (2.042)	–1439.701654 (1.042)	–27 (–3.2)
AQ27diNN	UB3LYP/6-31G(d)	–1440.665419 (2.139)	–1440.665431 (1.139)	–33 (–3.9)
AQ27diIN	UB97D/6-31G(d)	–1289.432887 (2.021)	–1289.43289 (1.021)	–6.0 (–0.7)
AQ27diIN	UB3LYP/6-31G(d)	–1290.329505 (2.041)	–1290.329508 (1.041)	–6.0 (–0.7)
AQ26diNN	UB97D/6-31G(d)	–1439.701717 (2.042)	–1439.701715 (1.042)	6.8 (0.8)
AQ26diNN	UB3LYP/6-31G(d)	–1440.665495 (2.139)	–1440.665496 (1.139)	–2.9 (–0.3)
AQ26diIN	UB97D/6-31G(d)	–1289.432907 (2.021)	–1289.432908 (1.042)	–2.7 (–0.3)
AQ26diIN	UB3LYP/6-31G(d)	–1290.329642 (2.04117)	–1290.329644 (1.041292)	–4.7 (–0.6)

*Not determined. [b]Energy in hartrees, triplet optimized geometry. [c]Energy in hartrees, triplet state frozen geometry, unrestricted wavefunction with broken symmetry. [d]Computed triplet-singlet state energy in J/mol, with Yamaguchi correction (eq. S1); triplet state is lower for positive value. [e]Computed triplet-singlet state energy in Kelvin, with Yamaguchi correction (eq. S1); triplet state is lower for positive value.

$$\Delta E(T-S) = \frac{E_S - E_T}{\langle S^2 \rangle_T - \langle S^2 \rangle_S} \qquad \text{(Eq . S1)}$$

from Yamaguchi, K. A Spin Correction Procedure for Unrestricted Hartree-Fock and Møller-Plesset Wavefunctions for Singlet Diradicals and Polyradicals. *Chem. Phys. Lett.***1988**, *149*, 537-542.

Computational summaries for biradicals. Computations were carried out using Gaussian 09:

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

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A27diIN singlet
1\1\GINC-SKYNET\SP\UB97D\6-31G(d)\C20H16N4O2\LAHTI\02-Jan-2015\0\\#P G
 FINPUT IOP(6/7=3) UB97D/6-31G(d) TEST GUESS=(READ,MIX)\\An27tDiIN froz
 en triplet geom\\0,1\C,0,3.692974,0.375327,0.009356\C,0,1.244004,1.853
 669,0.017105\C,0,-1.209731,1.864178,0.024473\C,0,-3.671274,0.406867,0.
 031422\C,0,-1.217563,0.411153,0.024153\C,0,1.239385,0.40063,0.01681\C,
 0,5.007505,-0.294211,0.0054\N,0,5.172983,-1.704965,0.003172\O,0,4.2947
 03,-2.62115,0.003849\C,0,6.630454,-2.019321,-0.000563\C,0,7.252006,-0.
 605387,-0.000444\N,0,6.13882,0.360066,0.00355\C,0,-4.991496,-0.251388,
 0.035071\N,0,-5.169045,-1.660684,0.035602\O,0,-4.298641,-2.584353,0.03
 3323\C,0,-6.629152,-1.962553,0.039507\C,0,-7.238575,-0.543348,0.04135\
 N,0,-6.117162,0.412542,0.03818\H,0,-6.853716,-2.560464,0.935029\H,0,-6
 .858557,-2.560186,-0.854978\H,0,-7.86352,-0.357778,0.930193\H,0,-7.868
 652,-0.357659,-0.843835\H,0,6.850217,-2.618045,-0.896732\H,0,6.854402,
 -2.619995,0.893269\H,0,7.883355,-0.426195,0.885173\H,0,7.878817,-0.424
 077,-0.888854\C,0,-2.466018,-0.285545,0.02768\H,0,-2.458378,-1.372517,
 0.02739\C,0,-3.656737,1.850164,0.031754\H,0,-4.61153,2.374024,0.034707
 \C,0,-2.470774,2.545401,0.028403\H,0,-2.47375,3.637921,0.02869\C,0,0.0
 20081,2.546486,0.020941\H,0,0.024762,3.639776,0.021183\C,0,3.690799,1.
 818697,0.009675\H,0,4.650044,2.334362,0.006905\C,0,2.510835,2.524066,0
 .013411\H,0,2.523173,3.616521,0.013604\C,0,0.007963,-0.282436,0.020344
 \H,0,0.003282,-1.375262,0.020114\C,0,2.481826,-0.306732,0.012906\H,0,2
 .464881,-1.393599,0.012712\\Version=EM64L-G09RevB.01\State=1-A\HF=-114
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 0247,0.0051681,0.0002615\Quadrupole=25.4798841,-11.7900425,-13.6898416
 ,-0.1596017,-0.1154268,-0.0060285\PG=C01 [X(C20H16N4O2)]\\@
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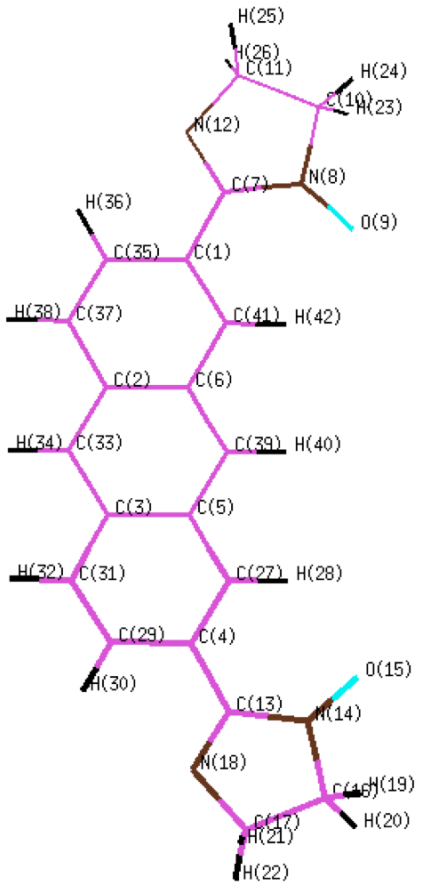

Mulliken atomic spin densities:					
		1			
1	C	0.014812	21	H	-0.009827
2	C	-0.001518	22	H	-0.009819
3	C	0.001516	23	H	0.018888
4	C	-0.014809	24	H	0.018898
5	C	-0.002882	25	H	0.009818
6	C	0.002884	26	H	0.009829
7	C	-0.089970	27	C	0.020280
8	N	0.323404	28	H	0.000891
9	O	0.459062	29	C	0.005073
10	C	-0.022438	30	H	0.000413
11	C	-0.014433	31	C	-0.005132
12	N	0.299878	32	H	0.000284
13	C	0.089966	33	C	0.000001
14	N	-0.323411	34	H	0.000000
15	O	-0.459066	35	C	-0.005074
16	C	0.022438	36	H	-0.000413
17	C	0.014433	37	C	0.005133
18	N	-0.299863	38	H	-0.000284
19	H	-0.018888	39	C	-0.000002
20	H	-0.018897	40	H	0.000000
			41	C	-0.020283
			42	H	-0.000891

A27diIN triplet
1\1\GINC-SKYNET\FOpt\UB97D\6-31G(d)\C20H16N4O2(3)\LAHTI\31-Dec-2014\0\
\#P GFINPUT IOP(6/7=3) UB97D/6-31G(d) TEST OPT\\An27tDiNN\\0,3\C,3.692
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54\C,-1.2097310348,1.8641775164,0.0244728385\C,-3.6712738174,0.4068670
626,0.0314221131\C,-1.2175625727,0.4111534676,0.024152827\C,1.23938522
3,0.4006304796,0.016809618\C,5.0075050131,-0.2942112193,0.0054004472\N
,5.1729830679,-1.7049650778,0.0031715687\O,4.2947028337,-2.6211497646,
0.0038488379\C,6.6304543546,-2.0193211692,-0.0005627913\C,7.2520058763
,-0.6053865674,-0.000444028\N,6.1388196544,0.360065852,0.003550452\C,-
4.9914964252,-0.2513876381,0.0350709741\N,-5.1690452151,-1.6606841493,
0.0356016827\O,-4.2986412143,-2.5843533297,0.0333230356\C,-6.629152269
,-1.9625534186,0.039507181\C,-7.2385753289,-0.5433476752,0.0413496291\
N,-6.1171620278,0.4125416699,0.038180206\H,-6.8537155922,-2.5604644218
,0.935029118\H,-6.8585566424,-2.5601857043,-0.8549778407\H,-7.86351984
72,-0.3577777028,0.9301934277\H,-7.8686523602,-0.3576592772,-0.8438345
47\H,6.8502174402,-2.618044725,-0.896732433\H,6.8544016796,-2.61999533
18,0.8932690264\H,7.8833554805,-0.426195225,0.8851729037\H,7.878816670
5,-0.4240774768,-0.8888541222\C,-2.4660184575,-0.285545466,0.027679770
9\H,-2.4583782711,-1.3725173963,0.0273899552\C,-3.6567371725,1.8501640
133,0.0317537763\H,-4.6115299413,2.3740238806,0.0347066422\C,-2.470774
4632,2.5454008722,0.0284030425\H,-2.473749851,3.6379213759,0.028690136
5\C,0.0200813019,2.546486162,0.0209413106\H,0.0247618679,3.6397760404,
0.0211825803\C,3.6907986386,1.8186967647,0.0096754866\H,4.6500444772,2
.3343622704,0.0069051275\C,2.5108350429,2.5240664315,0.013411186\H,2.5
231730596,3.6165207968,0.0136036798\C,0.0079629777,-0.2824355997,0.020
3438746\H,0.0032820876,-1.3752617182,0.0201136373\C,2.4818264256,-0.30
67316272,0.0129063674\H,2.4648812293,-1.3935994387,0.0127123616\\Versi
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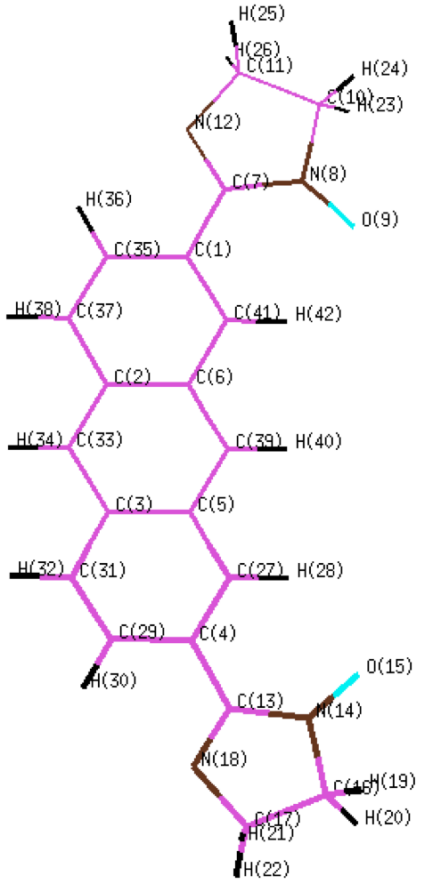

