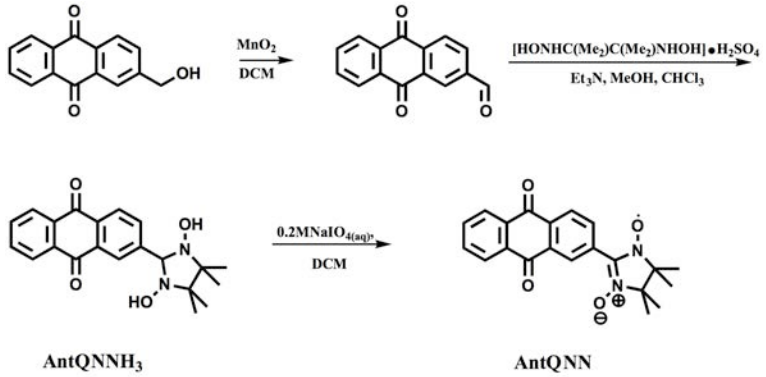
Supporting Material for

2-(9,10-Anthraquinon-2-yl)-4,4,5,5-tetramethyl-4,5-dihydro-1*H*-imidazole-3-oxide-1-oxyl: polymorphism in a conjugated anthraquinone-substituted nitronylnitroxide

Handan Akpinar,[a] John A. Schlueter[b] and Paul M. Lahti[a,]*

[a] *Department of Chemistry, University of Massachusetts, Amherst, Massachusetts 01003, United States; E-mail: lahti@chem.umass.edu*
[b] *Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, United States; E-mail: jaschlueter@anl.gov*

Synthesis:



2,3-Bis(hydroxylamino)-2,3-dimethylbutane hydrogen sulfate. This compound as prepared from 2-nitropropane according to the procedure of Ovcharenko, V.; Fokin, S.; Rey, P. *Mol. Cryst. Liq. Cryst. Sect. A* **1999**, *334*, 109.

9,10-Anthraquinone-2-carbaldehyde. 2-(Hydroxymethyl)anthracene-9,10-dione (Aldrich; 0.530 g, 2.22 mmol) was dissolved in 125 mL of dichloromethane. Manganese(IV) oxide (1.161 g, 13.35 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 0.516 g (98%) of 9,10-anthraquinone-2-carbaldehyde as yellow powder. Mp: 188-191 °C. FTIR (cm^{-1}): 1689, 1673, 1581. ^1H NMR (400 MHz, DMSO-d_6): δ 10.12 (s, 1H), 8.56 (s, 1H), 8.27-8.23 (m, 2H), 8.13-8.12 (m, 2H), 7.85-7.84 (m, 2H).

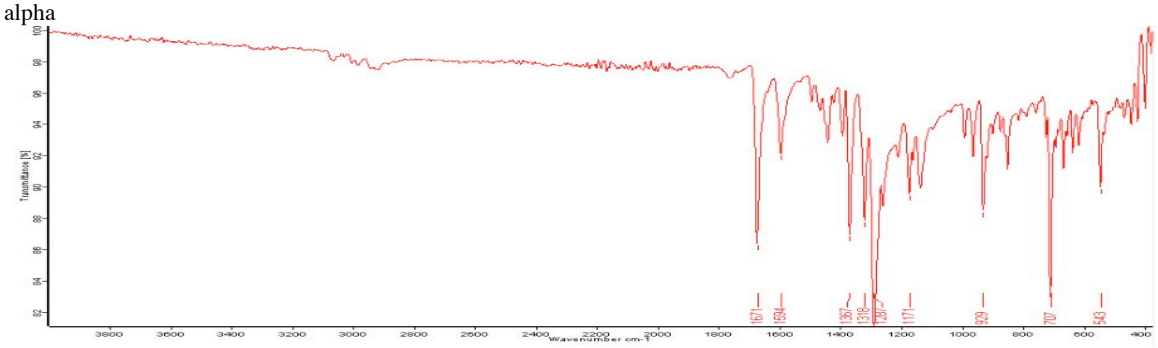
2-(9,10-Anthraquinon-2-yl)-4,4,5,5-tetramethyl-4,5-dihydro-*1H*-imidazole-3-oxide-1-oxyl (AntQNN). Bis(hydroxylamino)-2,3-dimethylbutane hydrogen sulfate (0.522 g, 2.12 mmol) and 9,10-anthraquinone-2-carbaldehyde (0.5 g, 2.12 mmol) were dissolved in 50 mL of methanol and 30 mL of chloroform. Triethylamine (0.214 g, 2.12 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 (**AntQmNNH3**) was dissolved in 150 mL of dichloromethane. The mixture was allowed to stir under nitrogen at 0-3 °C in an ice-bath for 15 min. To this mixture was added 0.2 M $NaIO_4$ (0.453 g, 2.12 mmol in 10.55 mL of H_2O). 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 **AntQmNN** (0.269 g, 35%), which could be recrystallized to either brown plates (alpha phase, FTIR (cm^{-1}): 1674, 1591) or black to brown-black clusters of needles (beta phase, FTIR (cm^{-1}): 1671, 1594) from dichloromethane/acetonitrile. Mp: 207-209 °C. UV-vis (λ_{max},[$\varepsilon = M^{-1}\ cm^{-1}$]): hexane 630 nm [300], toluene 632 nm [130] acetonitrile 610 nm [100]. EPR (9.647 GHz, dichloromethane): g = 2.0071, a_N = 7.04 gauss (2 N). MS (FAB): found m/z = 363.1, calculated for $C_{21}H_{19}N_2O_4$ m/z = 363.1.

Isolating AntQNN polymorphs. AntQNN was dissolved in a solvent mixture of acetonitrile/DCM, and allowed to evaporate at room temperature. Sometimes the alpha phase was obtained, and sometimes the beta phase, but no case was observed of forming a mixture of the two phases. The alpha phase forms brown prisms that are readily distinguished from the beta phase, which forms needles that are essentially black to the naked eye under lab lighting.

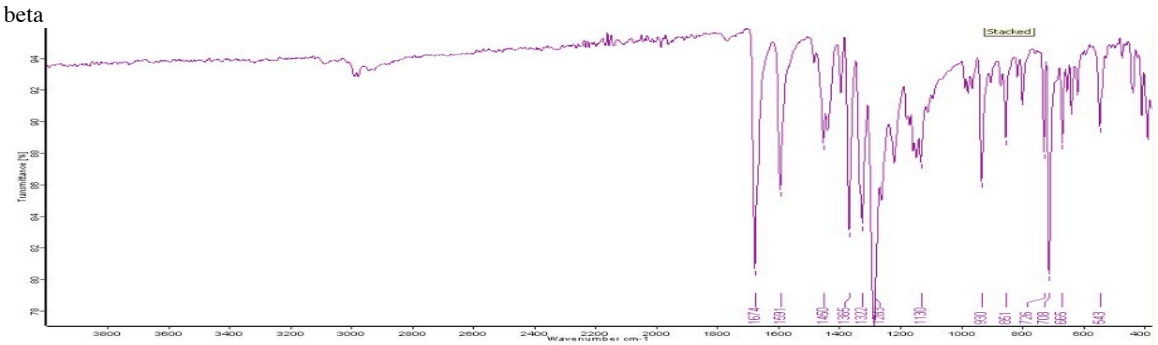
Figure S1. ATR FT-IR spectra for neat α-AntQNN and β-AntQNN.

FULL SCALE (4000 - 400 cm^{-1})

alpha



beta



FINGERPRINT REGION (400-2000 cm^{-1})

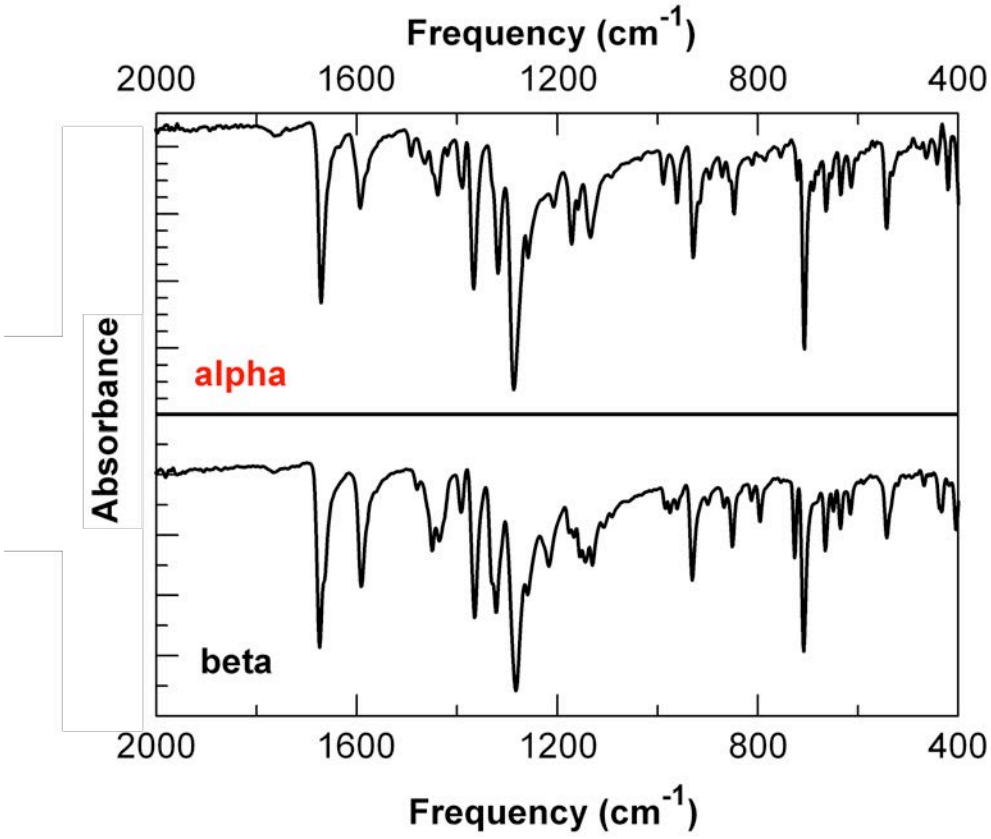


Figure S2. Plane-to-plane distance in angstroms for anthraquinone π-stacked dyads in α-AntQNN (upper), with a view of slip stacked pairs of anthraquinone π-stacked dyads (lower).

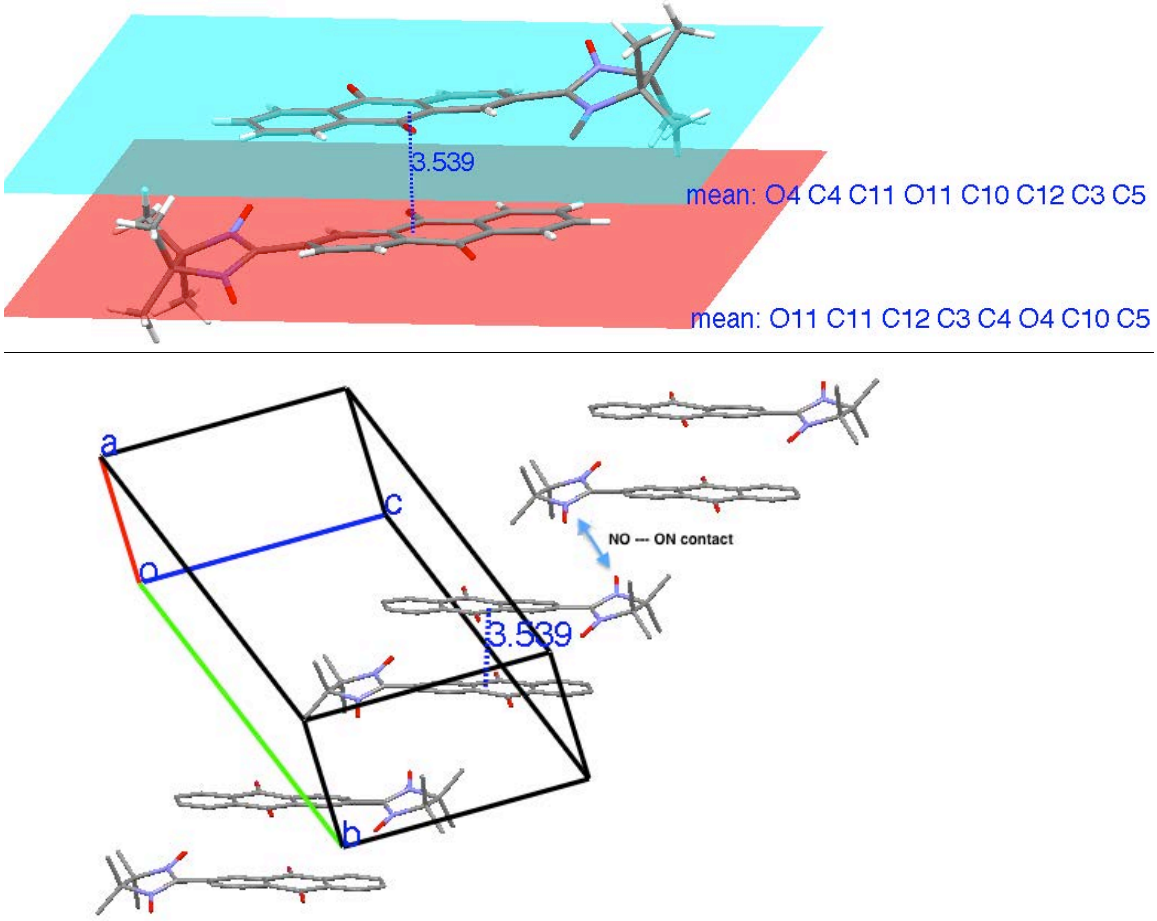


Figure S3. Plane-to-plane distance in angstroms for end-ring-only anthraquinone π-stacking in β-AntQNN.

