ELECTRONIC SUPPLEMENTARY INFORMATION

for

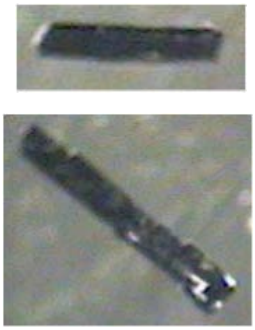
Radicals organized by disk shaped aromatics – polymorphism and co-crystals that tune inter-electron exchange.

Handan Akpinar,[a] *Joel T. Mague,*[b] *Miguel A. Novak,*[c,d] *Jonathan R. Friedman,*[e] *Paul M. Lahti**[a]

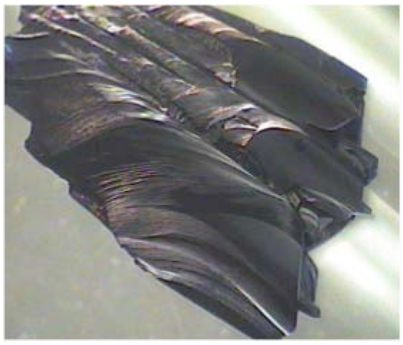
[a]Department of Chemistry, University of Massachusetts, Amherst, MA 01003 USA
[b]Department of Chemistry, Tulane University, New Orleans, LA 70118 USA
[c]Instituto de Física, Universidade Federal do Rio de Janeiro, Rio de Janeiro-RJ, 21945-970, Brazil
[d]Visiting Scholar, University of Massachusetts, Amherst, MA 01003 USA
[e]Department of Physics, Amherst College, Amherst, MA 01002 USA

*Includes details of magnetic data fitting.

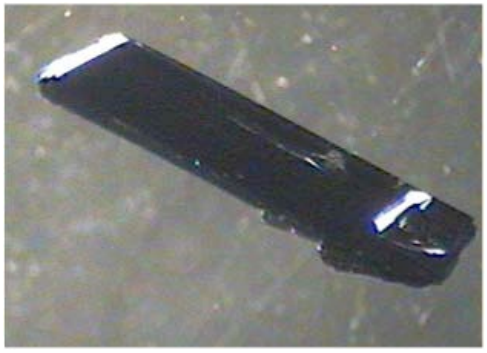
Figure S1. Pictures of crystals of PyrNN, $(PyrNN)_2 \cdot C_6F_6$, α-PyrIN, PyrIN recrystallized from C_6F_6, β-PyrIN.



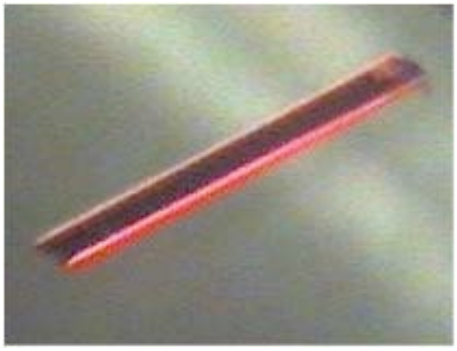
α-PyrNN (1.6 mm long)



$(PyrNN)_2 \cdot C_6F_6$ (longest dimension 6 mm)



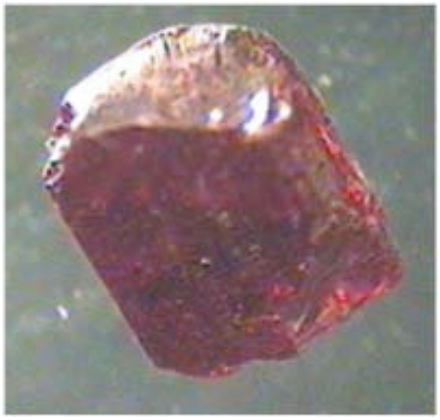
β-PyrNN (5 mm long)



α-PyrIN (1.5 mm long)

Attempted PyrIN with C_6F_6 (2 mm long)

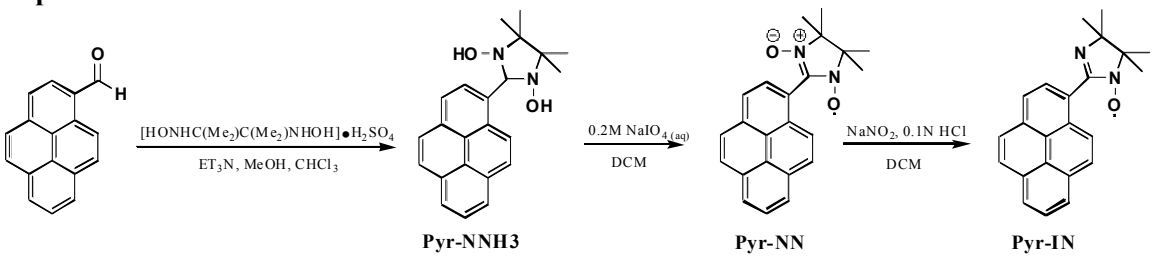
β-PyrIN (blade) (3.5 mm long)



β-PyrIN (block) (longest dimension 3 mm)

Attempted PyrIN with C_6F_6 (5 mm long)

Experimental Procedures:



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.

2-(1'-Pyrenyl)-4,4,5,5-tetramethyl-4,5-dihydro-*1H*-imidazole-3-oxide-1-oxyl (**PyrNN**). Bis(hydroxylamino)-2,3-dimethylbutane hydrogen sulfate (1.069 g, 4.34 mmol) and pyrene-1-carbaldehyde (1.0 g, 4.34 mmol) were dissolved in 50 mL of methanol and 30 mL of chloroform. Triethylamine (0.438 g, 4.34 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 (**PyrNNH3**) was dissolved in 120 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 $NaIO_4$ (0.928 g, 4.34 mmol in 21.6 mL of H_2O). A deep-blue 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 the solvent removed by rotary evaporation. Chromatography on silica gel with ethyl acetate yielded **PyrNN** (0.610 g, 39%). Recrystallization from acetonitrile alone gave dark-blue needles, mp: 190-191 °C; this is the α-allotope. Recrystallization from dichloromethane/acetonitrile gave long needles or plates, mp: 190-191 °C; this is the β-allotope. ESR (toluene, 9.647 GHz): 7.18 gauss (2 N). MS (FAB): found *m/z* = 357.2, calculated for $C_{23}H_{21}N_2O_2$ *m/z* = 357.2.

2-(1'-Pyrenyl)-4,4,5,5-tetramethyl-4,5-dihydro-*1H*-imidazole-1-oxyl (**PyrIN**). To a stirred solution of **PyrNN** (0.800 g, 2.24 mmol) in 160 mL of dichloromethane under nitrogen was added $NaNO_2$ (3.101 g, 44.80 mmol), then 12.3 mL of 0.1 M aq HCl solution. A color change was observed from deep-blue to orange. The reaction was stirred for 15 min, then 50 mL of water was added. The reaction was extracted with dichloromethane. The combined organic layers were dried over anhydrous magnesium sulfate and evaporated to dryness rotary evaporation. Chromatography on silica gel with ethyl acetate/hexane (1/1) as the eluent yielded **PyrIN** (0.540 g, 71 %), which could be recrystallized to give a mix of red-orange blades plus brick-like crystals from ethyl acetate/hexane solution, mp 150-151 °C; this is the β-allotrope. Recrystallization from layered chloroform under methylcyclohexane yielded clusters of dark red needles (mp 150-151 °C); this is the α-allotope. ESR (toluene, 9.647 GHz), a_N = 8.85, 4.00 gauss. MS (FAB): found *m/z* = 341.2, calculated for $C_{23}H_{21}N_2O$ *m/z* = 341.2.

Co-crystallization of PyrNN with C_6F_6. To a solution of **PyrNN** (0.055 g, 0.15 mmol) in 4 mL of dichloromethane was added 3 mL of C_6F_6 (4.836 g, 25.99 mmol); the solvent was allowed slowly to evaporate at room temperature. The mass of the solid residue was checked; it yielded **(PyrNN)$_2$·C_6F_6** (0.069 g, 100 %) as wavy plate shaped, dark blue crystals, mp 193-195 °C for several determinations.

Attempted co-crystallization of PyrIN with C_6F_6. To a solution of **Py-IN** (0.0303 g, 0.09 mmol) in 3 mL of dichloromethane was added 2 mL of excess **C_6F_6** (3.224 g, 17.33 mmol); and let the solvent slowly evaporate at room temperature. The mass of the solid residue was checked; it equaled the mass of the originally input **Pyr-IN** (0.0303 g, 0.09 mmol) as salmon colored, irregular prisms, some with holes seen under the microscope, mp 150-151 °C, the same as the **PyrIN** material that was input. These crystals did not give analysis-quality x-ray diffraction.

Crystallographic study and analysis procedures.

General X-ray Diffraction Procedures: For all structures, a suitable crystal was selected and affixed to the end of a Cryoloop™ with a drop of Paratone™ oil and placed in the cold nitrogen stream of the low temperature attachment of the Bruker-AXS Smart APEX CCD diffractometer. Full spheres of data were collected using a combination of ω and φ scans with scan widths varying between 0.3 and 0.5° and exposure times chosen to provide the maximum possible numbers of observable diffraction maxima. The raw intensity data were converted to F^2 values with SAINT [Bruker-AXS **2004**. SAINT+, Version 7.03, Madison, WI] and at the same time a global refinement of unit cell parameters was performed. Empirical absorption corrections and merging of symmetry equivalent reflections was performed with SADABS [Sheldrick, G. M. **2002**. *SADABS*, Version 2.05. University of Göttingen, Germany]. The structures were solved by direct methods (SHELXS) and refined by full-matrix least-squares procedures (SHELXL) [Sheldrick, G. M. *Acta Cryst.,* **2008**, *A64*, 112-122; Bruker-AXS, **2000**, *SHELXTL*, Version 6.10, Madison, WI]. In most instances at least some of the hydrogen atoms could be observed. Those attached to carbon were placed in idealized positions while those attached to nitrogen (in the alloys) were placed in positions derived from difference maps and all were included as riding contributions with isotropic displacement parameters tied to those of the attached atoms.