Mulliken atomic spin densities:					
		1			
1	C	0.019280	21	H	0.009878
2	C	-0.010516	22	H	0.009870
3	C	-0.010516	23	H	0.018893
4	C	0.019279	24	H	0.018902
5	C	0.009110	25	H	0.009869
6	C	0.009111	26	H	0.009880
7	C	-0.090435	27	C	-0.026107
8	N	0.323502	28	H	-0.000637
9	O	0.459102	29	C	-0.012314
10	C	-0.022445	30	H	-0.000064
11	C	-0.014489	31	C	0.010675
12	N	0.300973	32	H	-0.000519
13	C	-0.090432	33	C	0.011689
14	N	0.323510	34	H	-0.000534
15	O	0.459106	35	C	-0.012314
16	C	-0.022446	36	H	-0.000064
17	C	-0.014488	37	C	0.010675
18	N	0.300958	38	H	-0.000519
19	H	0.018893	39	C	-0.017263
20	H	0.018902	40	H	0.000790
			41	C	-0.026109
			42	H	-0.000637

A27diNN singlet
1\1\GINC-SKYNET\SP\UB97D\6-31G(d)\C20H16N4O4\LAHTI\02-Jan-2015\0\\#P G
FINPUT IOP(6/7=3) UB97D/6-31G(d) TEST GUESS=(READ,MIX)\\Ant27DiNN froz
en triplet state opt geom\\0,1\H,0,0.000009,-1.449748,0.000007\O,0,-4.
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31,-1.726887,0.350347\N,0,-6.174187,0.110921,-0.361037\C,0,0.00001,-0.
357005,0.000042\C,0,-1.228344,0.332321,0.000817\C,0,-2.471554,-0.36750
8,0.00102\H,0,-2.459264,-1.454347,0.015094\C,0,-3.685824,0.318983,-0.0
07902\C,0,-3.678074,1.764137,-0.004951\H,0,-4.625546,2.294661,-0.01688
8\C,0,-2.490454,2.458761,0.002585\H,0,-2.499826,3.551113,0.009026\C,0,
-1.22667,1.786042,0.000736\C,0,0.000014,2.473838,0.000134\H,0,0.000017
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0,2.471574,-0.367517,-0.000939\H,0,2.459279,-1.454354,-0.01508\C,0,3.6

85848,0.318968,0.008024\C,0,3.678101,1.764124,0.005171\H,0,4.625574,2.294643,0.017141\C,0,2.490483,2.458752,-0.002317\H,0,2.49986,3.551105,-0.008686\C,0,1.226697,1.786038,-0.000514\C,0,4.952626,-0.409943,0.0077\C,0,6.538264,-2.166248,-0.230069\C,0,7.271356,-0.895619,0.211213\H,0,-6.574018,-2.982406,-0.505035\H,0,-6.848728,-2.550495,1.210753\H,0,-7.981626,-0.506754,0.531656\H,0,-7.77527,-0.978415,-1.18325\H,0,7.981607,-0.506729,-0.531742\H,0,7.775371,-0.978431,1.18317\H,0,6.848728,-2.550492,-1.21079\H,0,6.574067,-2.982408,0.505004\\Version=EM64L-G09RevB.01\State=1-A\HF=-1290.540691\S2=1.039599\S2-1=0.\S2A=0.316446\RMSD=6.216e-09\Dipole=0.0000051,-0.8504313,-0.0000425\Quadrupole=29.3426079,-12.9457945,-16.3968134,0.0001387,-4.5143716,0.0004737\PG=C01 [X(C20H16N4O4)]\\@

Mulliken atomic spin densities:

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1	H	0.000000
2	O	-0.327583
3	O	-0.328445
4	N	-0.245319
5	N	-0.244598
6	C	0.000002
7	C	-0.004912
8	C	0.035718
9	H	-0.000861
10	C	-0.023731
11	C	0.004448
12	H	0.000530
13	C	-0.005904
14	H	0.000347
15	C	0.001203
16	C	-0.000002
17	H	0.000000
18	C	0.126656
19	C	0.017241
20	C	0.017263
21	O	0.327583
22	O	0.328445
23	N	0.245319
24	N	0.244598
25	C	0.004910
26	C	-0.035717
27	H	0.000861
28	C	0.023729
29	C	-0.004446
30	H	-0.000530
31	C	0.005902
32	H	-0.000347
33	C	-0.001200
34	C	-0.126655
35	C	-0.017240
36	C	-0.017263
37	H	-0.011601
38	H	-0.009893
39	H	-0.011496
40	H	-0.009854
41	H	0.011497
42	H	0.009853
43	H	0.009892
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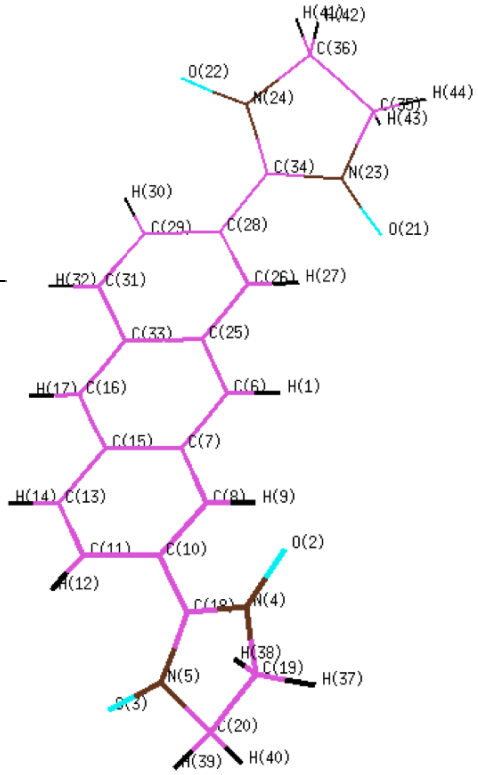
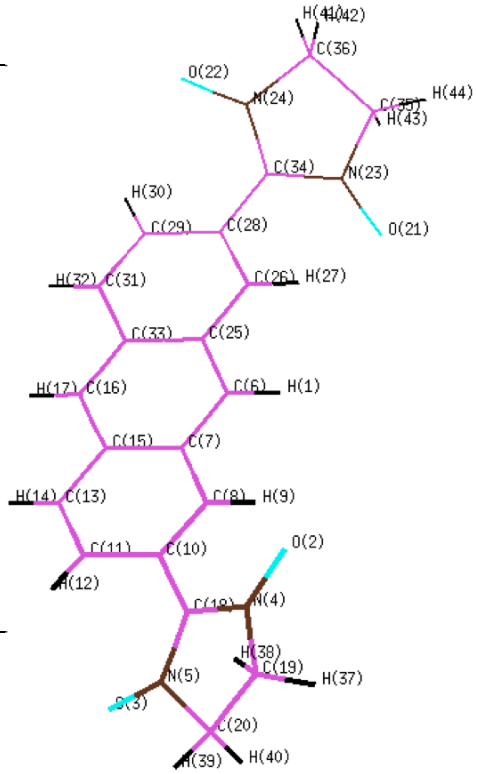


A27diNN triplet
1\1\GINC-SKYNET\FOpt\UB97D\6-31G(d)\C20H16N4O4(3)\LAHTI\02-Jan-2015\0\\#P GFINPUT IOP(6/7=3) UB97D/6-31G(d) TEST OPT\\Ant27DiNN\\0,3\H,0.0000088068,-1.4497481501,0.0000071316\O,-4.2395112599,-2.5580249254,0.7585323468\O,-6.4555609574,1.2739455051,-0.7960861863\N,-5.1135309305,-1.7268867003,0.3503465007\N,-6.1741868626,0.1109205026,-0.3610370434\C,0.0000100963,-0.3570047937,0.0000421702\C,-1.2283442839,0.3323211668,0.0008167689\C,-2.4715542425,-0.3675080958,0.0010199798\H,-2.4592637692,-1.4543470572,0.0150936726\C,-3.6858244367,0.3189828315,-0.0079023586\C,-3.678074175,1.7641367789,-0.0049511091\H,-4.6255456566,2.2946613845,-0.016887517\C,-2.4904535743,2.4587612929,0.0025845009\H,-2.4998258604,3.5511133189,0.0090263713\C,-1.2266700762,1.7860421135,0.0007364456\C,0.0000144889,2.4738383651,0.000134096\H,0.0000166942,3.5670688222,0.0001698805\C,-4.9526017044,-0.4099291573,-0.0076335334\C,-6.538237596,-2.1662474887,0.230040428\C,-7.2713189181,-0.8956185173,-0.2112574168\O,4.23953151,-2.5580191901,-0.7585265515\O,6.4556017923,1.2739092442,0.7961714251\N,5.1135543338,-1.7268879862,-0.3503325627\N,6.174218887,0.1108993429,0.3610865423\C,1.2283666535,0.3323174976,-0.0006875017\C,2.471573751,-0.3675168525,-0.000938501\H,2.4592785975,-1.4543544544,-0.0150803655\C,3.6858475264,0.3189679812,0.0080242661\C,3.6781008778,1.7641235153,0.0051705358\H,4.6255744949,2.2946433327,0.017141142\C,2.4904828679,2.4587523596,-0.0023167689\H,2.4998597717,3.5511049201,-0.0086857232\C,1.2266970414,1.7860379879,-0.0005135254\C,4.9526257625,-0.4099426793,0.0076996197\C,6.5382642738,-2.1662478635,-0.2300689809\C,7.2713561921,-0.8956194755,0.2112126386\H,-6.5740180193,-2.9824062353,-0.5050352865\H,-6.8487281324,-2.5504948279,1.2107526824\H,-7.9816260534,-0.5067539891,0.5316560508\H,-7.7752698504,-0.9784152798,-1.1832497568\H,7.9816067213,-0.5067291843,-0.5317417321\H,7.7753714319,-0.9784308228,1.1831695943\H,6.8487282324,-2.5504921771,-1.2107904791\H,6.5740665538,-2.98240836,0.5050041098\\Version=EM64L-G09RevB.01\State=3-A\HF=-1290.5407388\S2=2.043963\S2-1=0.\S2A=2.000911\RMSD=4.620e-09\RMSF=9.426e-06\Dipole=0.0000059,-0.8504745,-0.0000436\Quadrupole=29.3444778,-12.946206,-16.3982718,0.0001056,-4.5138531,0.0004793\PG=C01 [X(C20H16N4O4)]\\@

Mulliken atomic spin densities:					
		1			
1	H	0.001757	23	N	0.246048
2	O	0.328298	24	N	0.245321
3	O	0.329137	25	C	0.017375
4	N	0.246047	26	C	-0.048781
5	N	0.245321	27	H	0.001434
6	C	-0.038175	28	C	0.032325
7	C	0.017376	29	C	-0.020320
8	C	-0.048782	30	H	0.000234
9	H	0.001434	31	C	0.016803
10	C	0.032326	32	H	-0.000806
11	C	-0.020321	33	C	-0.019298
12	H	0.000234	34	C	-0.127680
13	C	0.016804	35	C	-0.017277
14	H	-0.000806	36	C	-0.017303
15	C	-0.019298	37	H	0.011656
16	C	0.020229	38	H	0.009933
17	H	-0.000896	39	H	0.011551
18	C	-0.127680	40	H	0.009893
19	C	-0.017277	41	H	0.011552
20	C	-0.017303	42	H	0.009892
21	O	0.328300	43	H	0.009932
22	O	0.329136	44	H	0.011656
			43	H	0.009892
			44	H	0.011601