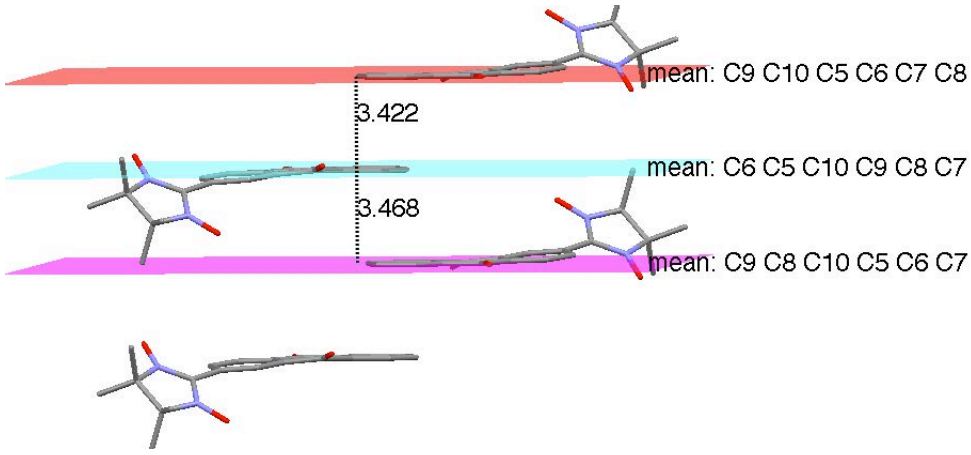
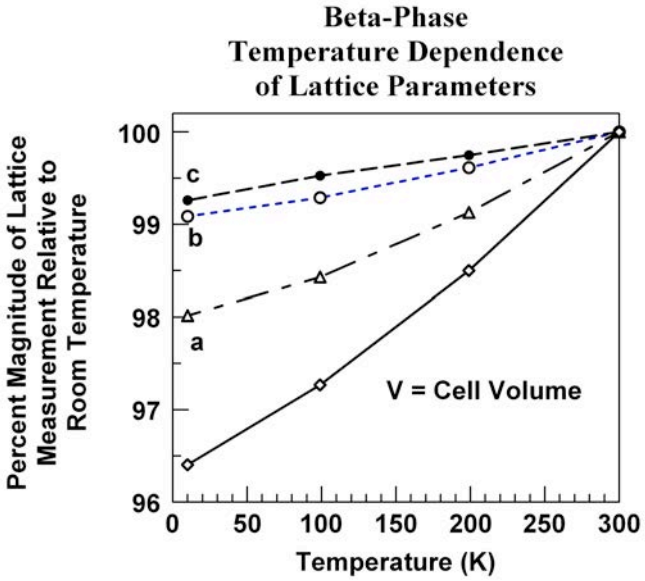
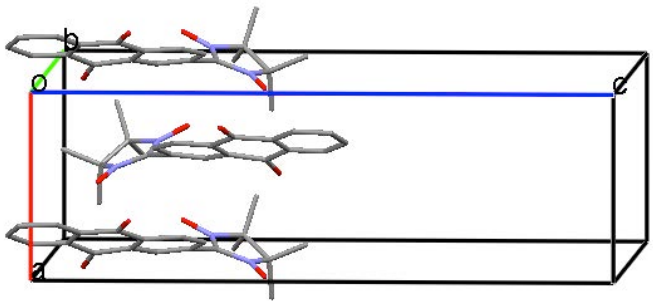


Figure S6. β-AntQNN crystallographic lattice parameter dependence on temperature.

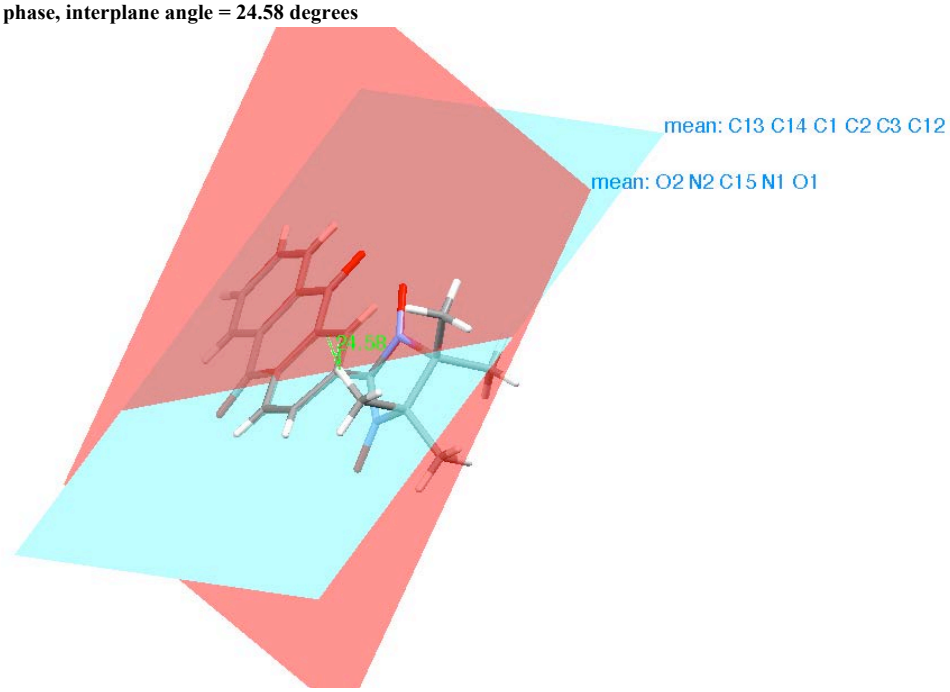




a-axis is the direction of propagation of the NO···ON close-contact chains in β-AntQNN

Figure S5. Inter-ring plane-plane torsions in α-AntQNN and β-AntQNN. The O-N-C-N-O atoms were used in the NN units for plane generation, and all of the benzene carbon atoms in the ring attached to the NN, for both structures.

Alpha phase, interplane angle = 24.58 degrees



Beta phase 300 K, interplane angle = 38.31 degrees

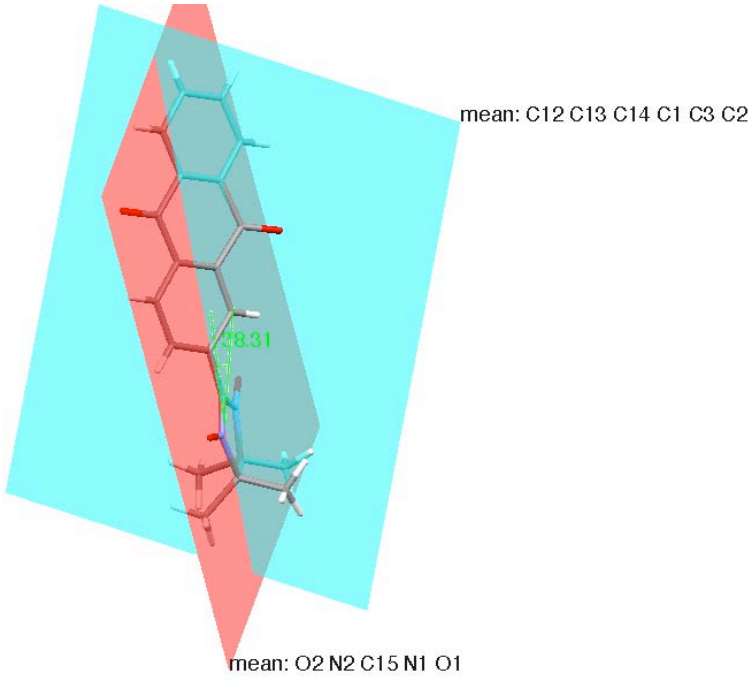


Figure S6. Solution UV-vis absorbance spectra for AntQNN (with digital curve smoothing

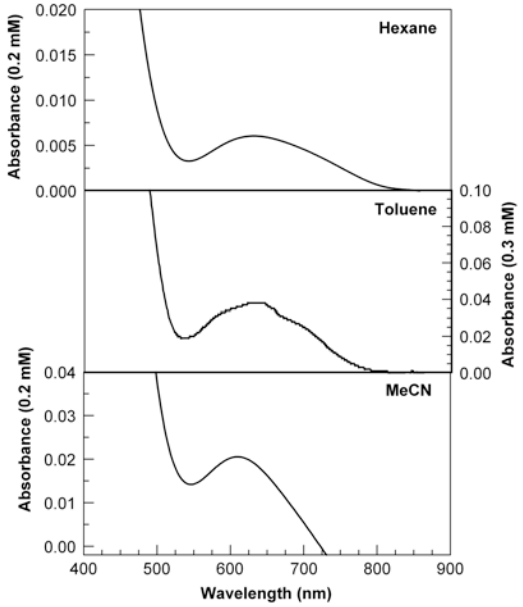
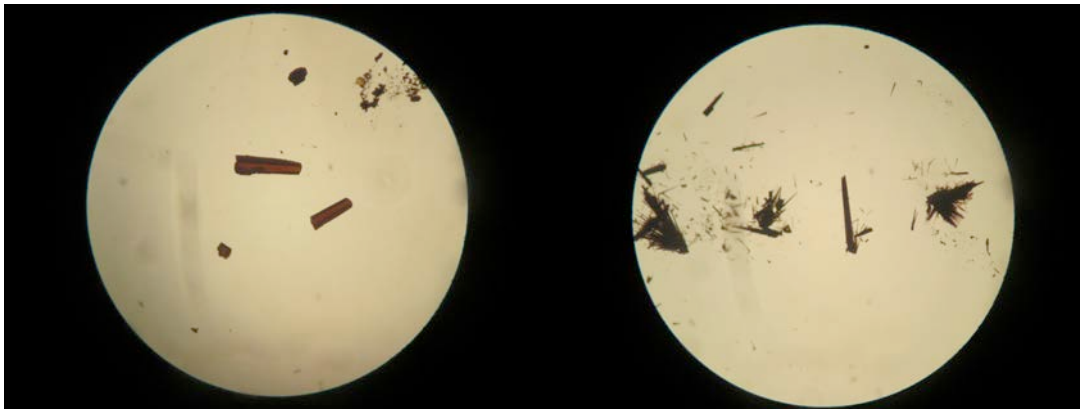


Figure S7. Visual comparison of solid samples of α-AntQNN and β-AntQNN.



alpha phase beta phase

Both pictures were taken at same magnification on a glass slide, with the "underside" white light lighting. Samples of β-AntQNN almost never show brown-transparent crystals, even with the crystals are visually small and thin. α-AntQNN appears dark cocoa brown under fluorescent lab light, and freqently forms brown translucent crystals on the side of a vial: these often form sheets of multiple side-by-side prisms, rather like a row of pre-use staples. β-AntQNN forms deep-colored, brown-black, sea-urchin like clusters of needles that typically taper to a point (where the tip does not break off).

Figure S8. ORTEP diagram for α-phase AntQNN at 293 K. Thermal ellipsoids shown for 50% probability.