α-PyrIN: In the latter stages of refinement for this structure, a definite electron density peak appeared about as far from N2 as O1 is from N1 suggesting partial occupancy of this site by oxygen. Trial refinements of oxygen site-occupancy factors (sof) treating this as representing a small amount of co-crystallized PyrNN and as a rotational disorder of the 5-membered ring did not provide a clear indication of which might be the better model. However the fact that the site occupancy factor of O1 refined to 0.96 while that for the peak near N2 refined to 0.09 suggests that the co-crystal model may be preferred.

β-PyrIN: Two independent molecules of the complex are present in the asymmetric unit. Although most of each molecule could be located in difference maps, it became evident that each was severely disordered. The disorder of the pyrenyl portions was treated by fitting a rigid model derived from a published structure of pyrene, since many resolved carbon sites as could be adequately identified using the FRAG function of SHELXL. Once this model was in place, sufficient numbers of atoms of the disordered iminoylnitroxide substituent could be located to define the orientations of the two components of this disorder and subsequent refinement enabled the remaining atoms to be located. Final refinement was carried out with restraints that the geometries of the two components of the disorder be the same and that the sof's for the two sum to 1.0.

Crystallographic packing representations in this article were created using the ORTEP [Farrugia, L. J. *J. Appl. Cryst*. **1997**, *30*, 565] and Mercury [Macrae, C. F.; Bruno, I. J.; Chisholm, J. A.; Edgington, P. R.; McCabe, P.; Pidcock, E.; Rodriguez-Monge, L.; Taylor, R.; van de Streek, J.; Wood, P. A. *J. Appl. Cryst*., **2008**, *41*, 466-470.] programs.

Figure S2. C_6F_6 contacts in $(PyrNN)_2 \cdot C_6F_6$ co-crystal.

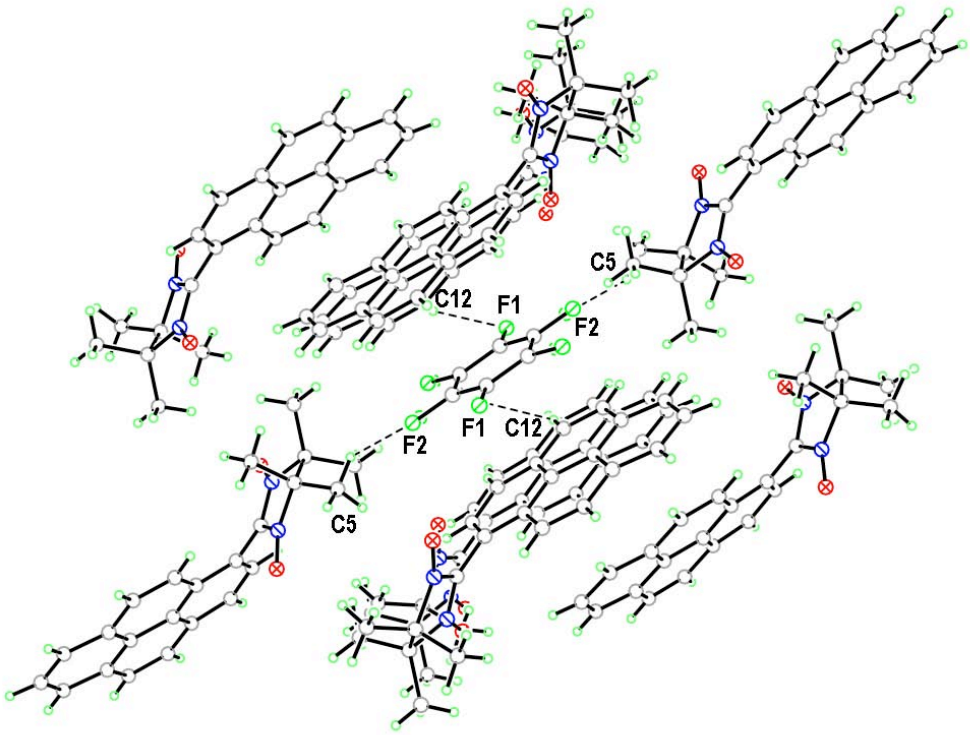
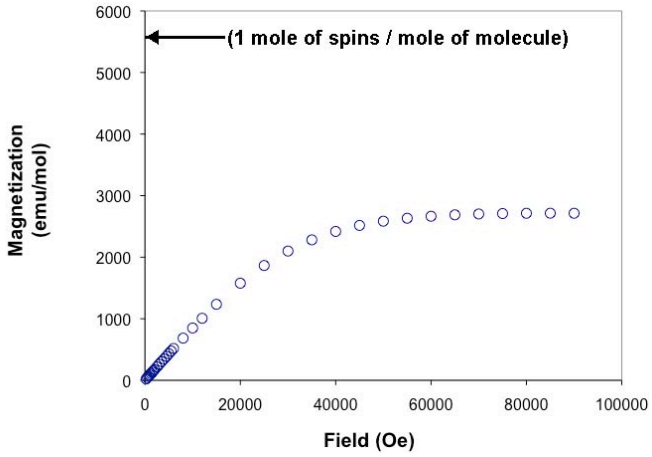
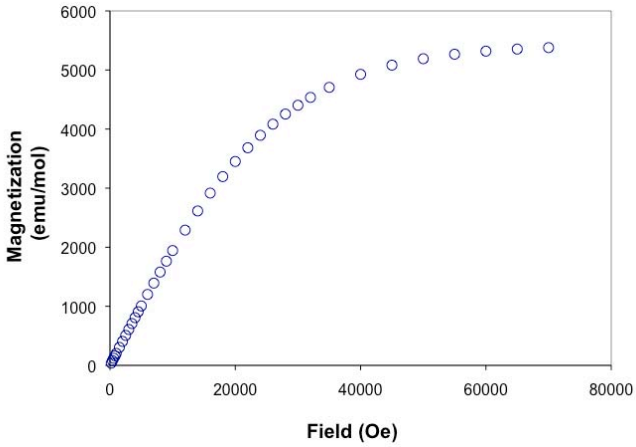


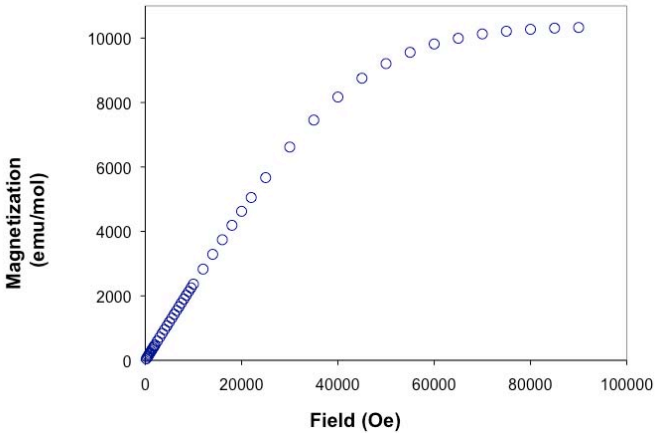
Figure S3. Magnetization versus field data for samples in this study. α-PyrIN and β-PyrNN show essentially zero magnetization at 1.8 K.



α-PyrNN, 1.8 K

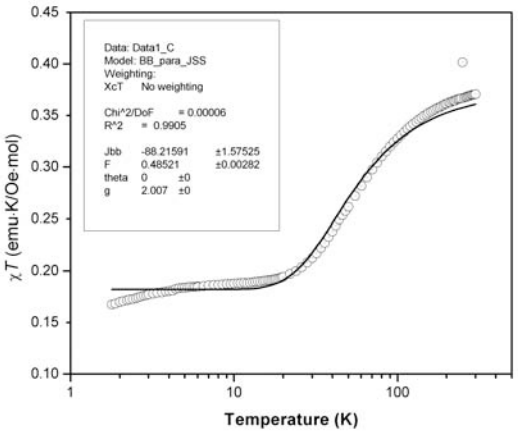


β-PyrIN, 1.8 K



$(PyrNN)_2 \cdot C_6F_6$, 1.8 K

Figure S4. Half-dimer model fit for α-PyrNN χT vs T data at 1000 Oe (dc), no mean field, fitted paramagnetic fraction.



Spin pairing model for S =1/2 spin units

$$H = -JS_1 \cdot S_2$$

$N\beta^2/k$ = 0.375 emu-K/Oe-mol, F = purity factor (fraction of paramagnetic S = ½ spins)

$$\chi T = \left[C \cdot \frac{2}{3 + \exp(-J_{BB}/kT)} \right] \cdot (1 - F) + (F) \cdot 0.375 \cdot \frac{T}{T - \theta} \quad , \quad C = \frac{Ng^2\beta^2}{k} = 0.375 g^2$$

$$\chi T = \left[C \cdot \frac{2}{3 + \exp(-J_{BB}/kT)} \right] \cdot \frac{T}{T - \theta_1} \cdot (1 - F) + (F) \cdot 0.375 \cdot \frac{T}{T - \theta_2} \quad , \quad C = \frac{Ng^2\beta^2}{k} = 0.375 g^2$$

Uncertainties are standard deviations; zero uncertainty means the parameter was fixed.

Figure S5. Half-dimer model fit for α-PyrNN χT vs T data at 1000 Oe (dc), fixed paramagnetic fraction of molecules with a mean field term.