AQ27diIN singlet
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86081,0.076317\C,0,1.28075,0.285701,0.075499\C,0,5.044713,-0.390046,0.
036259\N,0,5.212945,-1.794192,-0.044265\O,0,4.338222,-2.708451,-0.0966
8\C,0,6.674139,-2.101537,-0.061912\C,0,7.289043,-0.687023,0.01909\N,0,
6.170423,0.271695,0.074121\C,0,-5.045007,-0.388526,0.038983\N,0,-5.213
702,-1.792843,-0.037487\O,0,-4.339281,-2.707644,-0.085257\C,0,-6.67499
6,-2.099628,-0.056601\C,0,-7.289434,-0.684678,0.020214\N,0,-6.170498,0
.273772,0.073469\H,0,-6.899097,-2.746455,0.803957\H,0,-6.896379,-2.648
09,-0.983632\H,0,-7.91715,-0.547802,0.915593\H,0,-7.915847,-0.450989,-
0.855817\H,0,6.896658,-2.648014,-0.989831\H,0,6.89671,-2.750383,0.7975
35\H,0,7.91624,-0.552737,0.915216\H,0,7.916097,-0.451252,-0.855934\C,0
,-2.49905,-0.416785,0.03654\H,0,-2.470711,-1.500787,-0.025641\C,0,-3.7
09711,1.694824,0.158291\H,0,-4.659823,2.226874,0.189176\C,0,-2.504568,
2.391425,0.197737\H,0,-2.484825,3.479534,0.260205\C,0,0.000329,2.47910
3,0.201741\C,0,3.710108,1.69373,0.155834\H,0,4.660398,2.225494,0.18617
4\C,0,2.505198,2.390688,0.196033\H,0,2.485815,3.478806,0.258452\C,0,-0
.000165,-0.495318,0.030847\C,0,2.498745,-0.417525,0.034942\H,0,2.47004
5,-1.501517,-0.027256\O,0,0.000535,3.712602,0.272467\O,0,-0.000371,-1.
726329,-0.040164\\Version=EM64L-G09RevB.01\State=1-A\HF=-1289.4328897\
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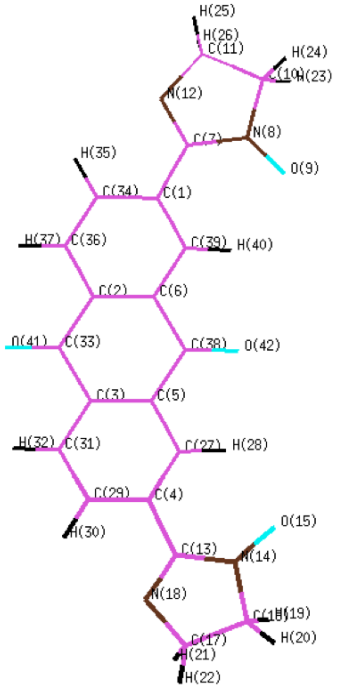
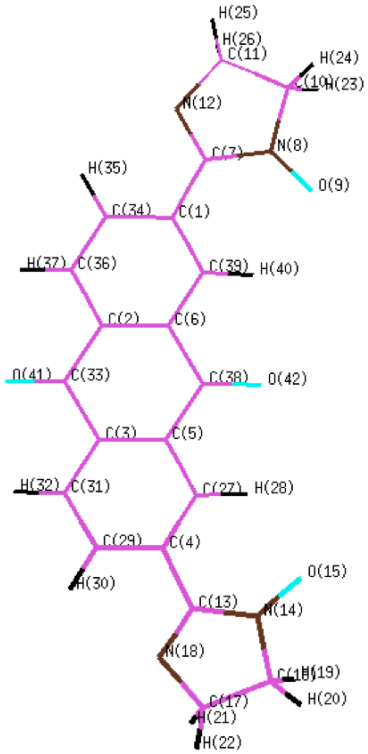
478765,-0.01476\Quadrupole=40.0253189,-26.8312527,-13.1940663,-0.01025
54,-0.0135372,-0.759631\PG=C01 [X(C20H14N4O4)]\\@

Mulliken atomic spin densities:					
		1			
1	C	-0.016868	21	H	0.010717
2	C	0.010909	22	H	0.010678
3	C	-0.010907	23	H	-0.017922
4	C	0.016866	24	H	-0.017925
5	C	0.007484	25	H	-0.010696
6	C	-0.007486	26	H	-0.010698
7	C	0.092142	27	C	-0.016656
8	N	-0.305024	28	H	-0.000861
9	O	-0.457845	29	C	-0.011664
10	C	0.021522	30	H	-0.000159
11	C	0.015219	31	C	0.005731
12	N	-0.320888	32	H	-0.000260
13	C	-0.092141	33	C	-0.000001
14	N	0.305024	34	C	0.011666
15	O	0.457845	35	H	0.000158
16	C	-0.021521	36	C	-0.005733
			37	H	0.000261
			38	C	0.000001



17	C	-0.015219	39	C	0.016658
18	N	0.320887	40	H	0.000861
19	H	0.017908	41	O	0.000001
20	H	0.017939	42	O	-0.000001

AQ27diIN triplet
1\1\GINC-SKYNET\FOpt\UB97D\6-31G(d)\C20H14N4O4(3)\LAHTI\31-Dec-2014\0\
\#P GFINPUT IOP(6/7=3) UB97D/6-31G(d) TEST OPT\\AQ27tDiIN\\0,3\C,3.723
2849258,0.2763602734,0.0745690381\C,1.2775894817,1.7000103024,0.156679
7624\C,-1.2771903917,1.7003860858,0.1575505538\C,-3.7233597931,0.27746
17675,0.0769859856\C,-1.2808222668,0.2860812624,0.0763170264\C,1.28074
96161,0.2857011291,0.0754994844\C,5.0447128082,-0.3900455328,0.0362585
747\N,5.2129453818,-1.7941918442,-0.044264815\O,4.3382219219,-2.708451
1777,-0.0966800862\C,6.6741386894,-2.1015366856,-0.061911907\C,7.28904
32856,-0.6870232906,0.0190895482\N,6.1704225041,0.2716945765,0.0741208
23\C,-5.0450068661,-0.3885263926,0.0389830297\N,-5.213702404,-1.792842
616,-0.0374866641\O,-4.339281131,-2.7076441267,-0.0852569383\C,-6.6749
963369,-2.0996277069,-0.0566012139\C,-7.2894335829,-0.6846781815,0.020
2139945\N,-6.1704983168,0.2737715712,0.0734690951\H,-6.8990968596,-2.7
464553576,0.8039574697\H,-6.8963785138,-2.6480899428,-0.9836316947\H,-
7.9171497672,-0.5478021598,0.9155928767\H,-7.9158472635,-0.4509885979,
-0.8558168583\H,6.8966584849,-2.6480136823,-0.9898314694\H,6.896710121
9,-2.7503828165,0.7975349521\H,7.9162395047,-0.552736785,0.9152156926\
H,7.9160966565,-0.451252279,-0.8559338247\C,-2.4990495645,-0.416784599
9,0.0365398609\H,-2.4707108095,-1.5007866636,-0.0256412503\C,-3.709710
5078,1.6948242506,0.1582905557\H,-4.6598230656,2.2268739596,0.18917554
57\C,-2.5045683476,2.3914250762,0.1977374436\H,-2.4848245337,3.4795338
327,0.2602047548\C,0.0003295,2.4791033462,0.2017409007\C,3.7101082591,
1.6937301859,0.1558344239\H,4.6603979676,2.2254943698,0.1861737514\C,2
.5051980006,2.390688115,0.196033271\H,2.4858145028,3.478806262,0.25845
21496\C,-0.0001649725,-0.49531793,0.0308466455\C,2.4987445286,-0.41752
49274,0.0349422604\H,2.4700452335,-1.5015166074,-0.0272555482\O,0.0005
350937,3.7126021467,0.2724666821\O,-0.0003711737,-1.7263286092,-0.0401
638821\\Version=EM64L-G09RevB.01\State=3-A\HF=-1289.4328874\S2=2.02122
3\S2-1=0.\S2A=2.000235\RMSD=6.208e-09\RMSF=3.561e-06\Dipole=-0.0000322
,-0.2479322,-0.0147652\Quadrupole=40.0227376,-26.8292866,-13.193451,-0
.0102888,-0.0135421,-0.7595536\PG=C01 [X(C20H14N4O4)]\\@



Mulliken atomic spin densities:					
		1			
1	C	0.016376	21	H	0.010709
2	C	-0.010932	22	H	0.010671
3	C	-0.010932	23	H	0.017922
4	C	0.016376	24	H	0.017924
5	C	0.007173	25	H	0.010689
6	C	0.007173	26	H	0.010691
7	C	-0.092064	27	C	-0.016560
8	N	0.305008	28	H	-0.000869
9	O	0.457806	29	C	-0.011595
10	C	-0.021520	30	H	-0.000157
11	C	-0.015213	31	C	0.005553
12	N	0.320763	32	H	-0.000240
13	C	-0.092064	33	C	0.001950
14	N	0.305008	34	C	-0.011595
15	O	0.457805	35	H	-0.000157
16	C	-0.021520	36	C	0.005553
17	C	-0.015213	37	H	-0.000240
18	N	0.320764	38	C	-0.001407
19	H	0.017907	39	C	-0.016560
20	H	0.017938	40	H	-0.000869
			41	O	-0.005109
			42	O	0.003055

AQ27diNN singlet
1\1\GINC-SKYNET\SP\UB97D\6-31G(d)\C20H14N4O6\LAHTI\02-Jan-2015\0\\#P G
FINPUT IOP(6/7=3) UB97D/6-31G(d) TEST GUESS=(READ,MIX)\\AntQ27DiNN tri
plet opt geom\\0,1\O,0,-0.000044,-1.716952,0.000016\O,0,4.293486,-2.52
7848,-0.928216\O,0,6.462967,1.209531,0.883246\N,0,5.155004,-1.735716,-
0.435652\N,0,6.198936,0.063693,0.398751\C,0,-0.000025,-0.483989,-0.000
027\C,0,1.279887,0.299848,-0.008555\C,0,2.495057,-0.401784,-0.023611\H
,0,2.466657,-1.487502,-0.046583\C,0,3.724909,0.293522,-0.012346\C,0,3.
714176,1.714459,0.008229\H,0,4.655219,2.256888,0.030346\C,0,2.503949,2
.406942,0.007074\H,0,2.485728,3.496815,0.01219\C,0,1.276503,1.718261,0
.000695\C,0,0.000019,2.498788,-0.000095\O,0,0.000037,3.734664,-0.00010
2\C,0,4.990958,-0.438757,-0.016189\C,0,6.577571,-2.184757,-0.294888\C,
0,7.293135,-0.950786,0.266832\O,0,-4.293289,-2.527673,0.928196\O,0,-6.
463149,1.209446,-0.883348\N,0,-5.154909,-1.735623,0.435681\N,0,-6.1990
03,0.063673,-0.398761\C,0,-1.279914,0.299886,0.008472\C,0,-2.495104,-0
.401707,0.023566\H,0,-2.466739,-1.487425,0.046598\C,0,-3.724937,0.2936
3,0.012262\C,0,-3.714164,1.714569,-0.008348\H,0,-4.655189,2.257027,-0.
030461\C,0,-2.503915,2.407015,-0.007228\H,0,-2.485661,3.496887,-0.0123
75\C,0,-1.276488,1.718299,-0.000841\C,0,-4.990974,-0.438668,0.016174\C
,0,-6.577443,-2.184783,0.294974\C,0,-7.293123,-0.950881,-0.26675\H,0,6
.585742,-3.05361,0.377007\H,0,6.923403,-2.493519,-1.290256\H,0,8.05707
4,-0.530433,-0.401246\H,0,7.726458,-1.096397,1.265235\H,0,-8.057057,-0
.53056,0.401353\H,0,-7.726489,-1.096559,-1.265125\H,0,-6.923216,-2.493
553,1.290361\H,0,-6.585566,-3.05365,-0.376904\\Version=EM64L-G09RevB.0
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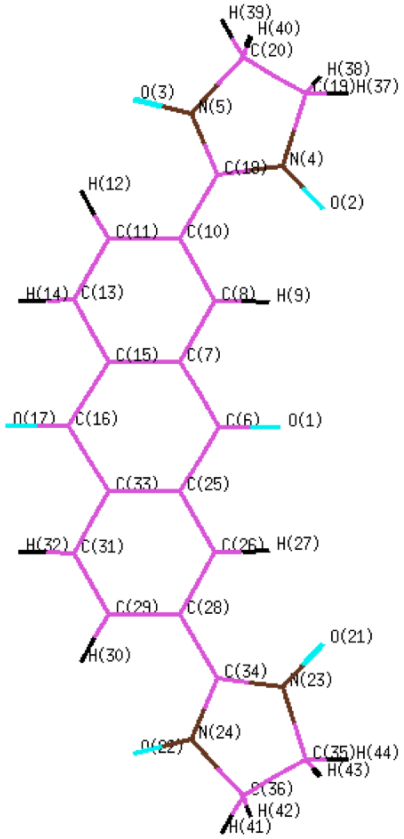
95e-09\Dipole=0.0000637,-1.1646109,0.0001234\Quadrupole=44.2746054,-27
.2508045,-17.0238009,0.0011331,-4.455377,-0.0002766\PG=C01 [X(C20H14N4
O6)]\\@