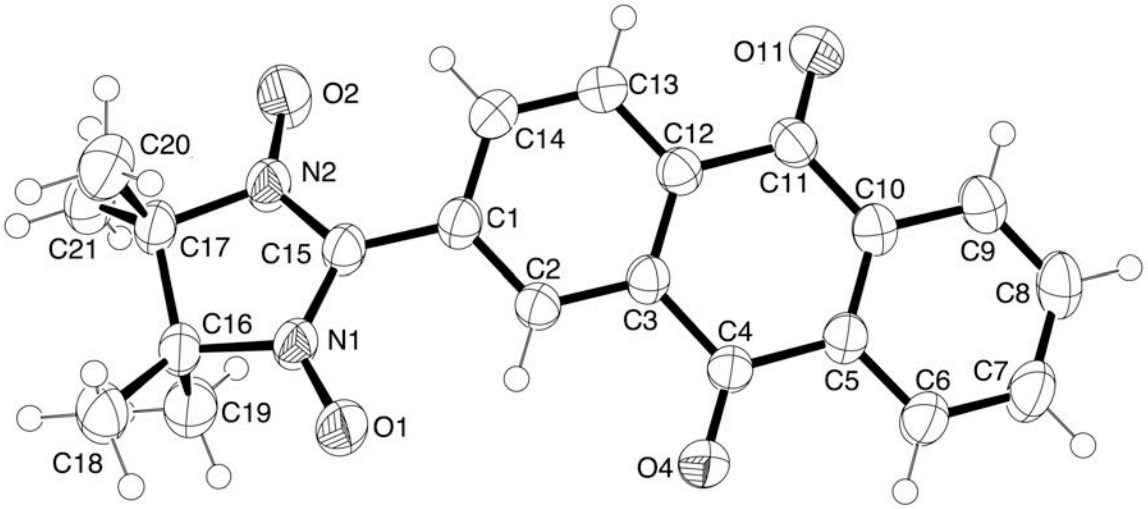


Figure S9. ORTEP diagram for β-phase AntQNN at 300 K. Thermal ellipsoids shown for 50% probability.

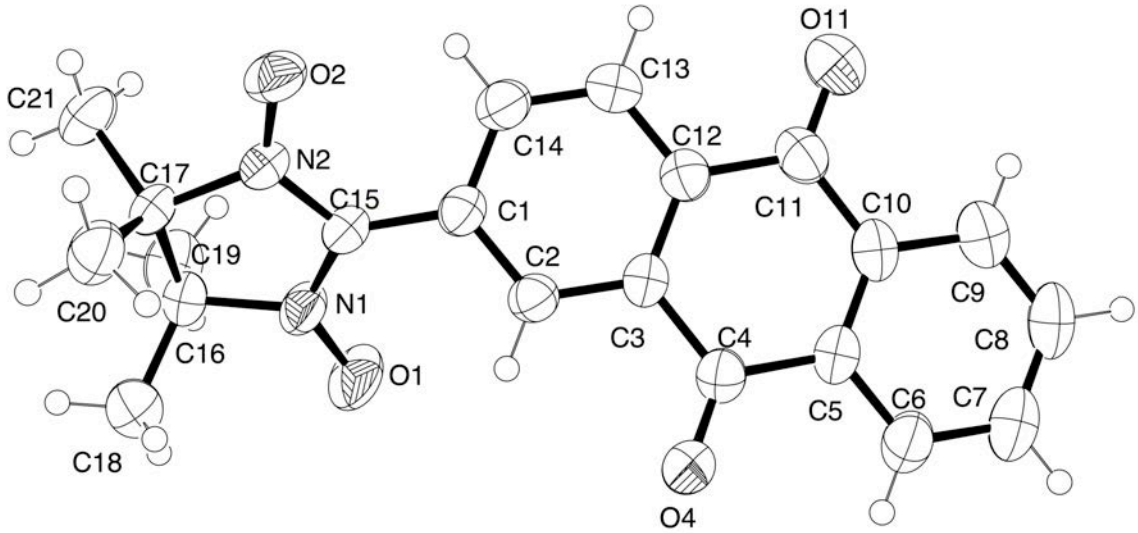
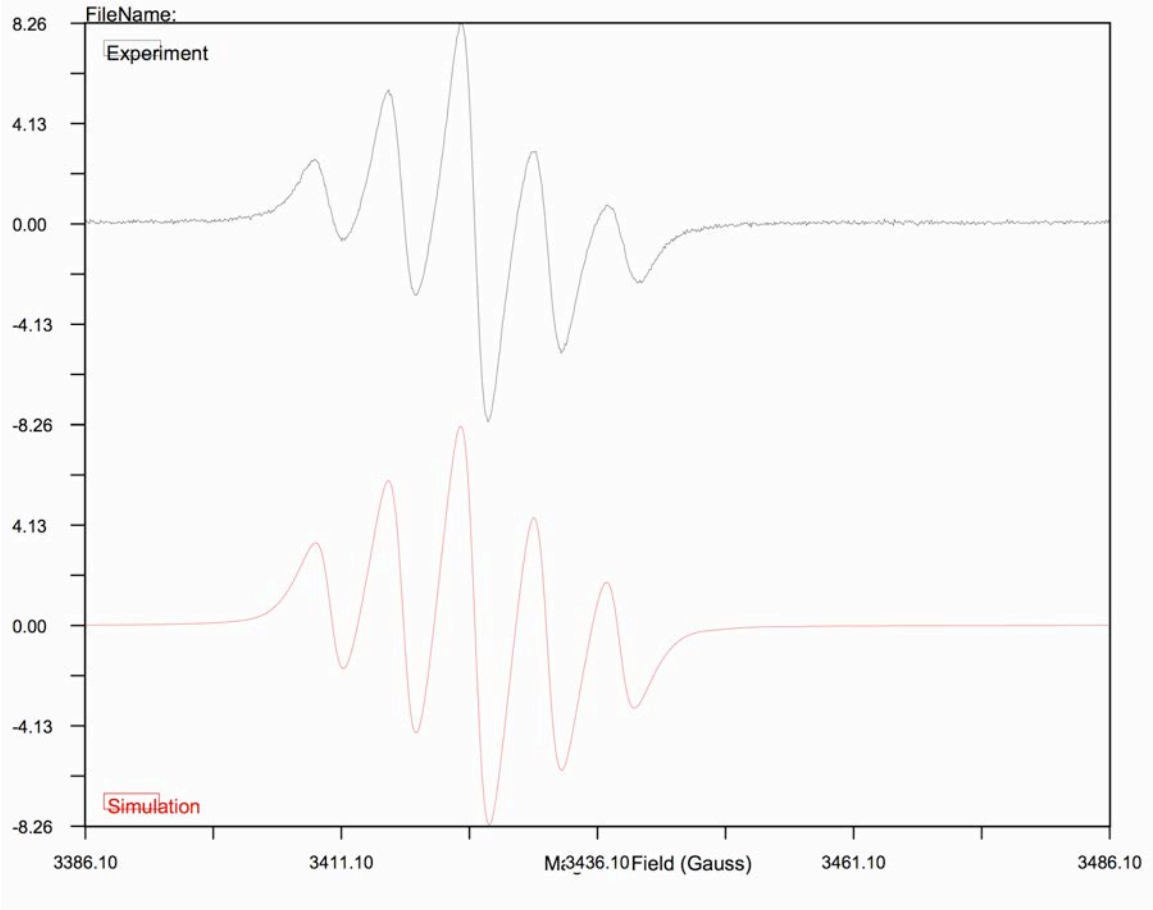


Figure S10. EPR spectrum of AntQNN, room temperature.

SPECTRUM Of **AntQNN**, 9.617 GHz, toluene, below, black trace. Red trace from WINSIM simulator (D. R. Duling, *J. Magn. Res.*, 1994, **B104**, 105-110), a(N) = 7.038 G (2N), correlation coefficient = 0.987.



Beta-Phase Single Crystal X-ray Diffraction. A black needle-like crystal of the β-phase with dimension 0.50 x 0.10 x 0.05 mm^3 was placed onto the tip of glass fiber and mounted on a Bruker APEX II 3-circle diffractometer equipped with an APEX II detector. Full data sets were collected at 300(2), 200(2), 100(2), and 10(2) K. The crystal temperature was maintained through use of an Oxford Cryostream 700 Plus low temperature device for temperatures down to 100 K and a model HFC-1645-LHE Cryocool-LHE (Cryo Industries of America) for the 10 K data collection. The data collection was carried out using MoKa radiation (l = 0.71073 Å) with a frame exposure time of 30 seconds and a detector distance of 5.00 cm. Three major sections of frames were collected with 0.30º w scans. Data to a resolution of 0.90 (300 K), 0.85 (200 K), 0.80 (100 K), 0.75 (10 K) Å were considered in the reduction. The resolution was limited by the weakly diffracting crystal. The raw intensity data were corrected for absorption (SADABS[1]). The structure was solved and refined using SHELXTL.* A direct-method solution was calculated, which provided most atomic positions from the E-map. Full-matrix least squares/difference Fourier cycles were performed, which located the remaining atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. Positions of aromatic H atoms were calculated by employing a "riding" model.

In order to search for possible symmetry lowering, a 20 μm crystal was mounted at the 15ID ChemMatCARS beamline of the Advanced Photon Source, Argonne National Laboratory. A complete data set was collected at 10 K with a Bruker 6000 CCD detector. No symmetry lowering was observed.

*. G. M. Sheldrick, Bruker AXS, Inc., Madison, WI, USA, 2001.

Crystallographic figures in this article were generated using the following programs:

Mercury: C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek and P. A. Wood, *J. Appl. Cryst*., 2008, **41**, 466-470. C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler and J. van de Streek, *J. Appl. Cryst.,* 2006, **39**, 453-457. Cf. www.ccdc.cam.ac.uk/products/mercury.

ORTEP-3 for Windows: L. J. Farrugia, *J. Appl. Cryst*., 1997, **30**, 565.

Table S1. Crystallographic data and structure refinement for **AntQNN** polymorphs.

	α-phase	β-phase	β-phase	β-phase	β-phase
CCDC Deposition Nr.	923571	923567	923568	923569	923570
Temperature	293 K	300 K	199 K	100 K	10 K
Chemical formula	$C_{21}H_{19}N_2O_4$	$C_{21}H_{19}N_2O_4$	$C_{21}H_{19}N_2O_4$	$C_{21}H_{19}N_2O_4$	$C_{21}H_{19}N_2O_4$
Chemical formula weight	363.38	363.38	363.38	363.38	363.38
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system, space group	Monoclinic, *P2₁/c*	Orthorhombic, *Pbca*	Orthorhombic, *Pbca*	Monoclinic, *Pbca*	Monoclinic, *Pbca*
a, b, c (angstroms)	8.2851(17) 18.895(4) 11.832(2)	7.3230(5) 21.4026(17) 22.3514(17)	7.2592(5) 21.3199(14) 22.2954(15)	7.2081(4) 21.2504(13) 22.2459(13)	7.1778(4) 21.2070(12) 22.1861(12)
α, β, γ (degrees)	90.0 107.70(3) 90.0	90.0 90.0 90.0	90.0 90.0 90.0	90.0 90.0 90.0	90.0 90.0 90.0
V(Å^3)	1764.6(6)	3503.2(5)	3450.6(4)	3407.5(3)	3377.2(3)
Z	4	8	8	8	8
D_{calc} (Mg/m^3)	1.368	1.378	1.399	1.417	1.429
F(000)	764	1528	1528	1528	1528
μ (mm^{-1})	0.096	0.096	0.098	0.099	0.100
R_{int}	0.017	0.067	0.068	0.070	0.092
Completeness to 2θ	0.992 (2θ = 55.04°)	1.000 (2θ = 46.64°)	0.998 (2θ = 49.62°)	0.999 (2θ = 52.80°)	0.998 (2θ = 56.48°)
N_{ref}, Parameters	3031, 244	2534, 245	2974, 245	3482, 245	4209, 244
Goodness of fit on F^2	0.822	1.025	1.016	1.031	1.031
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e-Å^{-3})	0.397, -0.423	0.173, -0.177	0.215, -0.225	0.317, -0.280	0.437, -0.292
R_1, wR_2 ($I > 2\sigma(I)$)	0.0533, 0.1644 (3031)	0.0436, 0.1126 (1812)	0.0431, 0.1099 (2176)	0.0430, 0.1086 (2568)	0.0483, 0.1118 (3007)
R_1, wR_2 (all)	0.0740 , 0.1951 (4036)	0.0690, 0.1309 (2534)	0.0673, 0.1258 (2974)	0.0665, 0.1232 (3482)	0.0771, 0.1275 (4209)

Equations used for magnetic analyses.