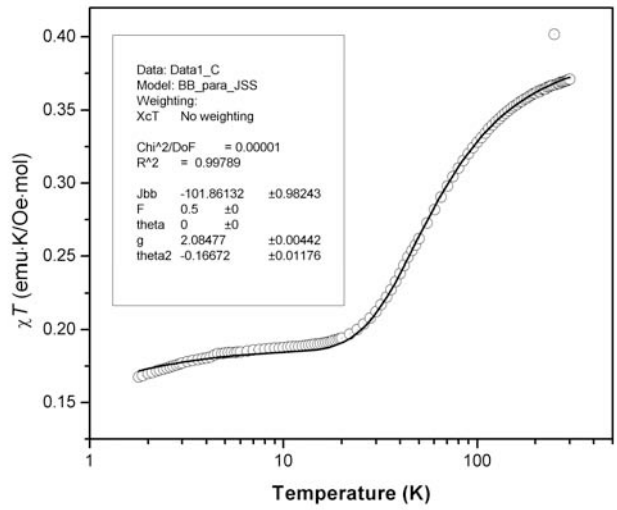
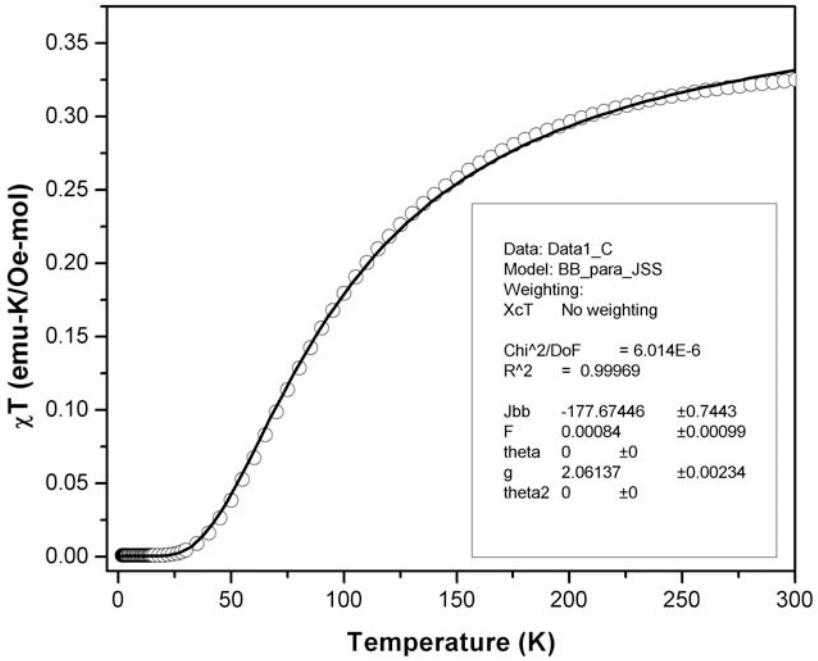


Figure S6. χT vs T data for β-PyrNN at 1000 Oe (dc), with fit to spin pairing model, showing fitted term output.



Spin pairing model for S =1/2 spin units

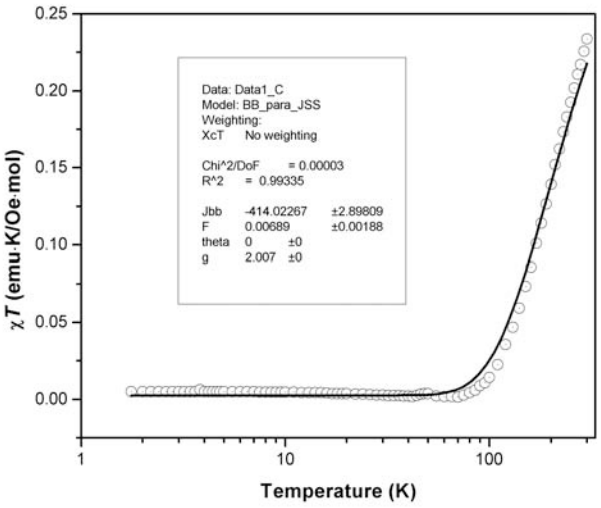
$$H = -JS_1 \cdot S_2$$

$N\beta^2/k$ = 0.375 emu-K/Oe-mol, F = purity factor (fraction of paramagnetic S = ½ spins)

$$\chi T = \left[C \cdot \frac{2}{3 + \exp(-J_{BB}/kT)} \right] \cdot \frac{T}{T - \theta_1} \cdot (1 - F) + (F) \cdot 0.375 \cdot \frac{T}{T - \theta_2} \quad , \quad C = \frac{Ng^2\beta^2}{k} = 0.375 g^2$$

Uncertainties are standard deviations; zero uncertainty means the parameter was fixed.

Figure S7. χT vs T data for α-PyrIN at 1000 Oe (dc), with fit to spin pairing model.



Spin pairing model for S =1/2 spin units

$$H = -JS_1 \cdot S_2$$

$N\beta^2/k$ = 0.375 emu-K/Oe-mol, F = purity factor (fraction of paramagnetic S = ½ spins)

$$\chi T = \left[C \cdot \frac{2}{3 + \exp(-J_{BB}/kT)} \right] \cdot \frac{T}{T-\theta} \cdot (1-F) + (F) \cdot 0.375 \quad , \quad C = \frac{Ng^2\beta^2}{k} = 0.375 g^2$$

Uncertainties are standard deviations; zero uncertainty means the parameter was fixed.

Figure S8. χT vs T data (left, at 1000 Oe) and M vs H data (right, at 1.8 K) for PyrIN crystallized from C_6F_6.

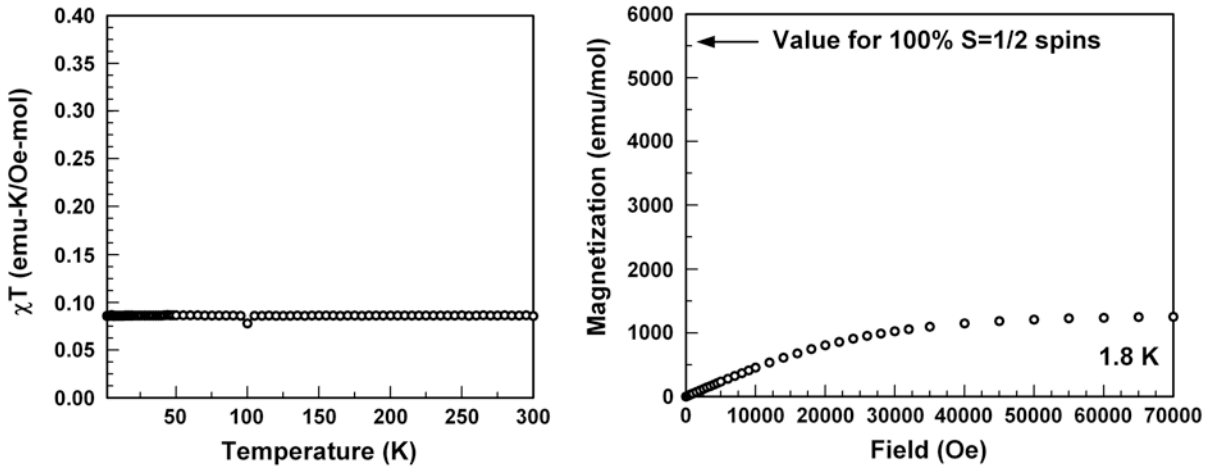
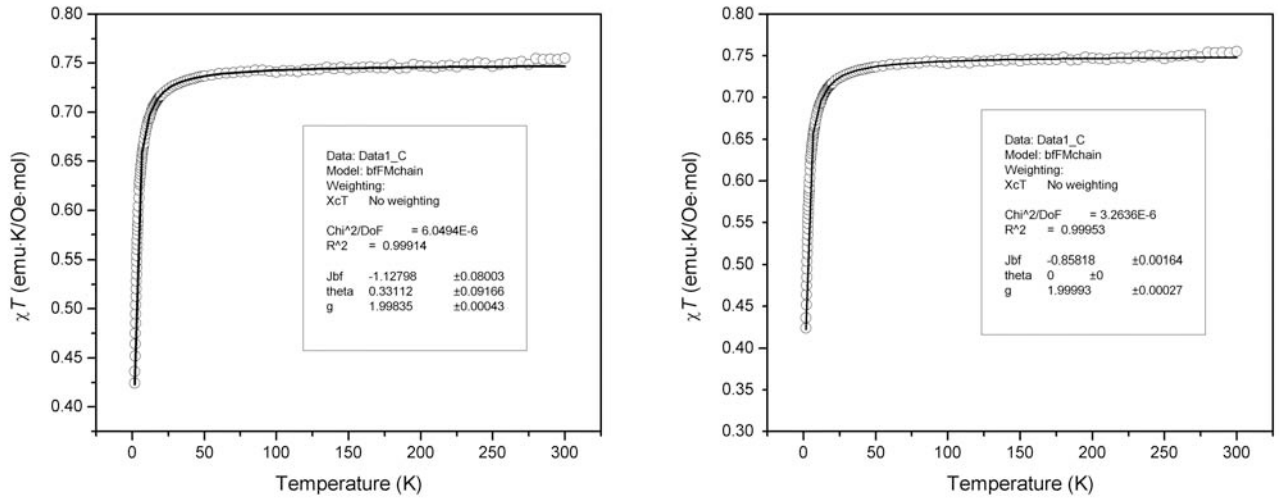


Figure S9. χT vs T data for $(PyrNN)_2 \cdot C_6F_6$ at 1000 Oe (dc); solid lines shows fits to 1-D chain model with (left) and without (right) mean field correction.