Mulliken atomic spin densities:					
		1			
1	O	-0.000002	22	O	-0.328289
2	O	0.334803	23	N	-0.241093
3	O	0.328278	24	N	-0.244432
4	N	0.241095	25	C	-0.010567
5	N	0.244431	26	C	0.023407
6	C	0.000002	27	H	-0.000373
7	C	0.010563	28	C	-0.025153
8	C	-0.023404	29	C	0.022557
9	H	0.000373	30	H	-0.000431
10	C	0.025150	31	C	-0.011137
11	C	-0.022553	32	H	0.000489
12	H	0.000430	33	C	0.022750
13	C	0.011133	34	C	0.129087
14	H	-0.000488	35	C	0.017168
15	C	-0.022745	36	C	0.017256
16	C	-0.000001	37	H	0.010864
17	O	0.000001	38	H	0.010341
18	C	-0.129087	39	H	0.010922
19	C	-0.017168	40	H	0.010446
20	C	-0.017256	41	H	-0.010923
21	O	-0.334792	42	H	-0.010446
			43	H	-0.010340
			44	H	-0.010864

AQ27diNN triplet
1\1\GINC-SKYNET\FOpt\UB97D\6-31G(d)\C20H14N4O6(3)\LAHTI\02-Jan-2015\0\
\#P GFINPUT IOP(6/7=3) UB97D/6-31G(d) TEST OPT GUESS=READ\\AntQ27DiNN
triplet opt\\0,3\O,-0.0000435681,-1.7169523691,0.0000157729\O,4.293485
6695,-2.5278476029,-0.9282155607\O,6.4629665844,1.2095306772,0.8832455
45\N,5.1550041408,-1.7357160561,-0.4356517763\N,6.1989355916,0.0636927
439,0.3987510303\C,-0.0000251238,-0.4839891773,-0.0000269757\C,1.27988
70914,0.2998478962,-0.0085547608\C,2.4950566653,-0.401783807,-0.023610
7399\H,2.4666574036,-1.4875018184,-0.0465827825\C,3.7249094932,0.29352
1505,-0.0123463356\C,3.7141760475,1.714458788,0.0082291016\H,4.6552190
085,2.2568875272,0.0303463051\C,2.503949312,2.4069420432,0.0070738319\
H,2.4857275762,3.4968145289,0.0121902834\C,1.2765025162,1.7182610423,0
.0006949729\C,0.0000188089,2.4987879745,-0.0000945705\O,0.0000369882,3
.7346637068,-0.0001018542\C,4.9909582102,-0.4387568263,-0.0161888772\C
,6.5775708382,-2.1847572834,-0.294887524\C,7.2931353471,-0.9507855011,
0.2668316404\O,-4.2932886254,-2.5276734506,0.9281958617\O,-6.463148836
6,1.2094457065,-0.8833476162\N,-5.1549093375,-1.735622784,0.4356813603

\N,-6.1990031436,0.0636728616,-0.3987609352\C,-1.2799135792,0.29988647
84,0.0084724319\C,-2.4951035496,-0.4017068532,0.0235655033\H,-2.466738
9093,-1.4874252744,0.0465982591\C,-3.7249365525,0.2936296837,0.0122623
88\C,-3.7141643616,1.71456875,-0.0083480913\H,-4.655189263,2.257027153
8,-0.0304609447\C,-2.5039154128,2.407014879,-0.0072282198\H,-2.4856613
334,3.4968867003,-0.0123750478\C,-1.2764879813,1.7182987804,-0.0008411
585\C,-4.9909740794,-0.4386678422,0.0161740181\C,-6.5774428495,-2.1847
833517,0.2949741534\C,-7.2931229232,-0.9508811018,-0.2667496381\H,6.58
57415634,-3.0536098291,0.3770073923\H,6.9234032442,-2.4935192153,-1.29
02562903\H,8.0570738689,-0.5304331958,-0.4012460335\H,7.7264575441,-1.
0963969804,1.2652354582\H,-8.0570567122,-0.5305597608,0.4013533509\H,-
7.726488801,-1.0965589599,-1.2651247553\H,-6.9232156817,-2.4935528244,
1.2903608644\H,-6.5855658886,-3.0536495618,-0.3769040369\\Version=EM64
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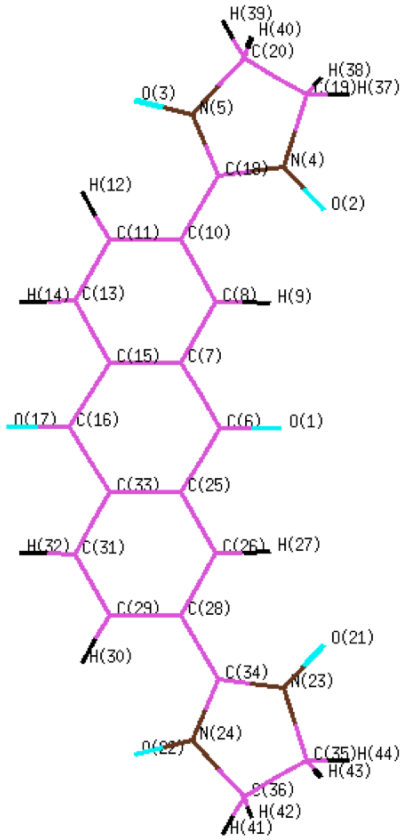
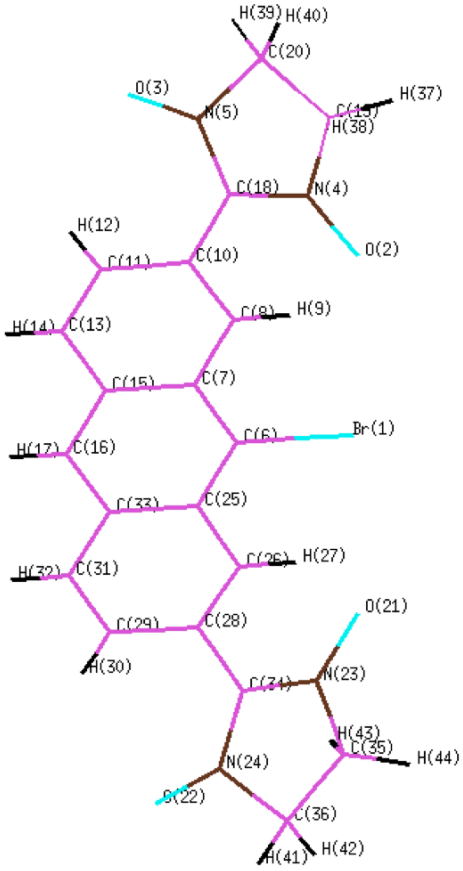
9\RMSD=5.901e-09\RMSF=4.683e-06\Dipole=0.0000593,-1.1638633,0.0001202\
Quadrupole=44.2631351,-27.2429615,-17.0201736,0.001042,-4.4558389,-0.0
002722\PG=C01 [X(C20H14N4O6)]\\@



Mulliken atomic spin densities:					
		1			
1	O	0.003075	22	O	0.328112
2	O	0.334585	23	N	0.240992
3	O	0.328100	24	N	0.244327
4	N	0.240994	25	C	0.009742
5	N	0.244325	26	C	-0.022920
6	C	-0.001371	27	H	0.000349
7	C	0.009742	28	C	0.024022
8	C	-0.022920	29	C	-0.022030
9	H	0.000350	30	H	0.000415
10	C	0.024022	31	C	0.010318
11	C	-0.022029	32	H	-0.000420
12	H	0.000415	33	C	-0.022249
13	C	0.010318	34	C	-0.128952
14	H	-0.000420	35	C	-0.017162
15	C	-0.022249	36	C	-0.017249
16	C	0.003209	37	H	0.010855
17	O	-0.013735	38	H	0.010335
18	C	-0.128952	39	H	0.010912
19	C	-0.017162	40	H	0.010441
20	C	-0.017249	41	H	0.010912
21	O	0.334574	42	H	0.010440
			43	H	0.010334
			44	H	0.010855
			44	H	-0.010864

BrA27diNN singlet
1\1\GINC-SKYNET\Stability\UB97D\6-31G(d)\C20H15Br1N4O4\LAHTI\26-Sep-20
11\0\\#P GFINPUT IOP(6/7=3) UB97D/6-31G(d) TEST STABLE=OPT GUESS=(READ
,MIX)\\XTL structure of BrAntDiNN\\0,1\Br,0,9.655,15.275,1.821\O,0,13.
581,15.201,-0.326\O,0,15.972,18.719,1.437\N,0,14.551,15.944,0.054\N,0,
15.68,17.623,0.871\C,0,9.655,17.185,1.821\C,0,10.845,17.841,1.491\C,0,
12.058,17.181,1.157\H,0,12.079,16.25,1.132\C,0,13.197,17.884,0.873\C,0
,13.176,19.311,0.875\H,0,13.946,19.79,0.669\C,0,12.032,19.963,1.177\H,
0,12.031,20.894,1.171\C,0,10.829,19.28,1.501\C,0,9.655,19.949,1.821\H,
0,9.655,20.879,1.821\C,0,14.442,17.176,0.59\C,0,15.977,15.552,-0.219\C
,0,16.731,16.569,0.678\O,0,5.73,15.201,3.968\O,0,3.339,18.719,2.206\N,
0,4.76,15.944,3.589\N,0,3.631,17.623,2.772\C,0,8.466,17.841,2.152\C,0,
7.253,17.181,2.486\H,0,7.232,16.25,2.51\C,0,6.114,17.884,2.77\C,0,6.13
5,19.311,2.768\H,0,5.365,19.79,2.973\C,0,7.279,19.963,2.466\H,0,7.28,2
0.894,2.471\C,0,8.482,19.28,2.141\C,0,4.869,17.176,3.052\C,0,3.334,15.
552,3.862\C,0,2.58,16.569,2.965\H,0,16.112427,14.49683,0.044612\H,0,16
.135944,15.692964,-1.294212\H,0,17.616855,17.033191,0.229666\H,0,16.96
0678,16.196492,1.682839\H,0,1.693906,17.033316,3.412733\H,0,2.349775,1
6.196766,1.960184\H,0,3.175056,15.692964,4.937212\H,0,3.198573,14.4968
3,3.598388\\Version=EM64L-G09RevB.01\State=1-A\HF=-3862.7816957\S2=1.0
36477\S2-1=0.\S2A=0.291583\RMSD=8.271e-09\Dipole=0.0004142,-0.2945369,
-0.0000046\Quadrupole=28.7062641,-13.5566767,-15.1495874,0.0065208,-16
.4115104,-0.0080038\PG=C01 [X(C20H15Br1N4O4)]\\@