Spin-Pairing

Spin-Pairing of two S = 1/2 systems (Bleaney-Bowers model, SP)
Derived from Bleaney, B.; Bowers, K. D. *Proc. R. Soc. London A*, **1952**, *214*, 451-465.

$$\chi = \frac{2Ng^2\beta^2}{3kT}\frac{3}{3+\exp\left(-2J/kT\right)} = \frac{2Ng^2\beta^2}{3kT}\frac{1}{3+\exp\left(-2J/kT\right)} = 0.375\left(\frac{g^2}{T}\right)\cdot\frac{2}{3+\exp\left(-2J/kT\right)}$$

$$H = -2J_{SP}\cdot S_1S_2$$

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

$$H = -2J\sum_{N=1}^{\infty} S_1S_{1+N}$$

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

$$\chi = \frac{Ng^2\beta^2}{kT-\theta}\cdot\frac{A+B\cdot\left(J/kT\right)+C\cdot\left(J/kT\right)^2}{1+D\cdot\left(J/kT\right)+E\cdot\left(J/kT\right)^2 F\cdot\left(J/kT\right)^3}\cdot(1-P)+P\cdot\frac{0.375}{T}$$

A = 0.25, B = 0.14995, C = 0.30094, D = 1.9862, E = 0.68854 and F = 6.0626

The fitted parameters were P, J/k, θ.

P was not used for the α-phase. θ was not used for β-phase.

All fittings were done using Origin version 7.5 for Windows (OriginLab, Northampton, MA 01060 USA).

Figure S11. Spin pairing fit for α-AntQNN magnetic susceptibility temperature dependence (external field 1000 Oe).

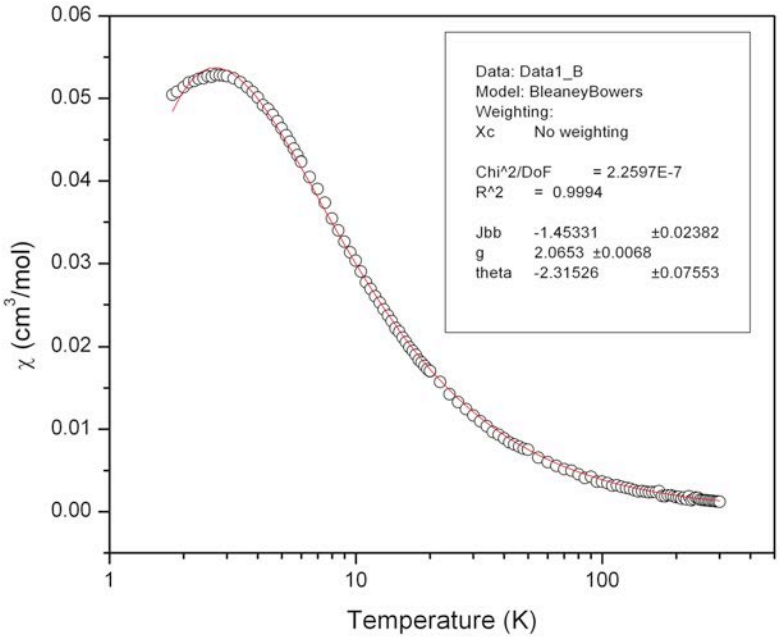


Figure S12. 1-D AFM Bonner-Fisher fit for α-AntQNN_magnetic susceptibility temperature dependence (external field 1000 Oe).

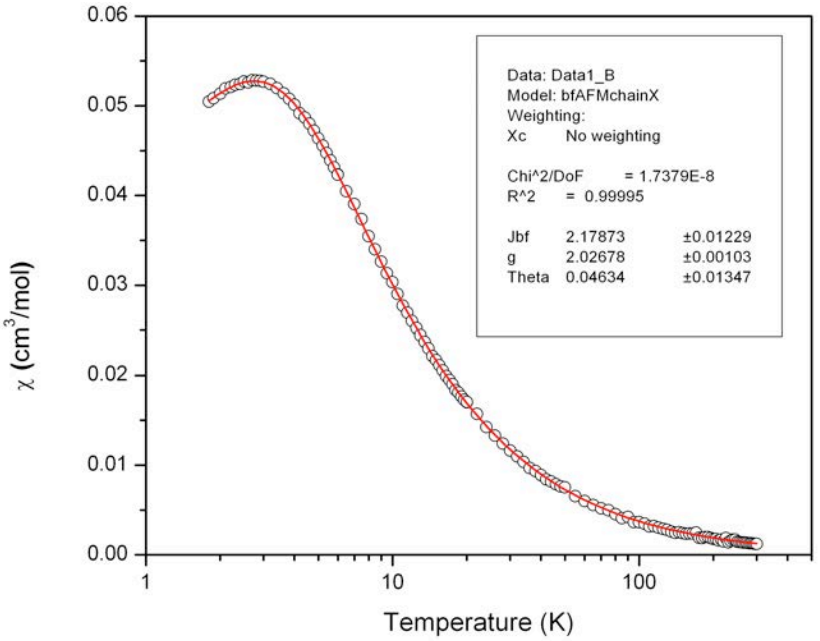


Figure S13. 1-D AFM Bonner-Fisher fit for β-AntQNN magnetic susceptibility temperature dependence (external field 1000 Oe).

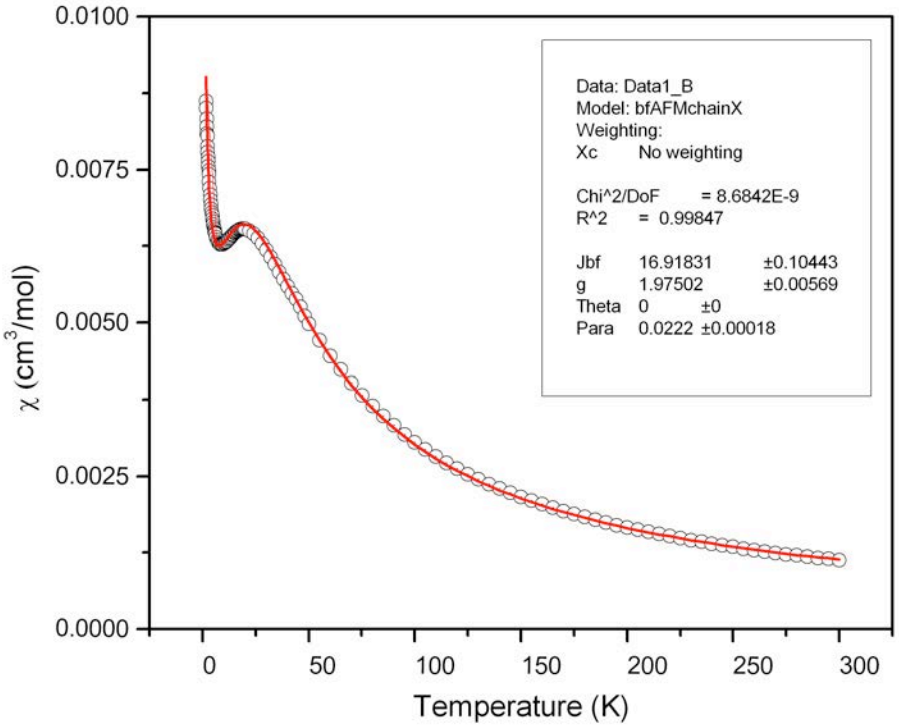
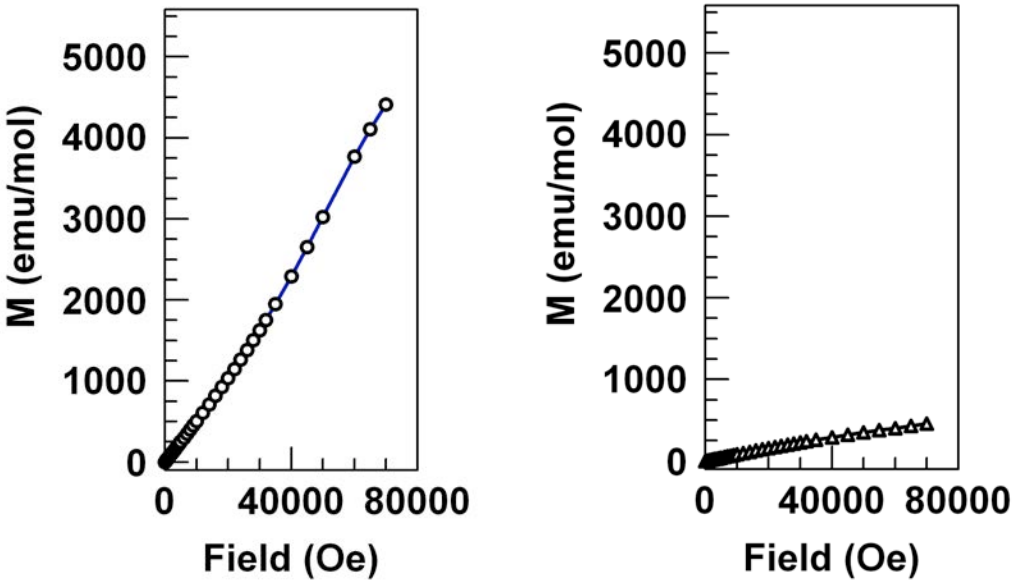


Figure S14. Molar magnetization plots at 1.8 K for α-AntQNN (left) and β-AntQNN (right). For reference, $S = 1/2$ is expected to saturate at about 5585 emu/mol.



Computational Modeling for Exchange Involving Close NO Contacts

Calculations with 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.

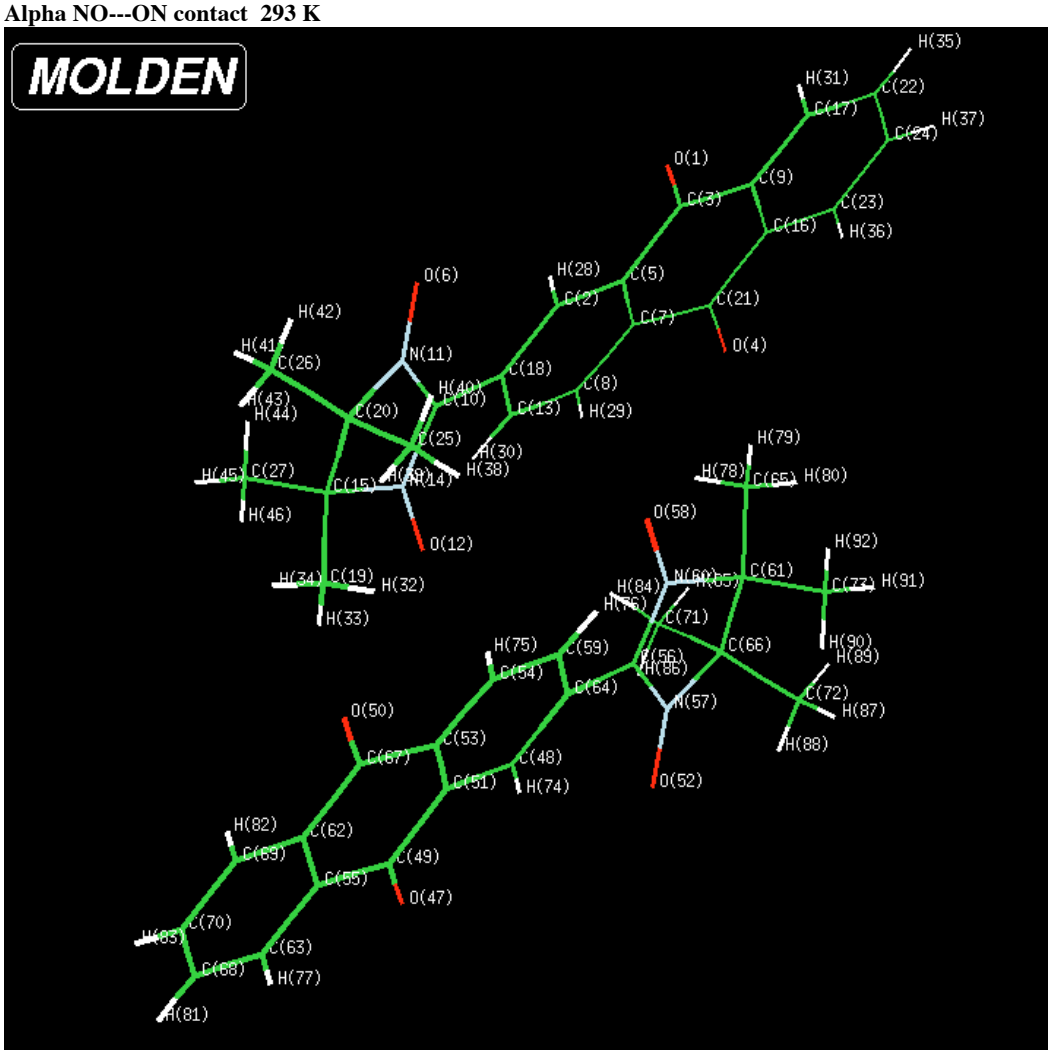
To compute ΔE(T-S), the S=0 energy was corrected for spin contamination effects using Yamaguchi's formula:

$$\Delta E_{T-S} = \frac{E_S - E_T}{< S^2_{HS} > - < S^2_{LS} >} \qquad (1)$$

(a) K. Yamaguchi, H. Fukui, T. Fueno, T. *Chem. Lett.* 1986, 625-628. (b) K. Yamaguchi, *Chem. Phys. Lett.* 1988, **149**, 537.