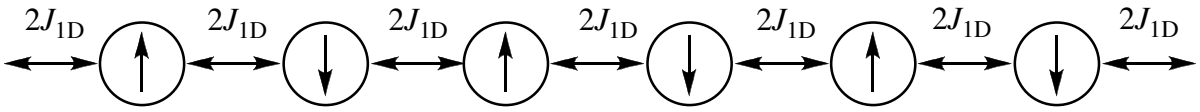
1-D linear Heisenberg chain model for S =1/2 spin units

From Swank, D. D.; Landee, C. P., Willet, R. D. *Phys. Rev. B*, **1979**, *20*, 2154.

$$\chi T = \frac{Ng^2\beta^2}{4k} \cdot \frac{T}{T-\theta} \cdot \left[\frac{1 + A \cdot \left(J_{BF}/2kT\right) + B \cdot \left(J_{BF}/2kT\right)^2 + C \cdot \left(J_{BF}/2kT\right)^3 + D \cdot \left(J_{BF}/2kT\right)^4 + E \cdot \left(\left(J_{BF}/2kT\right)\right)^5}{1 + F \cdot \left(J_{BF}/2kT\right) + G \cdot \left(J_{BF}/2kT\right)^2 + H \cdot \left(J_{BF}/2kT\right)^3 + I \cdot \left(J_{BF}/2kT\right)^4} \right]^{2/3}$$

$$H = -2J \sum_{N=1}^{\infty} S_1 \cdot S_{1+N}$$

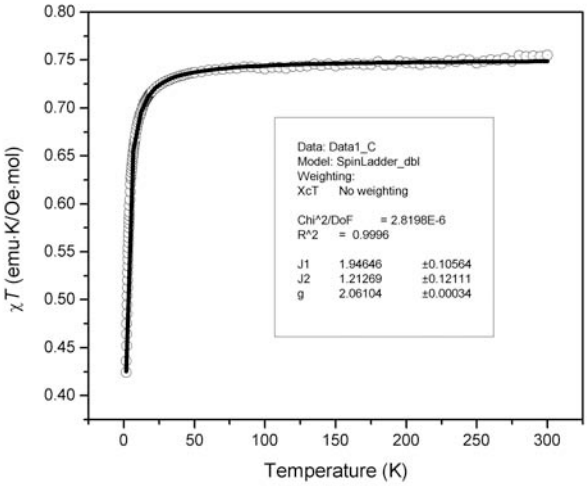
A = 5.7979916, B = 16.902653, C = 29.376885, D = 29.832959, E = 14.036918
and F = 2.7979916, G = 7.0086780 , H = 8.6538644, I = 4.5743114

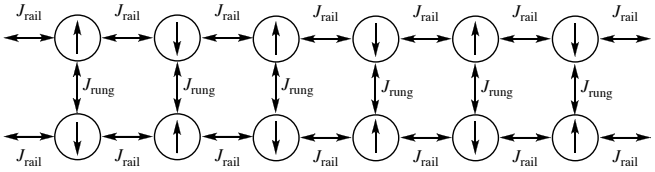


The fit without mean field correction gave g = 1.999 and J_{1D}/k = (–)1.716±0.003 K when converted to a Hamiltonian with J instead of $2J$.

Uncertainties are standard deviations; zero uncertainty means the parameter was fixed.

Figure S10. χT vs T data with spin ladder fitting for $(PyrNN)_2 \cdot C_6F_6$ at 1000 Oe (dc).





$H = J_{rail} \sum_{i=1}^{2} \sum_{j=1}^{\infty} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1} + J_{rung} \sum_{j=1}^{\infty} \mathbf{S}_{1,j} \cdot \mathbf{S}_{2,j}$,where index j refers to the position of the spin along the ladder length and index i = 1,2 refers to which side of the ladder on which the spin is located.

Derived from Johnston, D. C., et al. arXiv:cond-mat/0001147, 2000 (see Table VII in this reference).

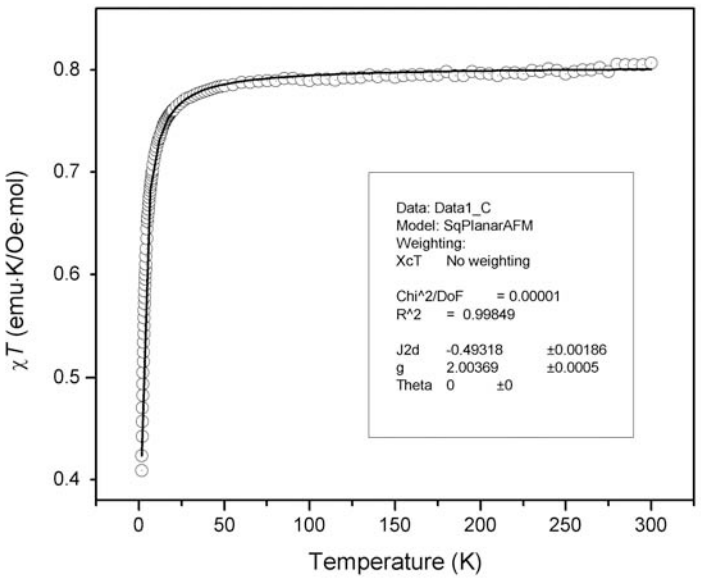
```
[INDVAR]: T
[DEPVAR]:XT
[PARAMS]: J1,J2,g
[EQUATIONS]:

C=2*2*0.5*g*g/4
E1=J1/T
DEL=0.4030*(J2/J1) +
0.0989*(J2/J1)^3
PRE=C*EXP(-DEL*J1/T)
N10=-0.05383784
N11=-0.67282213
N12=0.03896299
N13=0.01103114
N20=0.09740136
N21=0.12334838
N22=-0.0253489
N23=0.00655748
N30=0.01446744
N31=-0.03965984
N32=-0.03120146
N33=0.02118588
N40=0.001392519
N41=0.006657608
N42=-0.020207553
N43=0.008830122
N50=0.0001139343
N51=0.0001341951
N52=0.0016684229
N53=-0.0001396407
N60=0.0
N61=0.0000422531
N62=-0.0001609830
N63=0.0001335788
D10=0.44616216
D11=-0.82582213
D12=0.03896299
D13=-0.8786886
D20=0.32048245
D21=-0.40632550
D22=0.20252880
D23=-0.03801372
D24=0.07998604
D25=-0.00385344
D26=0.00379963
D30=0.13304199
D31=-0.25099527
D32=0.11749096
D33=-0.07871375
D34=0.04106834
D35=-0.01886681
D36=0.00157755
D37=-0.00387185
D38=0.00019055
D39=-0.00010728
D40=0.03718413
D41=-0.10249898
D42=0.04316152
D43=0.01936105
D50=0.002813608
D51=0.000402749
D52=0.001958564
D53=-0.003803837
D60=0.0002646763
D61=-0.0010424633
D62=0.0015813041
D63=-0.000291445
NUM1=E1*(N10+N11*(J2/J1)+N12*(J2/J1)*(J2/J1)+N13*(J2/J1)*(J2/J1)*(J2/J1))
NUM2=E1*E1*(N20+N21*(J2/J1)+N22*(J2/J1)*(J2/J1)+N23*(J2/J1)*(J2/J1)*(J2/J1))
NUM3=E1*E1*E1*(N30+N31*(J2/J1)+N32*(J2/J1)*(J2/J1)+N33*(J2/J1)*(J2/J1)*(J2/J1))
NUM4=E1*E1*E1*E1*(N40+N41*(J2/J1)+N42*(J2/J1)*(J2/J1)+N43*(J2/J1)*(J2/J1)*(J2/J1))
NUM5=E1*E1*E1*E1*E1*(N50+N51*(J2/J1)+N52*(J2/J1)*(J2/J1)+N53*(J2/J1)*(J2/J1)*(J2/J1))
NUM6=E1*E1*E1*E1*E1*E1*(N60+N61*(J2/J1)+N62*(J2/J1)*(J2/J1)+N63*(J2/J1)*(J2/J1)*(J2/J1))
NUM=NUM1+NUM2+NUM3+NUM4+NUM5+NUM6
DUM1=E1*(D10+D11*(J2/J1)+D12*(J2/J1)*(J2/J1)+D13*(J2/J1)*(J2/J1)*(J2/J1))
DUM2a=E1*E1*(D20+D21*(J2/J1)+D22*(J2/J1)*(J2/J1)+D23*(J2/J1)*(J2/J1)*(J2/J1))
DUM2b=E1*E1*(D24*(J2/J1)^4+D25*(J2/J1)^5+D26*(J2/J1)^6)
DUM3a=E1*E1*(D30+D31*(J2/J1)+D32*(J2/J1)*(J2/J1)+D33*(J2/J1)*(J2/J1)*(J2/J1))
DUM3b=E1*E1*(D34*(J2/J1)^4+D35*(J2/J1)^5+D36*(J2/J1)^6)
DUM3c=E1*E1*(D37*(J2/J1)^7+D38*(J2/J1)^8+D39*(J2/J1)^9)
DUM4=E1*(D40+D41*(J2/J1)+D42*(J2/J1)*(J2/J1)+D43*(J2/J1)*(J2/J1)*(J2/J1))
DUM5=E1*(D50+D51*(J2/J1)+D52*(J2/J1)*(J2/J1)+D53*(J2/J1)*(J2/J1)*(J2/J1))
DUM6=E1*(D60+D61*(J2/J1)+D62*(J2/J1)*(J2/J1)+D63*(J2/J1)*(J2/J1)*(J2/J1))
DUM=DUM1+DUM2a+DUM2b+DUM3a+DUM3b+DUM3c+DUM4+DUM5+DUM6

XT=PRE*(1+NUM)/(1+DUM)
```

Fitting to the above function gave g = 2.061, J_{rail}/k = (–)1.95±0.20 K, J_{rung}/k = (–)1.2±0.2 K. Uncertainties are standard deviations; zero uncertainty means the parameter was fixed. However, the statistical analysis also showed co-dependency of >0.9 for the two exchange constants, hence this model was rejected.

Figure S11. χT vs T data with 2-D square planar fitting for $(PyrNN)_2 \cdot C_6F_6$ at 1000 Oe (dc).



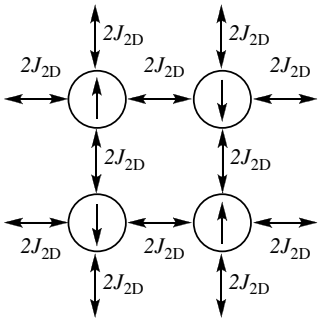
2-D Heisenberg Square Planar AFM system, all S = ½ spin units.

From Baker, G., Jr.; Gilbert, H. E.; Eve, J.; Rushbrooke, G. S. *Phys. Rev. Lett.*, **1967**, *25A*(*3*), 207.

$$\chi = \frac{Ng^2\beta^2}{kT} \cdot \left[1 + \frac{4x}{2} + \frac{16x^2}{(2!)(2^2)} + \frac{64x^3}{(3!)(2^3)} + \frac{416x^4}{(4!)(2^4)} + \frac{4544x^5}{(5!)(2^5)} + \frac{23488x^6}{(6!)(2^6)} - \frac{207616x^7}{(7!)(2^7)} + \frac{4205056x^8}{(8!)(2^8)} + \frac{198295552x^9}{(9!)(2^9)} - \frac{2574439424x^{10}}{(10!)(2^{10})}\right]$$

$$x = J/kT$$

$$H = -2J\sum_{i,j}^{i \neq j} S_i \cdot S_j \quad [\text{for i} < \text{j, j - i} = 1]$$



SQUARE PLANAR

Fitting to the above function gave g = 2.0037, J_{2D}/k = (–)0.986±0.004 K when converted to a Hamiltonian with J instead of 2J. Uncertainties are standard deviations; zero uncertainty means the parameter was fixed.