Mulliken atomic spin densities:					
		1			
1	Br	0.000002	22	O	-0.329856
2	O	0.339073	23	N	-0.236902
3	O	0.330090	24	N	-0.233576
4	N	0.236610	25	C	-0.003839
5	N	0.233752	26	C	0.028119
6	C	0.000052	27	H	-0.000239
7	C	0.003812	28	C	-0.020653
8	C	-0.028030	29	C	0.003571
9	H	0.000234	30	H	0.000536
10	C	0.020608	31	C	-0.004221
11	C	-0.003557	32	H	0.000253
12	H	-0.000535	33	C	0.000940
13	C	0.004196	34	C	0.123003
14	H	-0.000252	35	C	0.016620
15	C	-0.000939	36	C	0.015895
16	C	-0.000018	37	H	0.004725
17	H	0.000001	38	H	0.013910
18	C	-0.122980	39	H	0.004359
19	C	-0.016598	40	H	0.014386
20	C	-0.015911	41	H	-0.004347
21	O	-0.339252	42	H	-0.014389
			43	H	-0.013915
			44	H	-0.004739



BrA27diNN triplet
1\1\GINC-SKYNET\Stability\UB97D\6-31G(d)\C20H15Br1N4O4(3)\LAHTI\23-Sep
-2011\0\\#P GFINPUT IOP(6/7=3) UB97D/6-31G(d) TEST STABLE=OPT\\XTL str
ucture of BrAntDiNN\\0,3\Br,0,9.655,15.275,1.821\O,0,13.581,15.201,-0.
326\O,0,15.972,18.719,1.437\N,0,14.551,15.944,0.054\N,0,15.68,17.623,0
.871\C,0,9.655,17.185,1.821\C,0,10.845,17.841,1.491\C,0,12.058,17.181,
1.157\H,0,12.079,16.25,1.132\C,0,13.197,17.884,0.873\C,0,13.176,19.311
,0.875\H,0,13.946,19.79,0.669\C,0,12.032,19.963,1.177\H,0,12.031,20.89
4,1.171\C,0,10.829,19.28,1.501\C,0,9.655,19.949,1.821\H,0,9.655,20.879
,1.821\C,0,14.442,17.176,0.59\C,0,15.977,15.552,-0.219\C,0,16.731,16.5
69,0.678\O,0,5.73,15.201,3.968\O,0,3.339,18.719,2.206\N,0,4.76,15.944,
3.589\N,0,3.631,17.623,2.772\C,0,8.466,17.841,2.152\C,0,7.253,17.181,2
.486\H,0,7.232,16.25,2.51\C,0,6.114,17.884,2.77\C,0,6.135,19.311,2.768
\H,0,5.365,19.79,2.973\C,0,7.279,19.963,2.466\H,0,7.28,20.894,2.471\C,
0,8.482,19.28,2.141\C,0,4.869,17.176,3.052\C,0,3.334,15.552,3.862\C,0,
2.58,16.569,2.965\H,0,16.112427,14.49683,0.044612\H,0,16.135944,15.692
964,-1.294212\H,0,17.616855,17.033191,0.229666\H,0,16.960678,16.196492
,1.682839\H,0,1.693906,17.033316,3.412733\H,0,2.349775,16.196766,1.960
184\H,0,3.175056,15.692964,4.937212\H,0,3.198573,14.49683,3.598388\\Ve
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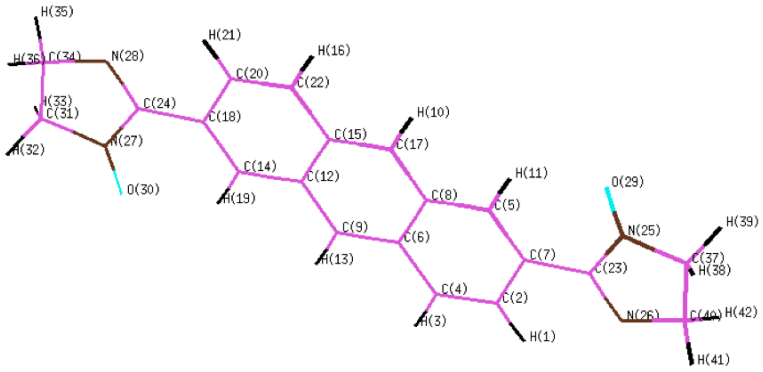
drupole=28.7071993,-13.5574215,-15.1497778,0.0065301,-16.4116034,-0.00
80105\PG=C01 [X(C20H15Br1N4O4)]\\@

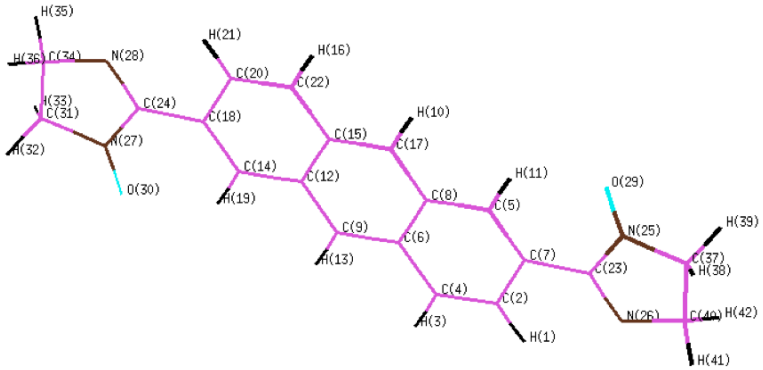
Mulliken atomic spin densities:					
		1			
1	Br	-0.000733	22	O	0.330200
2	O	0.339414	23	N	0.237318
3	O	0.330433	24	N	0.234003
4	N	0.237025	25	C	0.012982
5	N	0.234178	26	C	-0.037451
6	C	-0.027812	27	H	0.000654
7	C	0.012975	28	C	0.026773
8	C	-0.037375	29	C	-0.015002
9	H	0.000649	30	H	-0.000012
10	C	0.026732	31	C	0.012057
11	C	-0.015008	32	H	-0.000558
12	H	-0.000010	33	C	-0.014759
13	C	0.012038	34	C	-0.123604
14	H	-0.000557	35	C	-0.016651
15	C	-0.014783	36	C	-0.015928
16	C	0.014997	37	H	0.004758
17	H	-0.000622	38	H	0.013932
18	C	-0.123578	39	H	0.004393
19	C	-0.016629	40	H	0.014409
20	C	-0.015945	41	H	0.004382
21	O	0.339593	42	H	0.014412
			43	H	0.013938
			44	H	0.004771

```
A26diIN singlet
1\1\GINC-SKYNET\SP\UB97D\6-31G(d)\C20H16N4O2\LAHTI\04-Jan-2015\0\\#P G
 FINPUT IOP(6/7=3) UB97D/6-31G(d) TEST GUESS=(READ,MIX)\\Ant26DiIN trip
 let opt geom (frozen)\\0,1\H,0,-3.0846,-3.666016,0.000075\C,0,-2.20620
 5,-3.022382,0.000089\H,0,-3.324543,-1.193644,0.00011\C,0,-2.333732,-1.
 65392,0.000118\C,0,0.233667,-2.845356,0.000109\C,0,-1.182127,-0.799388
 ,0.000139\C,0,-0.903795,-3.644678,0.000083\C,0,0.131569,-1.419955,0.00
 0139\C,0,-1.279815,0.602167,0.000144\H,0,2.266983,-1.071441,0.00013\H,
 0,1.22127,-3.299299,0.000077\C,0,-0.131569,1.419955,0.000139\H,0,-2.26
 6983,1.071441,0.00013\C,0,-0.233667,2.845356,0.000109\C,0,1.182127,0.7
 99388,0.000139\H,0,3.324543,1.193644,0.00011\C,0,1.279815,-0.602167,0.
 000144\C,0,0.903795,3.644678,0.000083\H,0,-1.22127,3.299299,0.000077\C
 ,0,2.206205,3.022382,0.000089\H,0,3.0846,3.666016,0.000075\C,0,2.33373
 2,1.65392,0.000118\C,0,-0.863158,-5.119567,0.000088\C,0,0.863158,5.119
 567,0.000088\N,0,0.340439,-5.874968,-0.000353\N,0,-1.939318,-5.860807,
 0.00046\N,0,-0.340439,5.874968,-0.000353\N,0,1.939318,5.860807,0.00046
 \O,0,1.545213,-5.475533,-0.000979\O,0,-1.545213,5.475533,-0.000979\C,0
 ,0.001307,7.326127,-0.000031\H,0,-0.444928,7.784031,0.895043\H,0,-0.44
 4746,7.784395,-0.894999\C,0,1.545213,7.280665,0.000183\H,0,1.978076,7.
 771539,-0.886822\H,0,1.977869,7.771866,0.8871\C,0,-0.001307,-7.326127,
 -0.000031\H,0,0.444928,-7.784031,0.895043\H,0,0.444746,-7.784395,-0.89
 4999\C,0,-1.545213,-7.280665,0.000183\H,0,-1.977869,-7.771866,0.8871\H
 ,0,-1.978076,-7.771539,-0.886822\\Version=EM64L-G09RevB.01\HF=-1140.27
 37196\S2=1.021029\S2-1=0.\S2A=0.169723\RMSD=8.244e-09\Dipole=-0.000004
 ,-0.0000048,0.0003845\Quadrupole=-15.7861682,29.573445,-13.7872768,5.7
 241402,0.,0.\PG=C02 [X(C20H16N4O2)]\\@
```