Visualizations below were done with Molden v4.9 for Mac, G.Schaftenaar and J.H. Noordik, *J. Comput.-Aided Mol. Design*, **14**, 123-134 (2000).

Alpha NO---ON contact 293 K



Alpha AntQNN, NO--ON dyad, S=0 state; UB3LYP\6-31+G(d)\ **293 K geometry**

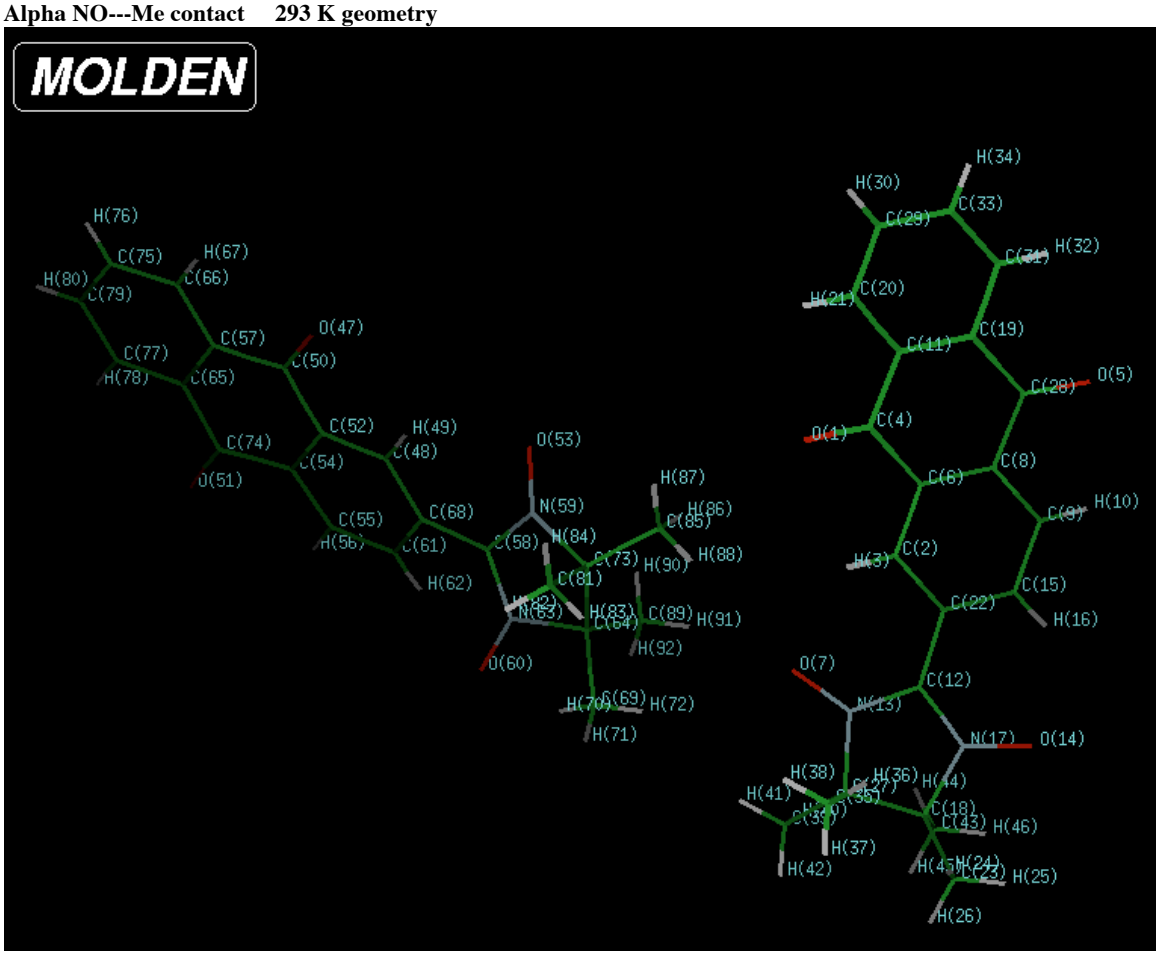
1\1\GINC-SKYNET\Stability\UB3LYP\6-31+G(d)\C42H38N4O8\LAHTI\12-Jan-201
3\0\\#P GFINPUT IOP(6/7=3) UB3LYP/6-31+G* test GUESS=(READ,MIX) STABLE
\\Handan AntQ-NN alpha isomer dyad contact\\0,1\O,0,0.6005,1.071,-5.94
8\C,0,-0.7365,0.892,-3.487\C,0,-0.0315,0.058,-5.726\O,0,-2.1495,-3.423
,-4.927\C,0,-0.8135,-0.101,-4.463\O,0,-0.5875,3.608,-2.452\C,0,-1.6105
,-1.228,-4.253\C,0,-2.3915,-1.313,-3.104\C,0,-0.0815,-1.059,-6.71\C,0,
-1.3305,1.751,-1.229\N,0,-0.9005,3.021,-1.361\O,0,-1.9245,0.412,0.607\
C,0,-2.3255,-0.331,-2.142\N,0,-1.5875,1.524,0.077\C,0,-1.5655,2.797,0.
875\C,0,-0.8375,-2.21,-6.466\C,0,0.6355,-0.947,-7.9\C,0,-1.4675,0.765,
-2.302\C,0,-1.0355,2.535,2.275\C,0,-0.6555,3.664,-0.019\C,0,-1.5955,-2
.372,-5.209\C,0,0.5945,-1.97,-8.829\C,0,-0.8705,-3.228,-7.426\C,0,-0.1
455,-3.107,-8.591\C,0,0.8355,3.459,0.265\C,0,-0.9965,5.139,-0.06\C,0,-
3.0085,3.276,0.956\H,0,-0.1995,1.638,-3.625\H,0,-2.9615,-2.039,-2.985\
H,0,-2.8555,-0.395,-1.38\H,0,1.1415,-0.185,-8.069\H,0,-0.1275,2.228,2.
221\H,0,-1.5755,1.865,2.702\H,0,-1.0685,3.346,2.787\H,0,1.0725,-1.89,-
9.624\H,0,-1.3845,-3.989,-7.277\H,0,-0.1555,-3.794,-9.218\H,0,1.0325,2
.519,0.287\H,0,1.0575,3.851,1.113\H,0,1.3545,3.879,-0.426\H,0,-1.9325,
5.245,-0.24\H,0,-0.4865,5.566,-0.752\H,0,-0.7855,5.54,0.787\H,0,-3.340
5,3.443,0.071\H,0,-3.0475,4.085,1.472\H,0,-3.5465,2.602,1.378\O,0,-0.6
015,-1.071,5.948\C,0,0.7365,-0.892,3.487\C,0,0.0305,-0.058,5.726\O,0,2
.1495,3.423,4.927\C,0,0.8125,0.101,4.464\O,0,0.5865,-3.608,2.452\C,0,1
.6105,1.228,4.253\C,0,2.3905,1.313,3.104\C,0,0.0805,1.059,6.711\C,0,1.
3295,-1.751,1.23\N,0,0.9005,-3.021,1.361\O,0,1.9235,-0.412,-0.607\C,0,
2.3255,0.331,2.142\N,0,1.5865,-1.524,-0.077\C,0,1.5655,-2.797,-0.875\C
,0,0.8375,2.21,6.467\C,0,-0.6355,0.947,7.9\C,0,1.4665,-0.765,2.302\C,0
,1.0345,-2.535,-2.275\C,0,0.6545,-3.664,0.02\C,0,1.5945,2.372,5.21\C,0
,-0.5955,1.97,8.83\C,0,0.8695,3.228,7.427\C,0,0.1455,3.107,8.592\C,0,-
0.8365,-3.459,-0.265\C,0,0.9955,-5.139,0.06\C,0,3.0075,-3.276,-0.956\H
,0,0.1985,-1.638,3.625\H,0,2.9615,2.039,2.986\H,0,2.8555,0.395,1.38\H,
0,-1.1415,0.185,8.069\H,0,0.1265,-2.228,-2.221\H,0,1.5745,-1.865,-2.70
1\H,0,1.0685,-3.346,-2.787\H,0,-1.0725,1.89,9.624\H,0,1.3835,3.989,7.2
78\H,0,0.1555,3.794,9.218\H,0,-1.0325,-2.519,-0.286\H,0,-1.0575,-3.851
,-1.113\H,0,-1.3545,-3.879,0.426\H,0,1.9325,-5.245,0.24\H,0,0.4865,-5.
566,0.752\H,0,0.7845,-5.54,-0.787\H,0,3.3395,-3.443,-0.071\H,0,3.0475,
-4.085,-1.471\H,0,3.5465,-2.602,-1.378\\Version=EM64L-G09RevB.01\State
=1-A\HF=-2443.3999076\S2=1.119506\S2-1=0.\S2A=0.943489\RMSD=7.534e-09\
Dipole=0.0002061,0.0009452,0.0028526\Quadrupole=-9.7580208,-7.4634528,
17.2214736,-16.6306614,-8.6798518,38.1026968\PG=C01 [X(C42H38N4O8)]\\@

Alpha AntQNN, NO--ON dyad, S=1 state, UB3LYP\6-31+G(d)\ **293 K geometry**

1\1\GINC-SKYNET\SP\UB3LYP\6-31+G(d)\C42H38N4O8(3)\LAHTI\09-Jan-2013\0\
\#P GFINPUT IOP(6/7=3) UB3LYP/6-31+G* test\\Handan AntQ-NN alpha isome
r dyad contact\\0,3\O,0,0.6005,1.071,-5.948\C,0,-0.7365,0.892,-3.487\C
,0,-0.0315,0.058,-5.726\O,0,-2.1495,-3.423,-4.927\C,0,-0.8135,-0.101,-
4.463\O,0,-0.5875,3.608,-2.452\C,0,-1.6105,-1.228,-4.253\C,0,-2.3915,-
1.313,-3.104\C,0,-0.0815,-1.059,-6.71\C,0,-1.3305,1.751,-1.229\N,0,-0.
9005,3.021,-1.361\O,0,-1.9245,0.412,0.607\C,0,-2.3255,-0.331,-2.142\N,
0,-1.5875,1.524,0.077\C,0,-1.5655,2.797,0.875\C,0,-0.8375,-2.21,-6.466
\C,0,0.6355,-0.947,-7.9\C,0,-1.4675,0.765,-2.302\C,0,-1.0355,2.535,2.2
75\C,0,-0.6555,3.664,-0.019\C,0,-1.5955,-2.372,-5.209\C,0,0.5945,-1.97
,-8.829\C,0,-0.8705,-3.228,-7.426\C,0,-0.1455,-3.107,-8.591\C,0,0.8355
,3.459,0.265\C,0,-0.9965,5.139,-0.06\C,0,-3.0085,3.276,0.956\H,0,-0.19
95,1.638,-3.625\H,0,-2.9615,-2.039,-2.985\H,0,-2.8555,-0.395,-1.38\H,0
,1.1415,-0.185,-8.069\H,0,-0.1275,2.228,2.221\H,0,-1.5755,1.865,2.702\
H,0,-1.0685,3.346,2.787\H,0,1.0725,-1.89,-9.624\H,0,-1.3845,-3.989,-7.
277\H,0,-0.1555,-3.794,-9.218\H,0,1.0325,2.519,0.287\H,0,1.0575,3.851,
1.113\H,0,1.3545,3.879,-0.426\H,0,-1.9325,5.245,-0.24\H,0,-0.4865,5.56
6,-0.752\H,0,-0.7855,5.54,0.787\H,0,-3.3405,3.443,0.071\H,0,-3.0475,4.
085,1.472\H,0,-3.5465,2.602,1.378\O,0,-0.6015,-1.071,5.948\C,0,0.7365,
-0.892,3.487\C,0,0.0305,-0.058,5.726\O,0,2.1495,3.423,4.927\C,0,0.8125
,0.101,4.464\O,0,0.5865,-3.608,2.452\C,0,1.6105,1.228,4.253\C,0,2.3905
,1.313,3.104\C,0,0.0805,1.059,6.711\C,0,1.3295,-1.751,1.23\N,0,0.9005,
-3.021,1.361\O,0,1.9235,-0.412,-0.607\C,0,2.3255,0.331,2.142\N,0,1.586