Archival summaries of computational estimates of exchange for dyad models.

All computations carried out using Gaussian 09 for SuSE Linux. 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 09, Revision B.01, Gaussian, Inc: Wallingford CT, 2010.

Alpha-PyrIN model dyad (replace pyrene and methyls by H) - singlet UB3LYP/6-31G*


```
1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C6H10N4O2\LAHTI\06-Mar-2011\0\\#P G
 FINPUT IOP(6/7=3) UB3LYP/6-31G* TEST GUESS=(READ,MIX)\\Pyrene-IN NO--O
 N contact (S-T xtl geom)\\0,1\C,0,-2.722,0.662,0.804\C,0,2.722,-0.662,
 -0.804\C,0,2.764,0.198,-2.098\C,0,-2.764,-0.198,2.098\H,0,0.134,1.434,
 2.382\H,0,-0.226,-1.353,-2.444\C,0,0.746,-0.933,-2.159\C,0,-0.813,0.93
 6,2.143\H,0,-2.564,-1.272,1.841\H,0,3.346,-1.584,-0.946\H,0,3.735,0.02
 3,-2.632\H,0,-3.735,-0.023,2.632\H,0,2.564,1.272,-1.841\H,0,2.929,-0.0
 1,0.086\H,0,-2.929,0.01,-0.086\H,0,-3.346,1.584,0.946\N,0,-1.64,0.335,
 2.921\N,0,1.64,-0.335,-2.921\N,0,1.281,-1.03,-0.825\N,0,-1.281,1.03,0.
 825\O,0,0.666,-1.503,0.177\O,0,-0.666,1.503,-0.177\\Version=EM64L-G09R
 evB.01\State=1-A\HF=-603.9013655\S2=1.021313\S2-1=0.\S2A=0.265423\RMSD
 =6.000e-09\Dipole=-0.0433768,0.0167506,-0.0333925\Quadrupole=13.068922
 7,-1.2248764,-11.8440463,0.7722017,0.7942993,4.3471792\PG=C01 [X(C6H10
 N4O2)]\\@
```


Alpha-PyrIN model dyad (replace pyrene and methyls by H) - triplet UB3LYP/6-31G*


```
1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C6H10N4O2(3)\LAHTI\06-Mar-2011\0\\#
 P GFINPUT IOP(6/7=3) UB3LYP/6-31G* TEST\\Pyrene-IN NO--ON contact (S-T
  xtl geom)\\0,3\C,0,-2.722,0.662,0.804\C,0,2.722,-0.662,-0.804\C,0,2.7
 64,0.198,-2.098\C,0,-2.764,-0.198,2.098\H,0,0.134,1.434,2.382\H,0,-0.2
 26,-1.353,-2.444\C,0,0.746,-0.933,-2.159\C,0,-0.813,0.936,2.143\H,0,-2
 .564,-1.272,1.841\H,0,3.346,-1.584,-0.946\H,0,3.735,0.023,-2.632\H,0,-
 3.735,-0.023,2.632\H,0,2.564,1.272,-1.841\H,0,2.929,-0.01,0.086\H,0,-2
 .929,0.01,-0.086\H,0,-3.346,1.584,0.946\N,0,-1.64,0.335,2.921\N,0,1.64
 ,-0.335,-2.921\N,0,1.281,-1.03,-0.825\N,0,-1.281,1.03,0.825\O,0,0.666,
 -1.503,0.177\O,0,-0.666,1.503,-0.177\\Version=EM64L-G09RevB.01\State=3
 -A\HF=-603.9007979\S2=2.034541\S2-1=0.\S2A=2.000569\RMSD=5.492e-09\Dip
 ole=-0.0459789,0.0186226,-0.0318582\Quadrupole=13.0472694,-1.2407639,-
 11.8065055,0.7905364,0.774011,4.3442889\PG=C01 [X(C6H10N4O2)]\\@
```


Alpha-PyrNN model dyad (replace pyrene and methyls by H) - singlet UB3LYP/6-31G*


```
1\1\GINC-SKYNET\Stability\UB3LYP\6-31G(d)\C6H10N4O4\LAHTI\07-Mar-2011\
 0\\#P GFINPUT IOP(6/7=3) UB3LYP/6-31G* TEST GUESS=(READ,MIX) STABLE=OP
 T\\Pyrene-NN NO--ON contact (S-T xtl geom)\\0,1\C,0,-3.769,0.069,-4.98
 2\C,0,-0.787,-2.065,-1.788\C,0,-2.69,-0.828,-6.873\C,0,-1.866,-1.169,0
 .104\C,0,-2.862,-2.037,-0.677\C,0,-1.694,0.04,-6.093\H,0,-0.025,-2.352
 ,-2.522\H,0,-4.531,0.356,-4.248\H,0,-3.807,-1.458,-0.85\H,0,-0.748,-0.
 538,-5.919\H,0,-2.957,-3.037,-0.178\H,0,-1.598,1.041,-6.591\H,0,-2.518
 ,-1.909,-6.627\H,0,-2.675,-0.532,-7.956\H,0,-1.88,-1.464,1.187\H,0,-2.
 037,-0.087,-0.142\N,0,-3.979,-0.365,-6.242\N,0,-0.577,-1.631,-0.527\N,
 0,-2.431,0.195,-4.795\N,0,-2.125,-2.192,-1.975\O,0,-5.119,-0.5,-6.825\
 O,0,0.563,-1.494,0.056\O,0,-2.71,-2.581,-3.05\O,0,-1.846,0.585,-3.72\\
 Version=EM64L-G09RevB.01\State=1-A\HF=-754.2345433\S2=1.116057\S2-1=0.
 \S2A=0.93528\RMSD=6.981e-09\Dipole=0.0002573,-0.0019517,0.000105\Quadr
 upole=-9.9394784,1.9114549,8.0280234,-2.2713527,-20.7590782,-2.9461819
 \PG=C01 [X(C6H10N4O4)]\\@
```


Alpha-PyrNN model dyad (replace pyrene by H) - triplet UB3LYP/6-31G*


```
1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C6H10N4O4(3)\LAHTI\07-Mar-2011\0\\#
 P GFINPUT IOP(6/7=3) UB3LYP/6-31G* TEST\\Pyrene-NN NO--ON contact (S-T
  xtl geom)\\0,3\C,0,-3.769,0.069,-4.982\C,0,-0.787,-2.065,-1.788\C,0,-
 2.69,-0.828,-6.873\C,0,-1.866,-1.169,0.104\C,0,-2.862,-2.037,-0.677\C,
```

0,-1.694,0.04,-6.093\H,0,-0.025,-2.352,-2.522\H,0,-4.531,0.356,-4.248\
H,0,-3.807,-1.458,-0.85\H,0,-0.748,-0.538,-5.919\H,0,-2.957,-3.037,-0.
178\H,0,-1.598,1.041,-6.591\H,0,-2.518,-1.909,-6.627\H,0,-2.675,-0.532
,-7.956\H,0,-1.88,-1.464,1.187\H,0,-2.037,-0.087,-0.142\N,0,-3.979,-0.
365,-6.242\N,0,-0.577,-1.631,-0.527\N,0,-2.431,0.195,-4.795\N,0,-2.125
,-2.192,-1.975\O,0,-5.119,-0.5,-6.825\O,0,0.563,-1.494,0.056\O,0,-2.71
,-2.581,-3.05\O,0,-1.846,0.585,-3.72\\Version=EM64L-G09RevB.01\State=3
-A\HF=-754.2344673\S2=2.120438\S2-1=0.\S2A=2.006135\RMSD=7.967e-09\Dip
ole=0.0002664,-0.0019474,0.0001154\Quadrupole=-9.929528,1.8878897,8.04
16383,-2.2819392,-20.7210841,-2.9430759\PG=C01 [X(C6H10N4O4)]\\@

Beta-PyrNN model dyad (replace pyrene and methyls by H) - singlet UB3LYP/6-31G*

1\1\GINC-SKYNET\Stability\UB3LYP\6-31G(d)\C14H26N4O4\LAHTI\31-Jul-2011
\0\\#P GFINPUT IOP(6/7=3) TEST SCF=DIRECT UB3LYP/6-31G* STABLE=OPT\\NN
-NN close contact, beta-PyrNN, no Pyr\\0,1\N,0,-0.45,0.685,21.965\O,0,
-1.568,1.604,25.078\N,0,-0.948,1.188,24.041\O,0,-0.468,0.656,20.688\C,
0,0.614,-0.011,22.764\C,0,-1.398,1.22,22.768\C,0,0.487,0.76,24.104\C,0
,0.722,-0.068,25.347\H,0,0.206,-0.875,25.297\H,0,0.456,0.434,26.121\H,
0,1.654,-0.288,25.412\C,0,1.951,0.118,22.061\H,0,2.197,1.045,22.008\H,
0,1.883,-0.244,21.174\H,0,2.62,-0.364,22.553\C,0,0.19,-1.474,22.857\H,
0,-0.655,-1.535,23.31\H,0,0.851,-1.969,23.347\H,0,0.107,-1.841,21.973\
C,0,1.296,2.061,24.142\H,0,1.125,2.567,23.344\H,0,2.232,1.853,24.194\H
,0,1.039,2.575,24.91\N,0,-3.688,-0.685,27.98\O,0,-2.57,-1.604,24.868\N
,0,-3.19,-1.188,25.905\O,0,-3.671,-0.656,29.257\C,0,-4.753,0.011,27.18
2\C,0,-2.74,-1.22,27.178\C,0,-4.626,-0.76,25.842\C,0,-4.861,0.068,24.5
98\H,0,-4.344,0.875,24.648\H,0,-4.594,-0.434,23.824\H,0,-5.793,0.288,2
4.533\C,0,-6.09,-0.118,27.885\H,0,-6.336,-1.045,27.937\H,0,-6.021,0.24
4,28.771\H,0,-6.759,0.364,27.393\C,0,-4.329,1.474,27.088\H,0,-3.484,1.
535,26.636\H,0,-4.99,1.969,26.598\H,0,-4.245,1.841,27.972\C,0,-5.435,-
2.061,25.804\H,0,-5.264,-2.567,26.601\H,0,-6.371,-1.853,25.752\H,0,-5.
178,-2.575,25.035\H,0,-2.330749,1.690866,22.437121\H,0,-1.807458,-1.69
114,27.509071\\Version=EM64L-G09RevB.01\State=1-A\HF=-1068.444933\S2=1
.099938\S2-1=0.\S2A=0.819323\RMSD=8.865e-09\Dipole=0.0003896,-0.000359
5,0.0003441\Quadrupole=20.7188095,2.0496639,-22.7684734,-1.1239089,2.6
033269,0.5862312\PG=C01 [X(C14H26N4O4)]\\@