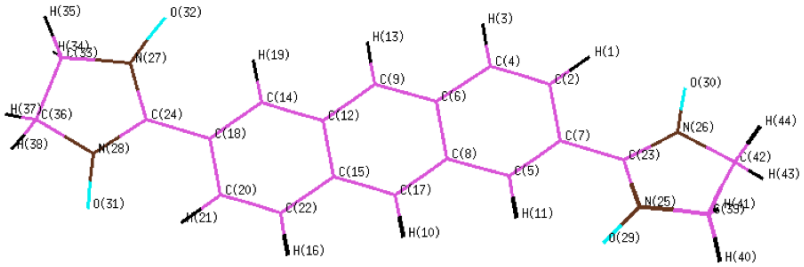
Mulliken atomic spin densities:					
		1			
1	H	-0.000128	21	H	0.000127
2	C	-0.011106	22	C	-0.010525
3	H	-0.000524	23	C	-0.090995
4	C	0.010520	24	C	0.090995
5	C	-0.025792	25	N	0.323934
6	C	-0.009186	26	N	0.301953
7	C	0.020687	27	N	-0.323934
8	C	0.010590	28	N	-0.301953
9	C	0.014162	29	O	0.458551
10	H	0.000647	30	O	-0.458551
11	H	-0.000674	31	C	0.022452
12	C	-0.010592	32	H	-0.018931
13	H	-0.000647	33	H	-0.018914
14	C	0.025797	34	C	0.014534
15	C	0.009188	35	H	-0.009950
16	H	0.000524	36	H	-0.009935
17	C	-0.014161	37	C	-0.022452
18	C	-0.020691	38	H	0.018931
19	H	0.000674	39	H	0.018914
20	C	0.011111	40	C	-0.014534
			41	H	0.009935
			42	H	0.009950

```
A26diIN triplet
1\1\GINC-SKYNET\FOpt\UB97D\6-31G(d)\C20H16N4O2(3)\LAHTI\03-Jan-2015\0\
 \#P GFINPUT IOP(6/7=3) UB97D/6-31G(d) TEST OPT\\Ant26DiIN triplet opt\
 \0,3\H,3.9958199541,-2.6434555104,0.0106051716\C,3.2556221331,-1.84473
 68842,0.0106193794\H,1.5673244233,-3.1655751712,0.010640229\C,1.910840
 7089,-2.1284839105,0.0106482758\C,2.7997339565,0.5586935492,0.01063900
 99\C,0.9297824935,-1.082566966,0.0106694071\C,3.724324781,-0.479511188
 8,0.0106125303\C,1.3954707376,0.2936724842,0.0106694364\C,-0.451298933
 2,-1.3404705261,0.0106735891\H,0.8041713679,2.3749754003,0.010660318\H
 ,3.1373270787,1.5918712782,0.0106065145\C,-1.3954707376,-0.2936724842,
 0.0106694364\H,-0.8041713679,-2.3749754003,0.010660318\C,-2.7997339565
 ,-0.5586935492,0.0106390099\C,-0.9297824935,1.082566966,0.0106694071\H
 ,-1.5673244233,3.1655751712,0.010640229\C,0.4512989332,1.3404705261,0.
 0106735891\C,-3.724324781,0.4795111888,0.0106125303\H,-3.1373270787,-1
 .5918712782,0.0106065145\C,-3.2556221331,1.8447368842,0.0106193794\H,-
 3.9958199541,2.6434555104,0.0106051716\C,-1.9108407089,2.1284839105,0.
 0106482758\C,5.1848028109,-0.2698646595,0.0106182814\C,-5.1848028109,0
 .2698646595,0.0106182814\N,5.7970714066,1.0124790364,0.0101774195\N,6.
 0446594411,-1.253838396,0.0109898635\N,-5.7970714066,-1.0124790364,0.0
 101774195\N,-6.0446594411,1.253838396,0.0109898635\O,5.2620002837,2.16
 3446559,0.0095505182\O,-5.2620002837,-2.163446559,0.0095505182\C,-7.27
 78633936,-0.8395457067,0.010498749\H,-7.6815257235,-1.3353869558,0.905
 5730346\H,-7.6819086919,-1.3352480926,-0.884469404\C,-7.4099016927,0.6
 993756969,0.0107133483\H,-7.9472124599,1.0730391337,-0.8762922428\H,-7
 .9475136759,1.0727962765,0.8976295713\C,7.2778633936,0.8395457067,0.01
 0498749\H,7.6815257235,1.3353869558,0.9055730346\H,7.6819086919,1.3352
 480926,-0.884469404\C,7.4099016927,-0.6993756969,0.0107133483\H,7.9475
 136759,-1.0727962765,0.8976295713\H,7.9472124599,-1.0730391337,-0.8762
 922428\\Version=EM64L-G09RevB.01\State=3-B\HF=-1140.2736957\S2=2.01930
 7\S2-1=0.\S2A=2.000199\RMSD=5.278e-09\RMSF=5.374e-05\Dipole=0.,0.,0.00
 03852\Quadrupole=30.2626957,-16.4833182,-13.7793775,-0.3839259,0.,0.\P
 G=C02 [X(C20H16N4O2)]\\@
```



Mulliken atomic spin densities:					
		1			
1	H	-0.000333	21	H	-0.000333
2	C	-0.006396	22	C	0.005297
3	H	-0.000278	23	C	-0.090078
4	C	0.005297	24	C	-0.090078
5	C	-0.020180	25	N	0.323815
6	C	-0.002965	26	N	0.299833
7	C	0.013771	27	N	0.323815
8	C	0.001536	28	N	0.299833
9	C	-0.002361	29	O	0.458484
10	H	0.000109	30	O	0.458484
11	H	-0.000899	31	C	-0.022441
12	C	0.001536	32	H	0.018926
13	H	0.000109	33	H	0.018909
14	C	-0.020180	34	C	-0.014424
15	C	-0.002965	35	H	0.009846
16	H	-0.000278	36	H	0.009831
17	C	-0.002361	37	C	-0.022441
18	C	0.013771	38	H	0.018926
19	H	-0.000899	39	H	0.018909
20	C	-0.006396	40	C	-0.014424
			41	H	0.009831
			42	H	0.009846

```
A26diNN singlet
1\1\GINC-SKYNET\SP\UB97D\6-31G(d)\C20H16N4O4\LAHTI\04-Jan-2015\0\\#P G
 FINPUT IOP(6/7=3) UB97D/6-31G(d) TEST GUESS=(READ,MIX)\\Ant26DiNN trip
 let opt geom\\0,1\H,0,-4.081207,2.506808,0.021676\C,0,-3.324367,1.7283
 07,0.007915\H,0,-1.684794,3.103927,-0.006158\C,0,-1.988311,2.05458,-0.
 000546\C,0,-2.774211,-0.659904,-0.002061\C,0,-0.968684,1.04822,-0.0007
 24\C,0,-3.742389,0.344801,0.008416\C,0,-1.383545,-0.344953,-0.001453\C
 ,0,0.401361,1.357284,-0.002228\H,0,-0.716113,-2.403894,-0.004379\H,0,-
 3.074038,-1.704578,-0.018404\C,0,1.383556,0.34504,-0.001481\H,0,0.7161
 23,2.403981,-0.004632\C,0,2.774222,0.65999,-0.002115\C,0,0.968695,-1.0
 48135,-0.000609\H,0,1.684801,-3.103847,-0.005796\C,0,-0.40135,-1.35719
 7,-0.002086\C,0,3.742385,-0.344725,0.008449\H,0,3.074071,1.704657,-0.0
 18581\C,0,3.324373,-1.728227,0.00811\H,0,4.081222,-2.506723,0.021983\C
 ,0,1.988319,-2.0545,-0.000312\C,0,-5.164386,0.006329,0.005633\C,0,5.16
 4379,-0.006306,0.005655\N,0,-5.692652,-1.210527,-0.353967\N,0,-6.18836
 9,0.853389,0.35542\N,0,5.692724,1.21054,-0.353862\N,0,6.188287,-0.8534
 91,0.355325\O,0,-5.090499,-2.256701,-0.759397\O,0,-6.128988,2.048017,0
 .791321\O,0,6.128772,-2.048179,0.791045\O,0,5.090638,2.256797,-0.75918
 2\C,0,7.184916,1.222103,-0.251235\H,0,7.463796,2.006884,0.465511\H,0,7
 .581142,1.481494,-1.242148\C,0,7.525808,-0.198095,0.210672\H,0,8.10543
 ,-0.780667,-0.518682\H,0,8.022513,-0.248345,1.188771\C,0,-7.184847,-1.
 222199,-0.251401\H,0,-7.463719,-2.007177,0.465129\H,0,-7.581024,-1.481
 352,-1.242398\C,0,-7.525833,0.197859,0.210844\H,0,-8.022388,0.247834,1
 .189036\H,0,-8.105651,0.780512,-0.518287\\Version=EM64L-G09RevB.01\Sta
 te=1-A\HF=-1290.5408354\S2=1.045859\S2-1=0.\S2A=0.365323\RMSD=4.875e-0
 9\Dipole=0.0002006,-0.0000872,-0.0678302\Quadrupole=40.0961607,-22.468
 7236,-17.6274371,11.9910469,0.0010591,-0.001743\PG=C01 [X(C20H16N4O4)]
 \\@
```



Mulliken atomic spin densities:							
		1					
1	H	0.000033		22	C	-0.017902	
2	C	-0.017011		23	C	-0.128065	
3	H	-0.000889		24	C	0.128061	
4	C	0.017898		25	N	0.246820	
5	C	-0.047860		26	N	0.245607	
6	C	-0.016463		27	N	-0.246824	
7	C	0.035835		28	N	-0.245607	
8	C	0.020222		29	O	0.328737	
9	C	0.029305		30	O	0.330159	
10	H	0.001334		31	O	-0.330149	
11	H	0.001356		32	O	-0.328744	
12	C	-0.020224		33	C	0.017335	
13	H	-0.001334		34	H	-0.011339	
14	C	0.047867		35	H	-0.010367	
15	C	0.016465		36	C	0.017332	
16	H	0.000889		37	H	-0.011237	
17	C	-0.029304		38	H	-0.010292	
18	C	-0.035837		39	C	-0.017334	
19	H	-0.001356		40	H	0.011336	
20	C	0.017015		41	H	0.010370	
21	H	-0.000033		42	C	-0.017332	
				43	H	0.010295	
				44	H	0.011234	

A26diNN triplet
1\1\GINC-SKYNET\FOpt\UB97D\6-31G(d)\C20H16N4O4(3)\LAHTI\03-Jan-2015\0\
\#P GFINPUT IOP(6/7=3) UB97D/6-31G(d) TEST OPT\\Ant26DiNN triplet opt\
\0,3\H,4.0742210384,-2.5123164747,0.0267742349\C,3.3195876615,-1.73168
32729,0.0125642756\H,1.6760863451,-3.1026429534,0.0025136905\C,1.98259
95702,-2.0541579786,0.0060854488\C,2.7762302889,0.6580671123,-0.000709
48\C,0.9658453505,-1.0448964119,0.0053716799\C,3.7415514455,-0.3493766
385,0.0103564228\C,1.3846737144,0.3470845733,0.0019210853\C,-0.4050760
921,-1.3500532856,0.0058578179\H,0.7231102744,2.4079134045,-0.00363884
39\H,3.079015335,1.7018536728,-0.0190805812\C,-1.3843803028,-0.3350126
979,0.0060190341\H,-0.7228223499,-2.3958510637,0.0055023204\C,-2.77593
84557,-0.6459961627,0.007407465\C,-0.9655497783,1.0569728126,0.0041691
199\H,-1.6757993096,3.114708183,-0.0035931934\C,0.405368344,1.36212325
3,0.0007025629\C,-3.7412215749,0.361491448,0.0173833106\H,-3.078781843
3,-1.689829395,-0.0070294226\C,-3.3192686539,1.7437933392,0.014334031\
H,-4.0738808324,2.5244669489,0.0277589216\C,-1.982300532,2.0662405876,
0.0039307304\C,5.1645042332,-0.0149659545,0.005478928\C,-5.1641770771,
0.0271254343,0.0166836128\N,5.6958443985,1.1997912525,-0.3566780809\N,
6.1864490813,-0.8643727842,0.3555357327\N,-5.6963790483,-1.1887921332,
-0.3402750081\N,-6.1852849772,0.8777953636,0.3660818405\O,5.0962338399
,2.2470168738,-0.7631604774\O,6.1241381637,-2.0581155882,0.7934480712\
O,-6.1218898633,2.0730161522,0.7997878582\O,-5.0977195932,-2.237420338
7,-0.7445413377\C,-7.1884851809,-1.1959329092,-0.2360114968\H,-7.46881
99813,-1.9787473606,0.4823155193\H,-7.5865287037,-1.4558049633,-1.2260
695114\C,-7.5248245763,0.2259819696,0.2239485843\H,-8.1035785985,0.809
0160828,-0.5057256037\H,-8.0203186229,0.2792405093,1.2025024742\C,7.18
81773675,1.2073746892,-0.2557502261\H,7.4700651954,1.9927196135,0.4591
963695\H,7.5840109309,1.4637836038,-1.2475976151\C,7.5256180323,-0.212
8959318,0.2084407833\H,8.0230932737,-0.2626939956,1.1861737441\H,8.102
9780634,-0.7983865856,-0.5203677915\\Version=EM64L-G09RevB.01\State=3-
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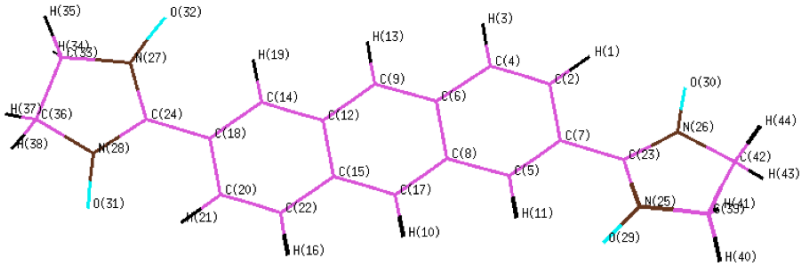
F=4.053e-06\Dipole=-0.0002788,-0.0000218,-0.0678456\Quadrupole=40.1535
881,-22.5334374,-17.6201507,11.8125942,-0.0832063,-0.0031201\PG=C01 [X
(C20H16N4O4)]\\@