5,-1.524,-0.077\C,0,1.5655,-2.797,-0.875\C,0,0.8375,2.21,6.467\C,0,-0.
6355,0.947,7.9\C,0,1.4665,-0.765,2.302\C,0,1.0345,-2.535,-2.275\C,0,0.
6545,-3.664,0.02\C,0,1.5945,2.372,5.21\C,0,-0.5955,1.97,8.83\C,0,0.869
5,3.228,7.427\C,0,0.1455,3.107,8.592\C,0,-0.8365,-3.459,-0.265\C,0,0.9
955,-5.139,0.06\C,0,3.0075,-3.276,-0.956\H,0,0.1985,-1.638,3.625\H,0,2
.9615,2.039,2.986\H,0,2.8555,0.395,1.38\H,0,-1.1415,0.185,8.069\H,0,0.
1265,-2.228,-2.221\H,0,1.5745,-1.865,-2.701\H,0,1.0685,-3.346,-2.787\H
,0,-1.0725,1.89,9.624\H,0,1.3835,3.989,7.278\H,0,0.1555,3.794,9.218\H,
0,-1.0325,-2.519,-0.286\H,0,-1.0575,-3.851,-1.113\H,0,-1.3545,-3.879,0
.426\H,0,1.9325,-5.245,0.24\H,0,0.4865,-5.566,0.752\H,0,0.7845,-5.54,-
0.787\H,0,3.3395,-3.443,-0.071\H,0,3.0475,-4.085,-1.471\H,0,3.5465,-2.
602,-1.378\\Version=EM64L-G09RevB.01\State=3-A\HF=-2443.3999114\S2=2.1
19655\S2-1=0.\S2A=2.006429\RMSD=3.806e-09\Dipole=0.000206,0.0009452,0.
0028523\Quadrupole=-9.7583859,-7.461299,17.219685,-16.6308792,-8.68006
03,38.100411\PG=C01 [X(C42H38N4O8)]\\@

Alpha NO---Me contact 293 K geometry



Alpha AntQNN, NO--Me dyad, S=0 state, UB3LYP\6-31+G(d)\ **293 K geometry**

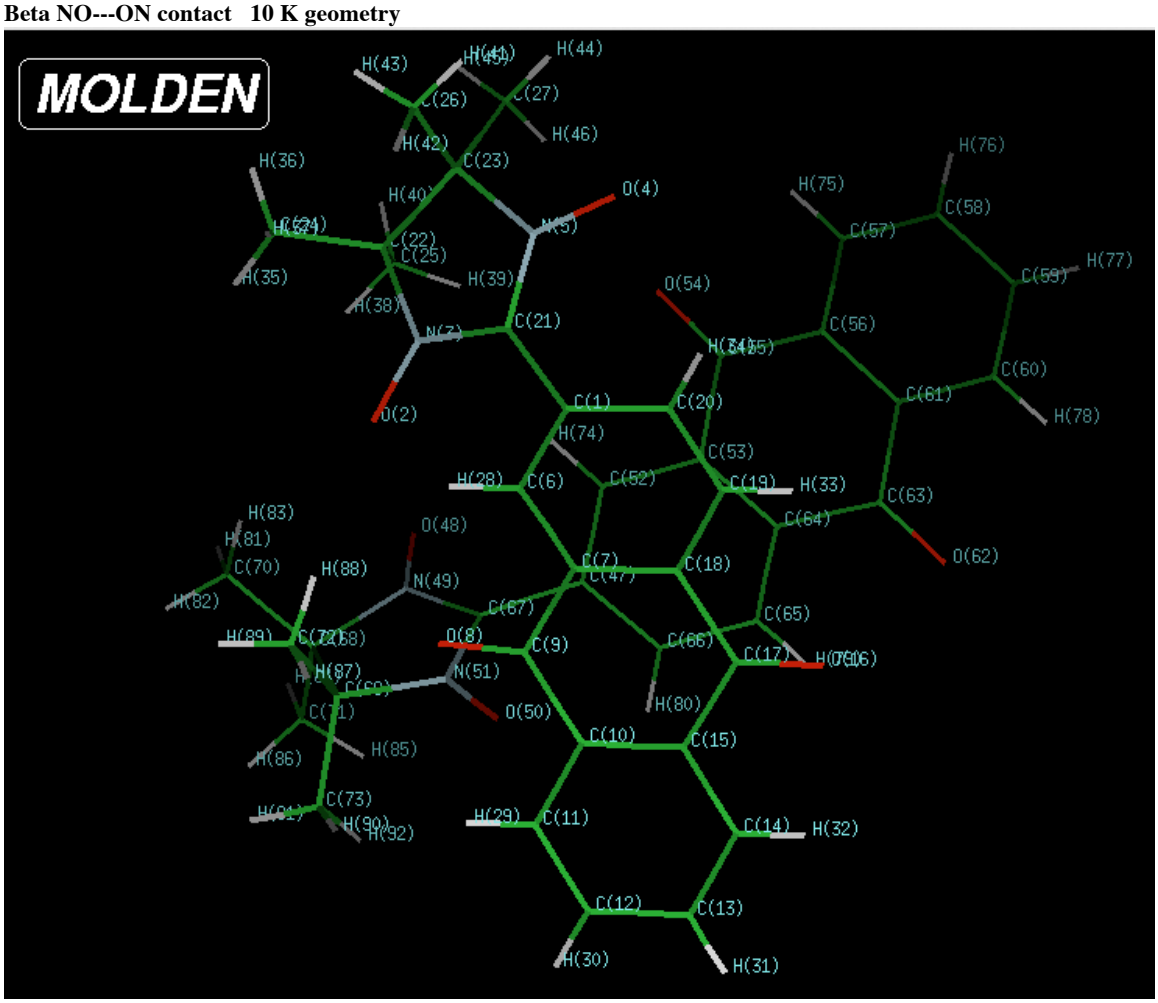
1\1\GINC-SKYNET\Stability\UB3LYP\6-31+G(d)\C42H38N4O8\LAHTI\14-Jan-201
3\0\\#P GFINPUT IOP(6/7=3) TEST UB3LYP/6-31+G* GUESS=(READ,MIX) STABLE
=OPT\\CH/NO contact dyad, Handan alpha-AntQ-NN\\0,1\O,0,7.091,1.071,-0
.311\C,0,5.754,0.892,2.15\H,0,6.291,1.638,2.012\C,0,6.459,0.058,-0.089
\O,0,4.341,-3.423,0.71\C,0,5.677,-0.101,1.174\O,0,5.903,3.608,3.185\C,
0,4.88,-1.228,1.384\C,0,4.099,-1.313,2.533\H,0,3.529,-2.039,2.652\C,0,
6.409,-1.059,-1.073\C,0,5.16,1.751,4.408\N,0,5.59,3.021,4.276\O,0,4.56
6,0.412,6.244\C,0,4.165,-0.331,3.495\H,0,3.635,-0.395,4.257\N,0,4.903,
1.524,5.714\C,0,4.925,2.797,6.512\C,0,5.653,-2.21,-0.829\C,0,7.126,-0.
947,-2.263\H,0,7.632,-0.185,-2.432\C,0,5.023,0.765,3.335\C,0,5.455,2.5

35,7.912\H,0,6.363,2.228,7.858\H,0,4.915,1.865,8.339\H,0,5.422,3.346,8
.424\C,0,5.835,3.664,5.618\C,0,4.895,-2.372,0.428\C,0,7.085,-1.97,-3.1
92\H,0,7.563,-1.89,-3.987\C,0,5.62,-3.228,-1.789\H,0,5.106,-3.989,-1.6
4\C,0,6.345,-3.107,-2.954\H,0,6.335,-3.794,-3.581\C,0,7.326,3.459,5.90
2\H,0,7.523,2.519,5.924\H,0,7.548,3.851,6.75\H,0,7.845,3.879,5.211\C,0
,5.494,5.139,5.577\H,0,4.558,5.245,5.397\H,0,6.004,5.566,4.885\H,0,5.7
05,5.54,6.424\C,0,3.482,3.276,6.593\H,0,3.15,3.443,5.708\H,0,3.443,4.0
85,7.109\H,0,2.944,2.602,7.015\O,0,8.886,8.377,-5.948\C,0,7.549,8.556,
-3.487\H,0,8.086,7.809,-3.625\C,0,8.254,9.389,-5.726\O,0,6.135,12.871,
-4.927\C,0,7.472,9.549,-4.464\O,0,7.698,5.839,-2.452\C,0,6.674,10.676,
-4.253\C,0,5.894,10.76,-3.104\H,0,5.323,11.486,-2.985\C,0,8.204,10.506
,-6.71\C,0,6.955,7.697,-1.23\N,0,7.384,6.427,-1.361\O,0,6.361,9.036,0.
607\C,0,5.96,9.779,-2.142\H,0,5.429,9.842,-1.38\N,0,6.698,7.924,0.077\
C,0,6.72,6.651,0.875\C,0,7.448,11.657,-6.467\C,0,8.92,10.395,-7.9\H,0,
9.426,9.633,-8.069\C,0,6.818,8.683,-2.302\C,0,7.25,6.912,2.275\H,0,8.1
58,7.22,2.221\H,0,6.71,7.583,2.701\H,0,7.216,6.101,2.787\C,0,7.63,5.78
4,-0.02\C,0,6.69,11.819,-5.209\C,0,8.88,11.417,-8.829\H,0,9.357,11.337
,-9.624\C,0,7.415,12.675,-7.427\H,0,6.901,13.436,-7.278\C,0,8.14,12.55
5,-8.592\H,0,8.129,13.242,-9.218\C,0,9.121,5.989,0.265\H,0,9.317,6.929
,0.286\H,0,9.342,5.597,1.113\H,0,9.639,5.568,-0.426\C,0,7.289,4.308,-0
.06\H,0,6.352,4.202,-0.24\H,0,7.799,3.881,-0.752\H,0,7.5,3.907,0.787\C
,0,5.277,6.171,0.956\H,0,4.945,6.005,0.071\H,0,5.237,5.362,1.471\H,0,4
.739,6.846,1.378\\Version=EM64L-G09RevB.01\State=1-A\HF=-2443.4031615\
S2=1.116415\S2-1=0.\S2A=0.919779\RMSD=4.484e-09\Dipole=0.0520014,-0.73
04091,1.9257878\Quadrupole=-4.7247862,-36.3316356,41.0564218,-2.771809
4,-4.3179798,10.7571049\PG=C01 [X(C42H38N4O8)]\\@