Beta-PyrNN model dyad (replace pyrene and methyls by H) - triplet UB3LYP/6-31G*

1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C14H26N4O4(3)\LAHTI\31-Jul-2011\0\\
#P GFINPUT IOP(6/7=3) TEST SCF=DIRECT UB3LYP/6-31G*\\NN-NN close conta
ct, beta-PyrNN, no Pyr\\0,3\N,0,-0.45,0.685,21.965\O,0,-1.568,1.604,25
.078\N,0,-0.948,1.188,24.041\O,0,-0.468,0.656,20.688\C,0,0.614,-0.011,
22.764\C,0,-1.398,1.22,22.768\C,0,0.487,0.76,24.104\C,0,0.722,-0.068,2
5.347\H,0,0.206,-0.875,25.297\H,0,0.456,0.434,26.121\H,0,1.654,-0.288,
25.412\C,0,1.951,0.118,22.061\H,0,2.197,1.045,22.008\H,0,1.883,-0.244,
21.174\H,0,2.62,-0.364,22.553\C,0,0.19,-1.474,22.857\H,0,-0.655,-1.535
,23.31\H,0,0.851,-1.969,23.347\H,0,0.107,-1.841,21.973\C,0,1.296,2.061
,24.142\H,0,1.125,2.567,23.344\H,0,2.232,1.853,24.194\H,0,1.039,2.575,
24.91\N,0,-3.688,-0.685,27.98\O,0,-2.57,-1.604,24.868\N,0,-3.19,-1.188
,25.905\O,0,-3.671,-0.656,29.257\C,0,-4.753,0.011,27.182\C,0,-2.74,-1.
22,27.178\C,0,-4.626,-0.76,25.842\C,0,-4.861,0.068,24.598\H,0,-4.344,0
.875,24.648\H,0,-4.594,-0.434,23.824\H,0,-5.793,0.288,24.533\C,0,-6.09
,-0.118,27.885\H,0,-6.336,-1.045,27.937\H,0,-6.021,0.244,28.771\H,0,-6
.759,0.364,27.393\C,0,-4.329,1.474,27.088\H,0,-3.484,1.535,26.636\H,0,
-4.99,1.969,26.598\H,0,-4.245,1.841,27.972\C,0,-5.435,-2.061,25.804\H,
0,-5.264,-2.567,26.601\H,0,-6.371,-1.853,25.752\H,0,-5.178,-2.575,25.0
35\H,0,-2.330749,1.690866,22.437121\H,0,-1.807458,-1.69114,27.509071\\
Version=EM64L-G09RevB.01\State=3-A\HF=-1068.4447149\S2=2.104891\S2-1=0
.\S2A=2.004708\RMSD=8.164e-09\Dipole=0.0004003,-0.000356,0.0003307\Qua
drupole=20.7063922,2.0353573,-22.7417495,-1.1301547,2.5918291,0.583937
2\PG=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rail model dyad (replace pyrene and methyls by H)- singlet UB3LYP/6-31G*

1\1\GINC-SKYNET\Stability\UB3LYP\6-31G(d)\C14H26N4O4\LAHTI\07-Mar-2011
\0\\#P GFINPUT IOP(6/7=3) UB3LYP/6-31G* TEST GUESS=(READ,MIX) STABLE=O
PT\\Pyrene-NN co C6F6 rail contact\\0,1\N,0,8.603,-7.075,2.422\O,0,8.2
41,-5.959,1.912\H,0,7.494,-7.089,4.277\H,0,11.065,-10.428,2.052\H,0,11
.033,-6.315,2.012\C,0,11.01,-7.227,2.31\H,0,11.762,-7.701,1.947\H,0,11
.05,-7.251,3.269\H,0,8.826,-8.297,0.043\C,0,8.426,-10.101,1.727\H,0,7.
665,-9.559,1.504\H,0,8.143,-10.839,2.273\H,0,8.827,-10.436,0.921\C,0,9
.442,-9.261,2.492\H,0,7.494,0.428,4.277\H,0,10.393,-10.824,3.412\C,0,8
.167,-7.604,3.583\N,0,8.739,-8.814,3.748\C,0,9.72,-7.885,1.838\O,0,8.6

28,-9.568,4.772\H,0,11.291,-9.542,3.324\H,0,10.39,-8.329,-0.044\C,0,9.
635,-7.865,0.323\C,0,10.66,-10.09,2.853\H,0,9.636,-6.956,0.015\C,0,8.1
67,-0.087,3.583\N,0,8.739,-1.297,3.748\O,0,8.628,-2.052,4.772\C,0,9.44
2,-1.745,2.492\C,0,9.72,-0.368,1.838\N,0,8.603,0.441,2.422\O,0,8.241,1
.557,1.912\C,0,8.426,-2.585,1.727\H,0,7.665,-2.043,1.504\H,0,8.143,-3.
322,2.273\H,0,8.827,-2.919,0.921\C,0,10.66,-2.574,2.853\H,0,11.291,-2.
026,3.324\H,0,11.065,-2.912,2.052\H,0,10.393,-3.307,3.412\C,0,9.635,-0
.349,0.323\H,0,8.826,-0.781,0.043\H,0,10.39,-0.813,-0.044\H,0,9.636,0.
56,0.015\C,0,11.01,0.289,2.31\H,0,11.05,0.265,3.269\H,0,11.033,1.201,2
.012\H,0,11.762,-0.185,1.947\\Version=EM64L-G09RevB.01\State=1-A\HF=-1
068.4358902\S2=1.105753\S2-1=0.\S2A=0.833149\RMSD=9.611e-09\Dipole=1.5
334172,-1.4105045,-1.570706\Quadrupole=8.2011381,-6.0415974,-2.1595408
,2.4671034,-2.1286845,12.2749315\PG=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rail model dyad (replace pyrene by H) - triplet UB3LYP/6-31G*

Test job not archived.

1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C14H26N4O4(3)\LAHTI\07-Mar-2011\0\\
#P GFINPUT IOP(6/7=3) UB3LYP/6-31G* TEST\\Pyrene-NN co C6F6 rail conta
ct\\0,3\N,0,8.603,-7.075,2.422\O,0,8.241,-5.959,1.912\H,0,7.494,-7.089
,4.277\H,0,11.065,-10.428,2.052\H,0,11.033,-6.315,2.012\C,0,11.01,-7.2
27,2.31\H,0,11.762,-7.701,1.947\H,0,11.05,-7.251,3.269\H,0,8.826,-8.29
7,0.043\C,0,8.426,-10.101,1.727\H,0,7.665,-9.559,1.504\H,0,8.143,-10.8
39,2.273\H,0,8.827,-10.436,0.921\C,0,9.442,-9.261,2.492\H,0,7.494,0.42
8,4.277\H,0,10.393,-10.824,3.412\C,0,8.167,-7.604,3.583\N,0,8.739,-8.8
14,3.748\C,0,9.72,-7.885,1.838\O,0,8.628,-9.568,4.772\H,0,11.291,-9.54
2,3.324\H,0,10.39,-8.329,-0.044\C,0,9.635,-7.865,0.323\C,0,10.66,-10.0
9,2.853\H,0,9.636,-6.956,0.015\C,0,8.167,-0.087,3.583\N,0,8.739,-1.297
,3.748\O,0,8.628,-2.052,4.772\C,0,9.442,-1.745,2.492\C,0,9.72,-0.368,1
.838\N,0,8.603,0.441,2.422\O,0,8.241,1.557,1.912\C,0,8.426,-2.585,1.72
7\H,0,7.665,-2.043,1.504\H,0,8.143,-3.322,2.273\H,0,8.827,-2.919,0.921
\C,0,10.66,-2.574,2.853\H,0,11.291,-2.026,3.324\H,0,11.065,-2.912,2.05
2\H,0,10.393,-3.307,3.412\C,0,9.635,-0.349,0.323\H,0,8.826,-0.781,0.04
3\H,0,10.39,-0.813,-0.044\H,0,9.636,0.56,0.015\C,0,11.01,0.289,2.31\H,
0,11.05,0.265,3.269\H,0,11.033,1.201,2.012\H,0,11.762,-0.185,1.947\\Ve
rsion=EM64L-G09RevB.01\State=3-A\HF=-1068.4358905\S2=2.105759\S2-1=0.\
S2A=2.004776\RMSD=3.243e-09\Dipole=1.533421,-1.4104874,-1.5707145\Quad
rupole=8.2012117,-6.041711,-2.1595007,2.467148,-2.1286768,12.2749227\P
G=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rung A model dyad (replace pyrene by H) - singlet UB3LYP/6-31G*