Mulliken atomic spin densities:					
		1			
1	H	-0.000347	22	C	0.005403
2	C	-0.007901	23	C	-0.125983
3	H	-0.000294	24	C	-0.125978
4	C	0.005408	25	N	0.245180
5	C	-0.036120	26	N	0.243975
6	C	-0.004130	27	N	0.245183
7	C	0.020910	28	N	0.243974
8	C	0.002217	29	O	0.327006
9	C	-0.007936	30	O	0.328442
10	H	0.000382	31	O	0.328431
11	H	0.000890	32	O	0.327013
12	C	0.002213	33	C	-0.017248
13	H	0.000382	34	H	0.011211
14	C	-0.036119	35	H	0.010273
15	C	-0.004125	36	C	-0.017242
16	H	-0.000293	37	H	0.011110
17	C	-0.007942	38	H	0.010200
18	C	0.020906	39	C	-0.017248
19	H	0.000890	40	H	0.011208
20	C	-0.007896	41	H	0.010276
21	H	-0.000348	42	C	-0.017242
			43	H	0.010203
			44	H	0.011106

```
AQ26diIN singlet
1\1\GINC-SKYNET\SP\UB97D\6-31G(d)\C20H14N4O4\LAHTI\04-Jan-2015\0\\#P G
 FINPUT IOP(6/7=3) UB97D/6-31G(d) TEST GUESS=(READ,MIX)\\AntQ26DiIN tri
 plet opt geom\\0,1\H,0,-2.410601,4.173811,-0.000168\C,0,-1.647,3.39689
 9,-0.000247\H,0,-3.051574,1.746737,-0.000491\C,0,-2.004854,2.050884,-0
 .000435\C,0,0.710664,2.782722,-0.000287\C,0,-1.016205,1.047069,-0.0005
 41\C,0,-0.280518,3.7824,-0.000153\C,0,0.349753,1.422759,-0.000495\C,0,
 -1.437254,-0.391429,-0.000694\H,0,1.765795,3.039789,-0.000217\C,0,-0.3
 49753,-1.422759,-0.000495\C,0,-0.710664,-2.782722,-0.000287\C,0,1.0162
 05,-1.047069,-0.000541\H,0,3.051574,-1.746737,-0.000491\C,0,1.437254,0
 .391429,-0.000694\C,0,0.280518,-3.7824,-0.000153\H,0,-1.765795,-3.0397
 89,-0.000217\C,0,1.647,-3.396899,-0.000247\H,0,2.410601,-4.173811,-0.0
 00168\C,0,2.004854,-2.050884,-0.000435\C,0,0.018618,5.232187,0.000051\
 C,0,-0.018618,-5.232187,0.000051\N,0,1.332592,5.761882,0.000778\N,0,-0
 .915017,6.145717,-0.000357\N,0,-1.332592,-5.761882,0.000778\N,0,0.9150
 17,-6.145717,-0.000357\O,0,2.445273,5.15699,0.001436\O,0,-2.445273,-5.
 15699,0.001436\C,0,-1.247621,-7.253098,0.00068\H,0,-1.767392,-7.624152
 ,-0.894385\H,0,-1.766913,-7.624258,0.895971\C,0,0.280518,-7.476469,0.0
 0021\H,0,0.62385,-8.033012,0.887152\H,0,0.623267,-8.033552,-0.88661\C,
 0,1.247621,7.253098,0.00068\H,0,1.767392,7.624152,-0.894385\H,0,1.7669
 13,7.624258,0.895971\C,0,-0.280518,7.476469,0.00021\H,0,-0.623267,8.03
 3552,-0.88661\H,0,-0.62385,8.033012,0.887152\O,0,2.630178,0.708409,-0.
 000527\O,0,-2.630178,-0.708409,-0.000527\\Version=EM64L-G09RevB.01\HF=
 -1289.4329079\S2=1.021217\S2-1=0.\S2A=0.170161\RMSD=4.947e-09\Dipole=-
 0.0000018,0.000002,-0.0000233\Quadrupole=-30.2598313,43.7106069,-13.4507
 756,-2.1636427,0.,0.\PG=C02 [X(C20H14N4O4)]\\@
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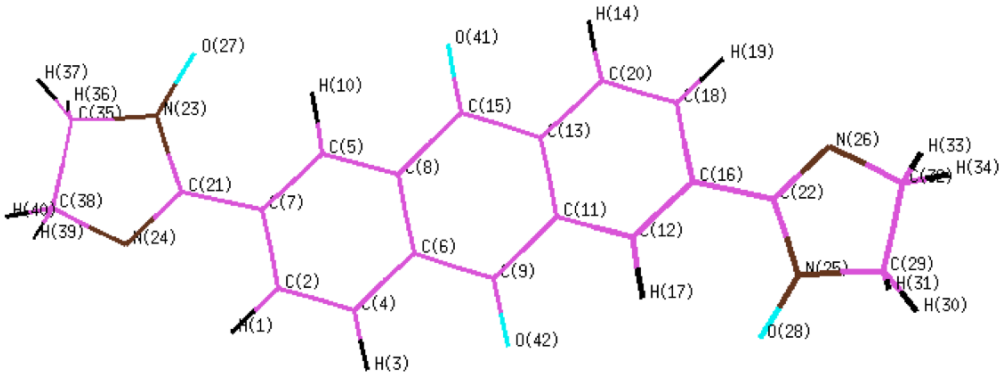

Mulliken atomic spin densities:

		1
1	H	-0.000161
2	C	-0.011437
3	H	-0.000246
4	C	0.005618
5	C	-0.016543
6	C	-0.010841
7	C	0.016545
8	C	0.007305
9	C	0.001685
10	H	-0.000885
11	C	-0.007305
12	C	0.016543
13	C	0.010841
14	H	0.000246
15	C	-0.001685
16	C	-0.016545
17	H	0.000885
18	C	0.011437
19	H	0.000161
20	C	-0.005618
21	C	-0.092236
22	C	0.092235
23	N	0.305992
24	N	0.320285
25	N	-0.305993
26	N	-0.320283
27	O	0.457665
28	O	-0.457665
29	C	0.021567
30	H	-0.017938
31	H	-0.017924
32	C	0.015181
33	H	-0.010686
34	H	-0.010671
35	C	-0.021567
36	H	0.017938
37	H	0.017924
38	C	-0.015181
39	H	0.010671
40	H	0.010686
41	O	0.004002
42	O	-0.004002

```
AQ26diIN triplet
1\1\GINC-SKYNET\FOpt\UB97D\6-31G(d)\C20H14N4O4(3)\LAHTI\03-Jan-2015\0\
 \#P GFINPUT IOP(6/7=3) UB97D/6-31G(d) TEST OPT\\AntQ26DiIN triplet opt
 \\0,3\H,4.0105981196,-2.6733496116,0.0095350168\C,3.2842633994,-1.8614
 896575,0.009614864\H,1.5474092944,-3.1573280312,0.0098583851\C,1.91806
 68559,-2.1322718134,0.0098024138\C,2.8225745173,0.5307138508,0.0096541
 729\C,0.9797320677,-1.0812722145,0.0099088068\C,3.7566185065,-0.522547
 38,0.0095203713\C,1.4422627142,0.2577758278,0.009862101\C,-0.482809737
 5,-1.4091875809,0.0100612786\H,3.1467897487,1.5671837313,0.0095847717\
 C,-1.4422627142,-0.2577758278,0.009862101\C,-2.8225745173,-0.530713850
 8,0.0096541729\C,-0.9797320677,1.0812722145,0.0099088068\H,-1.54740929
 44,3.1573280312,0.0098583851\C,0.4828097375,1.4091875809,0.0100612786\
 C,-3.7566185065,0.52254738,0.0095203713\H,-3.1467897487,-1.5671837313,
 0.0095847717\C,-3.2842633994,1.8614896575,0.009614864\H,-4.0105981196,
 2.6733496116,0.0095350168\C,-1.9180668559,2.1322718134,0.0098024138\C,
 5.2226073491,-0.3170182801,0.0093163531\C,-5.2226073491,0.3170182801,0
 .0093163531\N,5.8354915416,0.9602740844,0.0085898626\N,6.0743722573,-1
 .3073260836,0.0097247459\N,-5.8354915416,-0.9602740844,0.0085898626\N,
 -6.0743722573,1.3073260836,0.0097247459\O,5.3032132584,2.1094625411,0.
 0079310891\O,-5.3032132584,-2.1094625411,0.0079310891\C,-7.3181870107,
 -0.7798306339,0.0086873739\H,-7.7218150093,-1.2747309106,0.9037524728\
 H,-7.7218902989,-1.2742460066,-0.8866037544\C,-7.4430813378,0.75948907
 41,0.0091571879\H,-7.9764564162,1.1378115716,-0.8777851069\H,-7.977032
 1906,1.1372642887,0.8959770126\C,7.3181870107,0.7798306339,0.008687373
 9\H,7.7218150093,1.2747309106,0.9037524728\H,7.7218902989,1.2742460066
 ,-0.8866037544\C,7.4430813378,-0.7594890741,0.0091571879\H,7.977032190
 6,-1.1372642887,0.8959770126\H,7.9764564162,-1.1378115716,-0.877785106
 9\O,0.8756532017,2.5793240143,0.0098945816\O,-0.8756532017,-2.57932401
 43,0.0098945816\\Version=EM64L-G09RevB.01\State=3-B\HF=-1289.4329069\S
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 .,0.,0.0000225\Quadrupole=43.1290927,-29.6786546,-13.4504381,-6.881128
 6,0.,0.\PG=C02 [X(C20H14N4O4)]\\@
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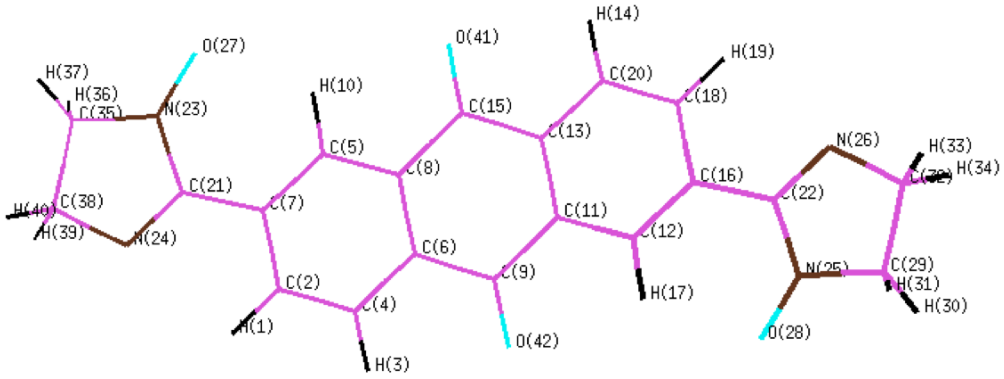
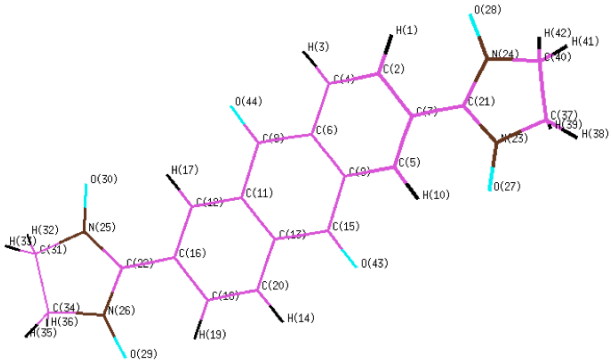