Alpha AntQNN, NO--Me dyad, S=1 state, UB3LYP\6-31+G(d)\ **293 K geometry**

1\1\GINC-SKYNET\SP\UB3LYP\6-31+G(d)\C42H38N4O8(3)\LAHTI\11-Jan-2013\0\
\#P GFINPUT IOP(6/7=3) TEST UB3LYP/6-31+G*\\CH/NO contact dyad, Handan
alpha-AntQ-NN\\0,3\O,0,7.091,1.071,-0.311\C,0,5.754,0.892,2.15\H,0,6.
291,1.638,2.012\C,0,6.459,0.058,-0.089\O,0,4.341,-3.423,0.71\C,0,5.677
,-0.101,1.174\O,0,5.903,3.608,3.185\C,0,4.88,-1.228,1.384\C,0,4.099,-1
.313,2.533\H,0,3.529,-2.039,2.652\C,0,6.409,-1.059,-1.073\C,0,5.16,1.7
51,4.408\N,0,5.59,3.021,4.276\O,0,4.566,0.412,6.244\C,0,4.165,-0.331,3
.495\H,0,3.635,-0.395,4.257\N,0,4.903,1.524,5.714\C,0,4.925,2.797,6.51
2\C,0,5.653,-2.21,-0.829\C,0,7.126,-0.947,-2.263\H,0,7.632,-0.185,-2.4
32\C,0,5.023,0.765,3.335\C,0,5.455,2.535,7.912\H,0,6.363,2.228,7.858\H
,0,4.915,1.865,8.339\H,0,5.422,3.346,8.424\C,0,5.835,3.664,5.618\C,0,4
.895,-2.372,0.428\C,0,7.085,-1.97,-3.192\H,0,7.563,-1.89,-3.987\C,0,5.
62,-3.228,-1.789\H,0,5.106,-3.989,-1.64\C,0,6.345,-3.107,-2.954\H,0,6.
335,-3.794,-3.581\C,0,7.326,3.459,5.902\H,0,7.523,2.519,5.924\H,0,7.54
8,3.851,6.75\H,0,7.845,3.879,5.211\C,0,5.494,5.139,5.577\H,0,4.558,5.2
45,5.397\H,0,6.004,5.566,4.885\H,0,5.705,5.54,6.424\C,0,3.482,3.276,6.
593\H,0,3.15,3.443,5.708\H,0,3.443,4.085,7.109\H,0,2.944,2.602,7.015\O
,0,8.886,8.377,-5.948\C,0,7.549,8.556,-3.487\H,0,8.086,7.809,-3.625\C,
0,8.254,9.389,-5.726\O,0,6.135,12.871,-4.927\C,0,7.472,9.549,-4.464\O,
0,7.698,5.839,-2.452\C,0,6.674,10.676,-4.253\C,0,5.894,10.76,-3.104\H,
0,5.323,11.486,-2.985\C,0,8.204,10.506,-6.71\C,0,6.955,7.697,-1.23\N,0
,7.384,6.427,-1.361\O,0,6.361,9.036,0.607\C,0,5.96,9.779,-2.142\H,0,5.
429,9.842,-1.38\N,0,6.698,7.924,0.077\C,0,6.72,6.651,0.875\C,0,7.448,1
1.657,-6.467\C,0,8.92,10.395,-7.9\H,0,9.426,9.633,-8.069\C,0,6.818,8.6
83,-2.302\C,0,7.25,6.912,2.275\H,0,8.158,7.22,2.221\H,0,6.71,7.583,2.7
01\H,0,7.216,6.101,2.787\C,0,7.63,5.784,-0.02\C,0,6.69,11.819,-5.209\C
,0,8.88,11.417,-8.829\H,0,9.357,11.337,-9.624\C,0,7.415,12.675,-7.427\
H,0,6.901,13.436,-7.278\C,0,8.14,12.555,-8.592\H,0,8.129,13.242,-9.218
\C,0,9.121,5.989,0.265\H,0,9.317,6.929,0.286\H,0,9.342,5.597,1.113\H,0
,9.639,5.568,-0.426\C,0,7.289,4.308,-0.06\H,0,6.352,4.202,-0.24\H,0,7.
799,3.881,-0.752\H,0,7.5,3.907,0.787\C,0,5.277,6.171,0.956\H,0,4.945,6
.005,0.071\H,0,5.237,5.362,1.471\H,0,4.739,6.846,1.378\\Version=EM64L-
G09RevB.01\State=3-A\HF=-2443.4031572\S2=2.116526\S2-1=0.\S2A=2.006102
\RMSD=2.402e-09\Dipole=0.051867,-0.7308434,1.9261997\Quadrupole=-4.725
5992,-36.3325265,41.0581257,-2.7714688,-4.3185725,10.7564961\PG=C01 [X
(C42H38N4O8)]\\@