1\1\GINC-SKYNET\Stability\UB3LYP\6-31G(d)\C14H26N4O4\LAHTI\07-Mar-2011
\0\\#P GFINPUT IOP(6/7=3) UB3LYP/6-31G* TEST GUESS=(READ,MIX) STABLE=O
PT\\Pyrene-NN co C6F6 rung contact\\0,1\C,0,0.49,-0.087,2.377\C,0,-0.4
9,0.087,-4.79\C,0,-1.765,1.745,-3.698\C,0,1.765,-1.745,1.285\C,0,-2.04
3,0.368,-3.045\C,0,2.043,-0.368,0.631\C,0,0.749,-2.585,0.52\C,0,-0.749
,2.585,-2.934\C,0,-2.983,2.574,-4.059\C,0,2.983,-2.574,1.646\C,0,1.958
,-0.349,-0.884\C,0,-1.958,0.349,-1.53\C,0,3.333,0.289,1.103\C,0,-3.333
,-0.289,-3.516\H,0,0.183,-0.428,-5.484\H,0,-0.184,0.428,3.071\N,0,1.06
2,-1.297,2.542\N,0,-1.062,1.297,-4.955\N,0,0.926,0.441,1.215\N,0,-0.92
6,-0.441,-3.628\O,0,0.951,-2.052,3.566\O,0,-0.951,2.052,-5.979\O,0,-0.
564,-1.557,-3.119\O,0,0.564,1.557,0.705\H,0,0.012,2.043,-2.711\H,0,-0.
012,-2.043,0.297\H,0,0.466,-3.322,1.067\H,0,-0.466,3.322,-3.48\H,0,1.1
5,-2.919,-0.286\H,0,-1.15,2.919,-2.128\H,0,3.614,-2.026,2.117\H,0,-3.6
14,2.026,-4.53\H,0,3.388,-2.912,0.845\H,0,-3.388,2.912,-3.258\H,0,2.71
6,-3.307,2.205\H,0,-2.716,3.307,-4.618\H,0,1.149,-0.781,-1.164\H,0,-1.
149,0.781,-1.25\H,0,-2.713,0.813,-1.163\H,0,2.713,-0.813,-1.251\H,0,1.
959,0.56,-1.192\H,0,-1.959,-0.56,-1.222\H,0,-3.373,-0.265,-4.476\H,0,3
.373,0.265,2.063\H,0,-3.356,-1.201,-3.218\H,0,3.356,1.201,0.805\H,0,4.
085,-0.185,0.74\H,0,-4.085,0.185,-3.154\\Version=EM64L-G09RevB.01\Stat
e=1-A\HF=-1068.4400981\S2=1.103753\S2-1=0.\S2A=0.818158\RMSD=7.694e-09
\Dipole=-0.0004032,0.0000143,0.0001796\Quadrupole=18.2978257,-1.495594
4,-16.8022313,-3.9678589,0.6929532,9.1282142\PG=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rung A model dyad (replace pyrene by H) - triplet UB3LYP/6-31G*

1\1\GINC-SKYNET\SP\UB3LYP\6-31G(d)\C14H26N4O4(3)\LAHTI\07-Mar-2011\0\\
#P GFINPUT IOP(6/7=3) UB3LYP/6-31G* TEST\\Pyrene-NN co C6F6 rung conta
ct\\0,3\C,0,0.49,-0.087,2.377\C,0,-0.49,0.087,-4.79\C,0,-1.765,1.745,-
3.698\C,0,1.765,-1.745,1.285\C,0,-2.043,0.368,-3.045\C,0,2.043,-0.368,

0.631\C,0,0.749,-2.585,0.52\C,0,-0.749,2.585,-2.934\C,0,-2.983,2.574,-
4.059\C,0,2.983,-2.574,1.646\C,0,1.958,-0.349,-0.884\C,0,-1.958,0.349,
-1.53\C,0,3.333,0.289,1.103\C,0,-3.333,-0.289,-3.516\H,0,0.183,-0.428,
-5.484\H,0,-0.184,0.428,3.071\N,0,1.062,-1.297,2.542\N,0,-1.062,1.297,
-4.955\N,0,0.926,0.441,1.215\N,0,-0.926,-0.441,-3.628\O,0,0.951,-2.052
,3.566\O,0,-0.951,2.052,-5.979\O,0,-0.564,-1.557,-3.119\O,0,0.564,1.55
7,0.705\H,0,0.012,2.043,-2.711\H,0,-0.012,-2.043,0.297\H,0,0.466,-3.32
2,1.067\H,0,-0.466,3.322,-3.48\H,0,1.15,-2.919,-0.286\H,0,-1.15,2.919,
-2.128\H,0,3.614,-2.026,2.117\H,0,-3.614,2.026,-4.53\H,0,3.388,-2.912,
0.845\H,0,-3.388,2.912,-3.258\H,0,2.716,-3.307,2.205\H,0,-2.716,3.307,
-4.618\H,0,1.149,-0.781,-1.164\H,0,-1.149,0.781,-1.25\H,0,-2.713,0.813
,-1.163\H,0,2.713,-0.813,-1.251\H,0,1.959,0.56,-1.192\H,0,-1.959,-0.56
,-1.222\H,0,-3.373,-0.265,-4.476\H,0,3.373,0.265,2.063\H,0,-3.356,-1.2
01,-3.218\H,0,3.356,1.201,0.805\H,0,4.085,-0.185,0.74\H,0,-4.085,0.185
,-3.154\\Version=EM64L-G09RevB.01\State=3-A\HF=-1068.4400956\S2=2.1037
83\S2-1=0.\S2A=2.004614\RMSD=5.210e-09\Dipole=-0.0004028,0.0000108,0.0
001825\Quadrupole=18.2975942,-1.4955214,-16.8020728,-3.9679858,0.69263
68,9.1279773\PG=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rung B model dyad (replace pyrene by H) - singlet UB3LYP/6-31G*

1\1\GINC-SKYNET\Stability\UB3LYP\6-31G(d)\C14H26N4O4\LAHTI\03-Nov-2011
\0\\#P GFINPUT IOP(6/7=3) TEST UB3LYP/6-31G* STABLE=OPT GUESS=(READ,MI
X)\\Pyrene-NN Co-xtl Rung B model\\0,1\O,0,-2.267,5.818,4.34\O,0,-1.92
9,2.154,7.161\N,0,-2.392,5.046,5.351\N,0,-2.275,3.285,6.666\C,0,-1.829
,3.826,5.506\C,0,-3.076,5.492,6.622\C,0,-3.379,4.112,7.266\C,0,-2.044,
6.317,7.393\H,0,-1.725,7.052,6.828\H,0,-1.288,5.745,7.641\H,0,-2.456,6
.682,8.203\C,0,-4.291,6.34,6.295\H,0,-4.787,6.531,7.119\H,0,-4.87,5.85
4,5.672\H,0,-4.002,7.181,5.885\C,0,-4.692,3.479,6.794\H,0,-4.745,3.527
,5.816\H,0,-5.448,3.964,7.186\H,0,-4.723,2.541,7.077\C,0,-3.286,4.071,
8.782\H,0,-3.369,3.144,9.09\H,0,-4.008,4.61,9.168\H,0,-2.421,4.433,9.0
65\O,0,-6.77,9.552,4.695\O,0,-7.107,5.888,1.873\N,0,-6.645,8.781,3.684
\N,0,-6.761,7.02,2.368\C,0,-7.207,7.56,3.528\C,0,-5.96,9.227,2.412\C,0
,-5.657,7.846,1.768\C,0,-6.993,10.051,1.641\H,0,-7.311,10.786,2.206\H,
0,-7.748,9.479,1.393\H,0,-6.58,10.417,0.831\C,0,-4.745,10.074,2.739\H,
0,-4.249,10.266,1.915\H,0,-4.166,9.588,3.363\H,0,-5.034,10.916,3.149\C
,0,-4.344,7.213,2.24\H,0,-4.291,7.261,3.218\H,0,-3.588,7.698,1.848\H,0
,-4.313,6.275,1.957\C,0,-5.75,7.806,0.252\H,0,-5.667,6.879,-0.056\H,0,
-5.028,8.344,-0.134\H,0,-6.615,8.168,-0.031\H,0,-1.153,3.313,4.813\H,0
,-7.884,7.047,4.221\\Version=EM64L-G09RevB.01\State=1-A\HF=-1068.54505
07\S2=1.109114\S2-1=0.\S2A=0.859428\RMSD=6.011e-09\Dipole=0.1258496,1.
0251651,0.0873705\Quadrupole=-2.7836774,-7.562799,10.3464764,5.658677,
-3.1294764,-6.1829852\PG=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rung B model dyad (replace pyrene by H) - triplet UB3LYP/6-31G*

1\1\GINC-SKYNET\Stability\UB3LYP\6-31G(d)\C14H26N4O4(3)\LAHTI\02-Nov-2
011\0\\#P GFINPUT IOP(6/7=3) TEST UB3LYP/6-31G* STABLE=OPT\\Pyrene-NN
Co-xtl Rung B model\\0,3\O,0,-2.267,5.818,4.34\O,0,-1.929,2.154,7.161\
N,0,-2.392,5.046,5.351\N,0,-2.275,3.285,6.666\C,0,-1.829,3.826,5.506\C
,0,-3.076,5.492,6.622\C,0,-3.379,4.112,7.266\C,0,-2.044,6.317,7.393\H,
0,-1.725,7.052,6.828\H,0,-1.288,5.745,7.641\H,0,-2.456,6.682,8.203\C,0
,-4.291,6.34,6.295\H,0,-4.787,6.531,7.119\H,0,-4.87,5.854,5.672\H,0,-4
.002,7.181,5.885\C,0,-4.692,3.479,6.794\H,0,-4.745,3.527,5.816\H,0,-5.
448,3.964,7.186\H,0,-4.723,2.541,7.077\C,0,-3.286,4.071,8.782\H,0,-3.3
69,3.144,9.09\H,0,-4.008,4.61,9.168\H,0,-2.421,4.433,9.065\O,0,-6.77,9
.552,4.695\O,0,-7.107,5.888,1.873\N,0,-6.645,8.781,3.684\N,0,-6.761,7.
02,2.368\C,0,-7.207,7.56,3.528\C,0,-5.96,9.227,2.412\C,0,-5.657,7.846,
1.768\C,0,-6.993,10.051,1.641\H,0,-7.311,10.786,2.206\H,0,-7.748,9.479
,1.393\H,0,-6.58,10.417,0.831\C,0,-4.745,10.074,2.739\H,0,-4.249,10.26
6,1.915\H,0,-4.166,9.588,3.363\H,0,-5.034,10.916,3.149\C,0,-4.344,7.21
3,2.24\H,0,-4.291,7.261,3.218\H,0,-3.588,7.698,1.848\H,0,-4.313,6.275,
1.957\C,0,-5.75,7.806,0.252\H,0,-5.667,6.879,-0.056\H,0,-5.028,8.344,-
0.134\H,0,-6.615,8.168,-0.031\H,0,-1.153,3.313,4.813\H,0,-7.884,7.047,
4.221\\Version=EM64L-G09RevB.01\State=3-A\HF=-1068.545048\S2=2.109194\
S2-1=0.\S2A=2.005089\RMSD=9.840e-09\Dipole=0.1259893,1.0249854,0.08749
09\Quadrupole=-2.7835724,-7.5628624,10.3464349,5.6587351,-3.1294121,-6
.1829461\PG=C01 [X(C14H26N4O4)]\\@