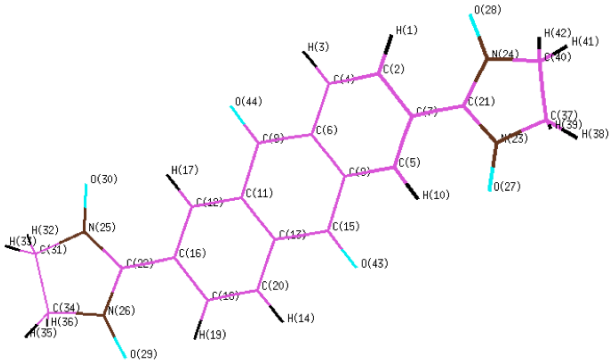
Mulliken atomic spin densities:					
1	H	-0.000142	21	C	-0.092206
2	C	-0.011832	22	C	-0.092206
3	H	-0.000256	23	N	0.306006
4	C	0.005739	24	N	0.320209
5	C	-0.016793	25	N	0.306006
6	C	-0.011047	26	N	0.320209
7	C	0.016505	27	O	0.457686
8	C	0.007189	28	O	0.457686
9	C	0.000296	29	C	-0.021567
10	H	-0.000863	30	H	0.017939
11	C	0.007189	31	H	0.017925
12	C	-0.016793	32	C	-0.015176
13	C	-0.011047	33	H	0.010682
14	H	-0.000256	34	H	0.010668
15	C	0.000296	35	C	-0.021567
16	C	0.016505	36	H	0.017939
17	H	-0.000863	37	H	0.017925
18	C	-0.011832	38	C	-0.015176
19	H	-0.000142	39	H	0.010668
20	C	0.005739	40	H	0.010682
			41	O	-0.000961
			42	O	-0.000961

```
AQ26diNN singlet
1\1\GINC-SKYNET\SP\UB97D\6-31G(d)\C20H14N4O6\LAHTI\04-Jan-2015\0\\#P G
 FINPUT IOP(6/7=3) UB97D/6-31G(d) TEST GUESS=(READ,MIX)\\AntQ26DiNN tri
 plet opt\\0,1\H,0,-2.532415,4.099994,-0.036699\C,0,-1.742093,3.354878,
 -0.016318\H,0,-3.096049,1.666154,-0.022249\C,0,-2.057319,1.996544,-0.0
 16575\C,0,0.635058,2.795923,0.011939\C,0,-1.045305,1.018612,-0.011042\
 C,0,-0.384201,3.774175,0.002735\C,0,0.312001,1.43036,-0.002543\C,0,-1.
 428323,-0.429139,-0.015048\H,0,1.683109,3.080859,0.033069\C,0,-0.31200
 1,-1.43036,-0.002543\C,0,-0.635058,-2.795923,0.011939\C,0,1.045305,-1.
 018612,-0.011042\H,0,3.096049,-1.666154,-0.022249\C,0,1.428323,0.42913
 9,-0.015048\C,0,0.384201,-3.774175,0.002735\H,0,-1.683109,-3.080859,0.
 033069\C,0,1.742093,-3.354878,-0.016318\H,0,2.532415,-4.099994,-0.0366
 99\C,0,2.057319,-1.996544,-0.016575\C,0,-0.04672,5.197384,0.007852\C,0
 ,0.04672,-5.197384,0.007852\N,0,1.152531,5.726469,0.416851\N,0,-0.8792
 61,6.211361,-0.395595\N,0,-1.152531,-5.726469,0.416851\N,0,0.879261,-6
 .211361,-0.395595\O,0,2.165176,5.127887,0.895324\O,0,-2.057319,6.13678
 1,-0.868902\O,0,2.057319,-6.136781,-0.868902\O,0,-2.165176,-5.127887,0
 .895324\C,0,-1.169898,-7.218988,0.286169\H,0,-1.996798,-7.483194,-0.38
 6713\H,0,-1.368675,-7.632531,1.283807\C,0,0.220686,-7.550508,-0.26728\
 H,0,0.838726,-8.161423,0.404493\H,0,0.211459,-8.007728,-1.26569\C,0,1.
 169898,7.218988,0.286169\H,0,1.996798,7.483194,-0.386713\H,0,1.368675,
 7.632531,1.283807\C,0,-0.220686,7.550508,-0.26728\H,0,-0.211459,8.0077
 28,-1.26569\H,0,-0.838726,8.161423,0.404493\O,0,2.611803,0.779662,-0.0
 3119\O,0,-2.611803,-0.779662,-0.03119\\Version=EM64L-G09RevB.01\HF=-14
 39.7017147\S2=1.041509\S2-1=0.\S2A=0.331666\RMSD=7.872e-09\Dipole=-0.0
 00018,-0.0000042,0.0445197\Quadrupole=-35.7063852,53.9691747,-18.26278
 95,6.7340162,-0.000006,-0.0000455\PG=C02 [X(C20H14N4O6)]\\@
```



Mulliken atomic spin densities:					
		1			
1	H	0.000389	22	C	0.129023
2	C	-0.021948	23	N	0.241261
3	H	-0.000442	24	N	0.244350
4	C	0.010541	25	N	-0.241260
5	C	-0.022932	26	N	-0.244350
6	C	-0.022325	27	O	0.334408
7	C	0.024434	28	O	0.328201
8	C	0.010009	29	O	-0.328201
9	C	0.002352	30	O	-0.334408
10	H	0.000320	31	C	0.017167
11	C	-0.010008	32	H	-0.010742
12	C	0.022930	33	H	-0.010476
13	C	0.022324	34	C	0.017246
14	H	0.000442	35	H	-0.010810
15	C	-0.002351	36	H	-0.010559
16	C	-0.024433	37	C	-0.017167
17	H	-0.000320	38	H	0.010742
18	C	0.021947	39	H	0.010476
19	H	-0.000389	40	C	-0.017246
20	C	-0.010540	41	H	0.010559
21	C	-0.129025	42	H	0.010810
			43	O	0.008331
			44	O	-0.008332

AQ26diNN triplet
1\1\GINC-SKYNET\FOpt\UB97D\6-31G(d)\C20H14N4O6(3)\LAHTI\03-Jan-2015\0\
\#P GFINPUT IOP(6/7=3) UB97D/6-31G(d) TEST OPT\\AntQ26DiNN triplet opt
\\0,3\H,4.0982826132,-2.5351835867,0.0316732705\C,3.3537005538,-1.7443
587077,0.0112923586\H,1.6640621584,-3.097173355,0.0172236235\C,1.99515
40828,-2.0586668002,0.0115493067\C,2.7963516604,0.633169606,-0.0169641
828\C,1.0179052334,-1.0459929309,0.0060164467\C,3.773914956,-0.3867499
34,-0.0077603269\C,1.4305699717,0.3110351539,-0.0024820915\C,-0.430103
5879,-1.4280325361,0.0100229881\H,3.0819954911,1.6810276807,-0.0380943
362\C,-1.4305699717,-0.3110351539,-0.0024820915\C,-2.7963516604,-0.633
169606,-0.0169641828\C,-1.0179052334,1.0459929309,0.0060164467\H,-1.66
40621584,3.097173355,0.0172236235\C,0.4301035879,1.4280325361,0.010022
9881\C,-3.773914956,0.386749934,-0.0077603269\H,-3.0819954911,-1.68102
76807,-0.0380943362\C,-3.3537005538,1.7443587077,0.0112923586\H,-4.098
2826132,2.5351835867,0.0316732705\C,-1.9951540828,2.0586668002,0.01154
93067\C,5.1973508805,-0.0502311324,-0.0128777486\C,-5.1973508805,0.050
2311324,-0.0128777486\N,5.7272458192,1.148662376,-0.4218760292\N,6.210
7658766,-0.883456711,0.3905697609\N,-5.7272458192,-1.148662376,-0.4218
760292\N,-6.2107658766,0.883456711,0.3905697609\O,5.1293485418,2.16171
20706,-0.9003498033\O,6.1353901287,-2.0614635025,0.8638769549\O,-6.135
3901287,2.0614635025,0.8638769549\O,-5.1293485418,-2.1617120706,-0.900
3498033\C,-7.2197761259,-1.1650214048,-0.2911946621\H,-7.4845407804,-1
.9917429843,0.3816879\H,-7.6334538311,-1.3635190118,-1.2888326393\C,-7
.550356836,0.2257859642,0.2622541317\H,-8.1608542285,0.8442383228,-0.4
09518756\H,-8.0075830815,0.2168685404,1.2606642698\C,7.2197761259,1.16
50214048,-0.2911946621\H,7.4845407804,1.9917429843,0.3816879\H,7.63345
38311,1.3635190118,-1.2888326393\C,7.550356836,-0.2257859642,0.2622541
317\H,8.0075830815,-0.2168685404,1.2606642698\H,8.1608542285,-0.844238
3228,-0.409518756\O,0.7814260077,2.6112760993,0.0261645645\O,-0.781426
0077,-2.6112760993,0.0261645645\\Version=EM64L-G09RevB.01\State=3-B\HF
=-1439.7017173\S2=2.041762\S2-1=0.\S2A=2.00081\RMSD=9.625e-09\RMSF=2.6
29e-05\Dipole=0.,0.,-0.0445058\Quadrupole=53.9852325,-35.7197827,-18.2
654498,6.6733744,0.,0.\PG=C02 [X(C20H14N4O6)]\\@



Mulliken atomic spin densities:					
		1			
1	H	0.000436	22	C	-0.129039
2	C	-0.022958	23	N	0.241282
3	H	-0.000468	24	N	0.244348
4	C	0.011041	25	N	0.241282
5	C	-0.023838	26	N	0.244348
6	C	-0.023039	27	O	0.334461
7	C	0.024801	28	O	0.328267
8	C	0.010414	29	O	0.328267
9	C	0.000949	30	O	0.334461
10	H	0.000389	31	C	-0.017171
11	C	0.010414	32	H	0.010745
12	C	-0.023838	33	H	0.010478
13	C	-0.023039	34	C	-0.017245
14	H	-0.000468	35	H	0.010810
15	C	0.000949	36	H	0.010560
16	C	0.024801	37	C	-0.017171
17	H	0.000389	38	H	0.010745
18	C	-0.022958	39	H	0.010478
19	H	0.000436	40	C	-0.017245
20	C	0.011041	41	H	0.010560
21	C	-0.129039	42	H	0.010810
			43	O	-0.005224
			44	O	-0.005224