Beta NO---ON contact 10 K geometry



Beta AntQNN, NO--ON dyad, S=0 state, UB3LYP\6-31+G(d)\ **10 K geometry**

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1\1\GINC-SKYNET\Stability\UB3LYP\6-31+G(d)\C42H38N4O8\LAHTI\12-Jan-201
 3\0\\#P GFINPUT IOP(6/7=3) UB3LYP/6-31+G* test GUESS=(READ,MIX) STABLE
 =OPT\\Handan AntQ-NN beta isomer dyad contact\\0,1\C,0,1.6175,-0.1795,
 -0.4185\O,0,0.7425,2.5815,0.0765\N,0,1.2995,2.2195,-1.0165\O,0,2.6945,
 -0.0755,-3.1695\N,0,2.2075,0.9485,-2.5675\C,0,1.7785,-0.0125,0.9625\C,
 0,1.5455,-1.0885,1.8165\O,0,2.3405,0.0875,3.7215\C,0,1.7595,-0.8985,3.
 2885\C,0,1.2965,-1.9925,4.1895\C,0,1.3655,-1.8075,5.5765\C,0,0.9615,-2
 .8195,6.4345\C,0,0.5025,-4.0345,5.9275\C,0,0.4315,-4.2215,4.5515\C,0,0
 .8195,-3.2035,3.6775\O,0,0.2905,-4.4875,1.7545\C,0,0.7165,-3.4335,2.20
 75\C,0,1.1195,-2.3205,1.3055\C,0,1.0165,-2.4915,-0.0785\C,0,1.2815,-1.
 4385,-0.9355\C,0,1.7365,0.9745,-1.3055\C,0,1.3585,3.1455,-2.2035\C,0,2
 .2235,2.3075,-3.2095\C,0,1.9695,4.4695,-1.7465\C,0,-0.0915,3.3595,-2.6
 505\C,0,3.6855,2.7365,-3.2875\C,0,1.6405,2.1595,-4.6125\H,0,2.0445,0.8
 285,1.3135\H,0,1.6905,-0.9865,5.9305\H,0,0.9985,-2.6835,7.3745\H,0,0.2
 385,-4.7305,6.5185\H,0,0.1155,-5.0485,4.2045\H,0,0.7655,-3.3365,-0.432
 5\H,0,1.2355,-1.5685,-1.8745\H,0,1.3595,4.9105,-1.1205\H,0,2.1145,5.04
 85,-2.5245\H,0,2.8255,4.2975,-1.3025\H,0,-0.5685,3.8805,-1.9705\H,0,-0
 .5305,2.4905,-2.7625\H,0,-0.1035,3.8435,-3.5005\H,0,4.1575,2.1775,-3.9
 385\H,0,4.1035,2.6355,-2.4075\H,0,3.7365,3.6745,-3.5675\H,0,2.2515,1.6
 295,-5.1675\H,0,1.5235,3.0465,-5.0115\H,0,0.7725,1.7085,-4.5595\C,0,-1
 .9715,-0.1795,0.4185\O,0,-2.8465,2.5815,-0.0765\N,0,-2.2895,2.2195,1.0
 165\O,0,-0.8945,-0.0755,3.1695\N,0,-1.3815,0.9485,2.5675\C,0,-1.8105,-
 0.0125,-0.9615\C,0,-2.0425,-1.0885,-1.8165\O,0,-1.2485,0.0875,-3.7215\
 C,0,-1.8295,-0.8985,-3.2885\C,0,-2.2925,-1.9925,-4.1895\C,0,-2.2235,-1
```

.8075,-5.5765\C,0,-2.6275,-2.8195,-6.4345\C,0,-3.0865,-4.0345,-5.9275\
C,0,-3.1575,-4.2215,-4.5515\C,0,-2.7695,-3.2035,-3.6775\O,0,-3.2985,-4
.4875,-1.7545\C,0,-2.8725,-3.4335,-2.2075\C,0,-2.4695,-2.3205,-1.3055\
C,0,-2.5715,-2.4915,0.0795\C,0,-2.3075,-1.4385,0.9355\C,0,-1.8525,0.97
45,1.3055\C,0,-2.2305,3.1455,2.2035\C,0,-1.3655,2.3075,3.2095\C,0,-1.6
195,4.4695,1.7465\C,0,-3.6805,3.3595,2.6505\C,0,0.0965,2.7365,3.2875\C
,0,-1.9485,2.1595,4.6125\H,0,-1.5445,0.8285,-1.3135\H,0,-1.8985,-0.986
5,-5.9305\H,0,-2.5905,-2.6835,-7.3745\H,0,-3.3495,-4.7305,-6.5185\H,0,
-3.4735,-5.0485,-4.2045\H,0,-2.8235,-3.3365,0.4325\H,0,-2.3535,-1.5685
,1.8745\H,0,-2.2295,4.9105,1.1205\H,0,-1.4745,5.0485,2.5245\H,0,-0.763
5,4.2975,1.3025\H,0,-4.1575,3.8805,1.9705\H,0,-4.1195,2.4905,2.7625\H,
0,-3.6925,3.8435,3.5005\H,0,0.5685,2.1775,3.9385\H,0,0.5145,2.6355,2.4
075\H,0,0.1475,3.6745,3.5675\H,0,-1.3375,1.6295,5.1675\H,0,-2.0655,3.0
465,5.0115\H,0,-2.8155,1.7085,4.5595\\Version=EM64L-G09RevB.01\State=1
-A\HF=-2443.5898751\S2=1.10133\S2-1=0.\S2A=0.813001\RMSD=2.589e-09\Dip
ole=-0.481475,2.2014102,-0.2098822\Quadrupole=-20.0727948,-4.433621,24
.5064158,5.4962294,-5.2472811,1.0291394\PG=C01 [X(C42H38N4O8)]\\@

Beta AntQNN, NO--ON dyad, S=1 state, UB3LYP\6-31+G(d)\ **10 K geometry**

1\1\GINC-SKYNET\SP\UB3LYP\6-31+G(d)\C42H38N4O8(3)\LAHTI\10-Jan-2013\0\
\#P GFINPUT IOP(6/7=3) UB3LYP/6-31+G* test\\Handan AntQ-NN beta isomer
 dyad contact\\0,3\C,0,1.6175,-0.1795,-0.4185\O,0,0.7425,2.5815,0.0765
\N,0,1.2995,2.2195,-1.0165\O,0,2.6945,-0.0755,-3.1695\N,0,2.2075,0.948
5,-2.5675\C,0,1.7785,-0.0125,0.9625\C,0,1.5455,-1.0885,1.8165\O,0,2.34
05,0.0875,3.7215\C,0,1.7595,-0.8985,3.2885\C,0,1.2965,-1.9925,4.1895\C
,0,1.3655,-1.8075,5.5765\C,0,0.9615,-2.8195,6.4345\C,0,0.5025,-4.0345,
5.9275\C,0,0.4315,-4.2215,4.5515\C,0,0.8195,-3.2035,3.6775\O,0,0.2905,
-4.4875,1.7545\C,0,0.7165,-3.4335,2.2075\C,0,1.1195,-2.3205,1.3055\C,0
,1.0165,-2.4915,-0.0785\C,0,1.2815,-1.4385,-0.9355\C,0,1.7365,0.9745,-
1.3055\C,0,1.3585,3.1455,-2.2035\C,0,2.2235,2.3075,-3.2095\C,0,1.9695,
4.4695,-1.7465\C,0,-0.0915,3.3595,-2.6505\C,0,3.6855,2.7365,-3.2875\C,
0,1.6405,2.1595,-4.6125\H,0,2.0445,0.8285,1.3135\H,0,1.6905,-0.9865,5.
9305\H,0,0.9985,-2.6835,7.3745\H,0,0.2385,-4.7305,6.5185\H,0,0.1155,-5
.0485,4.2045\H,0,0.7655,-3.3365,-0.4325\H,0,1.2355,-1.5685,-1.8745\H,0
,1.3595,4.9105,-1.1205\H,0,2.1145,5.0485,-2.5245\H,0,2.8255,4.2975,-1.
3025\H,0,-0.5685,3.8805,-1.9705\H,0,-0.5305,2.4905,-2.7625\H,0,-0.1035
,3.8435,-3.5005\H,0,4.1575,2.1775,-3.9385\H,0,4.1035,2.6355,-2.4075\H,
0,3.7365,3.6745,-3.5675\H,0,2.2515,1.6295,-5.1675\H,0,1.5235,3.0465,-5
.0115\H,0,0.7725,1.7085,-4.5595\C,0,-1.9715,-0.1795,0.4185\O,0,-2.8465
,2.5815,-0.0765\N,0,-2.2895,2.2195,1.0165\O,0,-0.8945,-0.0755,3.1695\N
,0,-1.3815,0.9485,2.5675\C,0,-1.8105,-0.0125,-0.9615\C,0,-2.0425,-1.08
85,-1.8165\O,0,-1.2485,0.0875,-3.7215\C,0,-1.8295,-0.8985,-3.2885\C,0,
-2.2925,-1.9925,-4.1895\C,0,-2.2235,-1.8075,-5.5765\C,0,-2.6275,-2.819
5,-6.4345\C,0,-3.0865,-4.0345,-5.9275\C,0,-3.1575,-4.2215,-4.5515\C,0,
-2.7695,-3.2035,-3.6775\O,0,-3.2985,-4.4875,-1.7545\C,0,-2.8725,-3.433
5,-2.2075\C,0,-2.4695,-2.3205,-1.3055\C,0,-2.5715,-2.4915,0.0795\C,0,-
2.3075,-1.4385,0.9355\C,0,-1.8525,0.9745,1.3055\C,0,-2.2305,3.1455,2.2
035\C,0,-1.3655,2.3075,3.2095\C,0,-1.6195,4.4695,1.7465\C,0,-3.6805,3.
3595,2.6505\C,0,0.0965,2.7365,3.2875\C,0,-1.9485,2.1595,4.6125\H,0,-1.
5445,0.8285,-1.3135\H,0,-1.8985,-0.9865,-5.9305\H,0,-2.5905,-2.6835,-7
.3745\H,0,-3.3495,-4.7305,-6.5185\H,0,-3.4735,-5.0485,-4.2045\H,0,-2.8
235,-3.3365,0.4325\H,0,-2.3535,-1.5685,1.8745\H,0,-2.2295,4.9105,1.120
5\H,0,-1.4745,5.0485,2.5245\H,0,-0.7635,4.2975,1.3025\H,0,-4.1575,3.88
05,1.9705\H,0,-4.1195,2.4905,2.7625\H,0,-3.6925,3.8435,3.5005\H,0,0.56
85,2.1775,3.9385\H,0,0.5145,2.6355,2.4075\H,0,0.1475,3.6745,3.5675\H,0
,-1.3375,1.6295,5.1675\H,0,-2.0655,3.0465,5.0115\H,0,-2.8155,1.7085,4.
5595\\Version=EM64L-G09RevB.01\State=3-A\HF=-2443.5898149\S2=2.102576\
S2-1=0.\S2A=2.004723\RMSD=2.910e-09\Dipole=-0.4802925,2.1999007,-0.209
3092\Quadrupole=-20.0739605,-4.4428634,24.5168239,5.5031729,-5.2416195
,1.0248464\PG=C01 [X(C42H38N4O8)]\\@

Beta AntQNN, NO--ON dyad, S=0 state, UB3LYP\6-31+G(d)\ **293 K geometry**

1\1\GINC-SKYNET\Stability\UB3LYP\6-31+G(d)\C42H38N4O8\LAHTI\22-Feb-201
3\0\\#P GFINPUT IOP(6/7=3) UB3LYP/6-31+G* test GUESS=(READ,MIX) STABLE
\\Handan AntQ-NN beta isomer dyad contact 300 K\\0,1\C,0,2.496,2.906,5
.153\O,0,1.598,5.652,5.645\N,0,2.153,5.296,4.546\O,0,3.577,3.028,2.409
\N,0,3.083,4.045,3.008\C,0,2.657,3.062,6.526\H,0,2.909,3.889,6.871\C,0
,2.441,1.986,7.388\O,0,3.222,3.168,9.286\C,0,2.66,2.172,8.856\C,0,2.22
8,1.068,9.757\C,0,2.296,1.251,11.137\H,0,2.595,2.061,11.482\C,0,1.923,
0.235,11.993\H,0,1.96,0.366,12.912\C,0,1.494,-0.979,11.488\H,0,1.253,-
1.665,12.068\C,0,1.423,-1.171,10.124\H,0,1.134,-1.988,9.788\C,0,1.782,
-0.146,9.244\O,0,1.298,-1.434,7.324\C,0,1.684,-0.37,7.777\C,0,2.037,0.
756,6.873\C,0,1.925,0.588,5.497\H,0,1.689,-0.242,5.15\C,0,2.164,1.645,
4.641\H,0,2.104,1.52,3.722\C,0,2.6,4.061,4.267\C,0,2.219,6.238,3.376\C
,0,3.09,5.41,2.369\C,0,2.826,7.547,3.852\H,0,2.223,7.977,4.464\H,0,2.9
81,8.12,3.098\H,0,3.659,7.369,4.296\C,0,0.773,6.447,2.929\H,0,0.303,6.
956,3.594\H,0,0.346,5.595,2.819\H,0,0.762,6.922,2.094\C,0,4.545,5.844,
2.29\H,0,5.009,5.295,1.654\H,0,4.954,5.749,3.154\H,0,4.591,6.761,2.014
\C,0,2.508,5.26,0.966\H,0,3.109,4.743,0.425\H,0,2.389,6.128,0.574\H,0,
1.659,4.813,1.017\C,0,6.157,2.906,6.023\O,0,5.259,5.652,5.531\N,0,5.81
4,5.296,6.63\O,0,7.238,3.028,8.767\N,0,6.744,4.045,8.168\C,0,6.318,3.0
62,4.65\H,0,6.57,3.889,4.305\C,0,6.103,1.986,3.787\O,0,6.884,3.168,1.8
9\C,0,6.322,2.172,2.32\C,0,5.89,1.068,1.419\C,0,5.958,1.251,0.039\H,0,
6.256,2.061,-0.306\C,0,5.585,0.235,-0.817\H,0,5.622,0.366,-1.737\C,0,5
.155,-0.979,-0.312\H,0,4.914,-1.665,-0.892\C,0,5.084,-1.171,1.052\H,0,
4.796,-1.988,1.388\C,0,5.444,-0.146,1.932\O,0,4.959,-1.434,3.852\C,0,5
.345,-0.37,3.399\C,0,5.698,0.756,4.303\C,0,5.587,0.588,5.679\H,0,5.35,
-0.242,6.026\C,0,5.825,1.645,6.535\H,0,5.765,1.52,7.454\C,0,6.261,4.06
1,6.909\C,0,5.88,6.238,7.8\C,0,6.751,5.41,8.807\C,0,6.487,7.547,7.323\
H,0,5.884,7.977,6.712\H,0,6.643,8.12,8.078\H,0,7.32,7.369,6.88\C,0,4.4
35,6.447,8.247\H,0,3.965,6.956,7.582\H,0,4.007,5.595,8.357\H,0,4.423,6
.922,9.081\C,0,8.206,5.844,8.886\H,0,8.67,5.295,9.522\H,0,8.616,5.749,
8.022\H,0,8.252,6.761,9.162\C,0,6.17,5.26,10.21\H,0,6.77,4.743,10.751\
H,0,6.051,6.128,10.601\H,0,5.321,4.813,10.159\\Version=EM64L-G09RevB.0
1\State=1-A\HF=-2443.3987451\S2=1.100044\S2-1=0.\S2A=0.79886\RMSD=6.09
6e-09\Dipole=-0.482346,2.1953732,0.1844929\Quadrupole=-20.024836,-4.45
35365,24.4783725,5.6709245,5.3353549,-0.8646254\PG=C01 [X(C42H38N4O8)]

Beta AntQNN, NO--ON dyad, S=1 state, UB3LYP\6-31+G(d)\ **293 K geometry**

1\1\GINC-SKYNET\SP\UB3LYP\6-31+G(d)\C42H38N4O8(3)\LAHTI\20-Feb-2013\0\
\#P GFINPUT IOP(6/7=3) UB3LYP/6-31+G* test\\Handan AntQ-NN beta isomer
dyad contact 300 K\\0,3\C,0,2.496,2.906,5.153\O,0,1.598,5.652,5.645\N
,0,2.153,5.296,4.546\O,0,3.577,3.028,2.409\N,0,3.083,4.045,3.008\C,0,2
.657,3.062,6.526\H,0,2.909,3.889,6.871\C,0,2.441,1.986,7.388\O,0,3.222
,3.168,9.286\C,0,2.66,2.172,8.856\C,0,2.228,1.068,9.757\C,0,2.296,1.25
1,11.137\H,0,2.595,2.061,11.482\C,0,1.923,0.235,11.993\H,0,1.96,0.366,
12.912\C,0,1.494,-0.979,11.488\H,0,1.253,-1.665,12.068\C,0,1.423,-1.17
1,10.124\H,0,1.134,-1.988,9.788\C,0,1.782,-0.146,9.244\O,0,1.298,-1.43
4,7.324\C,0,1.684,-0.37,7.777\C,0,2.037,0.756,6.873\C,0,1.925,0.588,5.
497\H,0,1.689,-0.242,5.15\C,0,2.164,1.645,4.641\H,0,2.104,1.52,3.722\C
,0,2.6,4.061,4.267\C,0,2.219,6.238,3.376\C,0,3.09,5.41,2.369\C,0,2.826
,7.547,3.852\H,0,2.223,7.977,4.464\H,0,2.981,8.12,3.098\H,0,3.659,7.36
9,4.296\C,0,0.773,6.447,2.929\H,0,0.303,6.956,3.594\H,0,0.346,5.595,2.
819\H,0,0.762,6.922,2.094\C,0,4.545,5.844,2.29\H,0,5.009,5.295,1.654\H
,0,4.954,5.749,3.154\H,0,4.591,6.761,2.014\C,0,2.508,5.26,0.966\H,0,3.
109,4.743,0.425\H,0,2.389,6.128,0.574\H,0,1.659,4.813,1.017\C,0,6.157,
2.906,6.023\O,0,5.259,5.652,5.531\N,0,5.814,5.296,6.63\O,0,7.238,3.028
,8.767\N,0,6.744,4.045,8.168\C,0,6.318,3.062,4.65\H,0,6.57,3.889,4.305
\C,0,6.103,1.986,3.787\O,0,6.884,3.168,1.89\C,0,6.322,2.172,2.32\C,0,5
.89,1.068,1.419\C,0,5.958,1.251,0.039\H,0,6.256,2.061,-0.306\C,0,5.585
,0.235,-0.817\H,0,5.622,0.366,-1.737\C,0,5.155,-0.979,-0.312\H,0,4.914
,-1.665,-0.892\C,0,5.084,-1.171,1.052\H,0,4.796,-1.988,1.388\C,0,5.444
,-0.146,1.932\O,0,4.959,-1.434,3.852\C,0,5.345,-0.37,3.399\C,0,5.698,0
.756,4.303\C,0,5.587,0.588,5.679\H,0,5.35,-0.242,6.026\C,0,5.825,1.645
,6.535\H,0,5.765,1.52,7.454\C,0,6.261,4.061,6.909\C,0,5.88,6.238,7.8\C
,0,6.751,5.41,8.807\C,0,6.487,7.547,7.323\H,0,5.884,7.977,6.712\H,0,6.
643,8.12,8.078\H,0,7.32,7.369,6.88\C,0,4.435,6.447,8.247\H,0,3.965,6.9
56,7.582\H,0,4.007,5.595,8.357\H,0,4.423,6.922,9.081\C,0,8.206,5.844,8
.886\H,0,8.67,5.295,9.522\H,0,8.616,5.749,8.022\H,0,8.252,6.761,9.162\
C,0,6.17,5.26,10.21\H,0,6.77,4.743,10.751\H,0,6.051,6.128,10.601\H,0,5
.321,4.813,10.159\\Version=EM64L-G09RevB.01\State=3-A\HF=-2443.3987124
\S2=2.100777\S2-1=0.\S2A=2.004554\RMSD=3.495e-09\Dipole=-0.4814117,2.1
943214,0.1839652\Quadrupole=-20.0262426,-4.4601401,24.4863826,5.676675
9,5.3312528,-0.8614352\PG=C01 [X(C42H38N4O8)]\\@