Alpha-PyrIN model dyad (replace pyrene and methyls by H) - singlet UB97D/6-31+G*

1\1\GINC-SKYNET\SP\UB97D\6-31+G(d)\C6H10N4O2\LAHTI\06-Mar-2011\0\\#P G
FINPUT IOP(6/7=3) UB97D/6-31+G(d) TEST GUESS=(READ,MIX)\\Pyrene-IN NO-
-ON contact (S-T xtl geom)\\0,1\C,0,-2.722,0.662,0.804\C,0,2.722,-0.66
2,-0.804\C,0,2.764,0.198,-2.098\C,0,-2.764,-0.198,2.098\H,0,0.134,1.43
4,2.382\H,0,-0.226,-1.353,-2.444\C,0,0.746,-0.933,-2.159\C,0,-0.813,0.
936,2.143\H,0,-2.564,-1.272,1.841\H,0,3.346,-1.584,-0.946\H,0,3.735,0.
023,-2.632\H,0,-3.735,-0.023,2.632\H,0,2.564,1.272,-1.841\H,0,2.929,-0
.01,0.086\H,0,-2.929,0.01,-0.086\H,0,-3.346,1.584,0.946\N,0,-1.64,0.33
5,2.921\N,0,1.64,-0.335,-2.921\N,0,1.281,-1.03,-0.825\N,0,-1.281,1.03,
0.825\O,0,0.666,-1.503,0.177\O,0,-0.666,1.503,-0.177\\Version=EM64L-G0
9RevB.01\State=1-A\HF=-603.5371774\S2=0.976501\S2-1=0.\S2A=0.122152\RM
SD=6.451e-09\Dipole=-0.0349822,0.0093073,-0.0259334\Quadrupole=14.3286
194,-1.4049456,-12.9236738,0.9339682,0.6123585,4.4313792\PG=C01 [X(C6H
10N4O2)]\\@

Alpha-PyrIN model dyad (replace pyrene and methyls by H) - triplet UB97D/6-31+G*

1\1\GINC-SKYNET\SP\UB97D\6-31+G(d)\C6H10N4O2(3)\LAHTI\06-Mar-2011\0\\#
P GFINPUT IOP(6/7=3) UB97D/6-31+G(d) TEST\\Pyrene-IN NO--ON contact (S
-T xtl geom)\\0,3\C,0,-2.722,0.662,0.804\C,0,2.722,-0.662,-0.804\C,0,2
.764,0.198,-2.098\C,0,-2.764,-0.198,2.098\H,0,0.134,1.434,2.382\H,0,-0
.226,-1.353,-2.444\C,0,0.746,-0.933,-2.159\C,0,-0.813,0.936,2.143\H,0,
-2.564,-1.272,1.841\H,0,3.346,-1.584,-0.946\H,0,3.735,0.023,-2.632\H,0
,-3.735,-0.023,2.632\H,0,2.564,1.272,-1.841\H,0,2.929,-0.01,0.086\H,0,
-2.929,0.01,-0.086\H,0,-3.346,1.584,0.946\N,0,-1.64,0.335,2.921\N,0,1.
64,-0.335,-2.921\N,0,1.281,-1.03,-0.825\N,0,-1.281,1.03,0.825\O,0,0.66
6,-1.503,0.177\O,0,-0.666,1.503,-0.177\\Version=EM64L-G09RevB.01\State
=3-A\HF=-603.5362612\S2=2.017373\S2-1=0.\S2A=2.000171\RMSD=7.124e-09\D
ipole=-0.0470072,0.0170996,-0.0169064\Quadrupole=14.2923061,-1.438191,
-12.8541152,0.9632094,0.5771795,4.4317974\PG=C01 [X(C6H10N4O2)]\\@

Alpha-PyrNN model dyad (replace pyrene and methyls by H) - singlet UB97D/6-31+G*

1\1\GINC-SKYNET\SP\UB97D\6-31+G(d)\C6H10N4O4\LAHTI\06-Mar-2011\0\\#P G
FINPUT IOP(6/7=3) UB97D/6-31+G(d) TEST GUESS=(READ,MIX)\\Pyrene-NN NO-
-ON contact (S-T xtl geom)\\0,1\C,0,-3.769,0.069,-4.982\C,0,-0.787,-2.
065,-1.788\C,0,-2.69,-0.828,-6.873\C,0,-1.866,-1.169,0.104\C,0,-2.862,
-2.037,-0.677\C,0,-1.694,0.04,-6.093\H,0,-0.025,-2.352,-2.522\H,0,-4.5
31,0.356,-4.248\H,0,-3.807,-1.458,-0.85\H,0,-0.748,-0.538,-5.919\H,0,-
2.957,-3.037,-0.178\H,0,-1.598,1.041,-6.591\H,0,-2.518,-1.909,-6.627\H
,0,-2.675,-0.532,-7.956\H,0,-1.88,-1.464,1.187\H,0,-2.037,-0.087,-0.14
2\N,0,-3.979,-0.365,-6.242\N,0,-0.577,-1.631,-0.527\N,0,-2.431,0.195,-
4.795\N,0,-2.125,-2.192,-1.975\O,0,-5.119,-0.5,-6.825\O,0,0.563,-1.494
,0.056\O,0,-2.71,-2.581,-3.05\O,0,-1.846,0.585,-3.72\\Version=EM64L-G0
9RevB.01\State=1-A\HF=-753.8155552\S2=1.017398\S2-1=0.\S2A=0.24967\RMS
D=9.618e-09\Dipole=-0.0000732,-0.0020321,-0.0001123\Quadrupole=-10.552
9235,2.2312632,8.3216604,-2.4257613,-22.0672785,-3.1689674\PG=C01 [X(C
6H10N4O4)]\\@

Alpha-PyrNN model dyad (replace pyrene and methyls by H) - triplet UB97D/6-31+G*

1\1\GINC-SKYNET\SP\UB97D\6-31+G(d)\C6H10N4O4(3)\LAHTI\06-Mar-2011\0\\#
P GFINPUT IOP(6/7=3) UB97D/6-31+G(d) TEST\\Pyrene-NN NO--ON contact (S
-T xtl geom)\\0,3\C,0,-3.769,0.069,-4.982\C,0,-0.787,-2.065,-1.788\C,0
,-2.69,-0.828,-6.873\C,0,-1.866,-1.169,0.104\C,0,-2.862,-2.037,-0.677\
C,0,-1.694,0.04,-6.093\H,0,-0.025,-2.352,-2.522\H,0,-4.531,0.356,-4.24
8\H,0,-3.807,-1.458,-0.85\H,0,-0.748,-0.538,-5.919\H,0,-2.957,-3.037,-
0.178\H,0,-1.598,1.041,-6.591\H,0,-2.518,-1.909,-6.627\H,0,-2.675,-0.5
32,-7.956\H,0,-1.88,-1.464,1.187\H,0,-2.037,-0.087,-0.142\N,0,-3.979,-
0.365,-6.242\N,0,-0.577,-1.631,-0.527\N,0,-2.431,0.195,-4.795\N,0,-2.1
25,-2.192,-1.975\O,0,-5.119,-0.5,-6.825\O,0,0.563,-1.494,0.056\O,0,-2.
71,-2.581,-3.05\O,0,-1.846,0.585,-3.72\\Version=EM64L-G09RevB.01\State
=3-A\HF=-753.8153488\S2=2.032707\S2-1=0.\S2A=2.000519\RMSD=2.800e-09\D
ipole=-0.000059,-0.002025,-0.0000898\Quadrupole=-10.533596,2.1873294,8
.3462665,-2.4424338,-22.0005786,-3.1638463\PG=C01 [X(C6H10N4O4)]\\@

Beta-PyrNN model dyad (replace pyrene and methyls by H) - singlet UB97D/6-31+G*

1\1\GINC-SKYNET\Stability\UB97D\6-31+G(d)\C14H26N4O4\LAHTI\29-Jul-2011
\0\\#P GFINPUT IOP(6/7=3) TEST SCF=DIRECT UB97D/6-31+G(d) STABLE=OPT\\
NN-NN close contact, beta-PyrNN, no Pyr\\0,1\N,0,-0.45,0.685,21.965\O,
0,-1.568,1.604,25.078\N,0,-0.948,1.188,24.041\O,0,-0.468,0.656,20.688\

C,0,0.614,-0.011,22.764\C,0,-1.398,1.22,22.768\C,0,0.487,0.76,24.104\C
,0,0.722,-0.068,25.347\H,0,0.206,-0.875,25.297\H,0,0.456,0.434,26.121\
H,0,1.654,-0.288,25.412\C,0,1.951,0.118,22.061\H,0,2.197,1.045,22.008\
H,0,1.883,-0.244,21.174\H,0,2.62,-0.364,22.553\C,0,0.19,-1.474,22.857\
H,0,-0.655,-1.535,23.31\H,0,0.851,-1.969,23.347\H,0,0.107,-1.841,21.97
3\C,0,1.296,2.061,24.142\H,0,1.125,2.567,23.344\H,0,2.232,1.853,24.194
\H,0,1.039,2.575,24.91\N,0,-3.688,-0.685,27.98\O,0,-2.57,-1.604,24.868
\N,0,-3.19,-1.188,25.905\O,0,-3.671,-0.656,29.257\C,0,-4.753,0.011,27.
182\C,0,-2.74,-1.22,27.178\C,0,-4.626,-0.76,25.842\C,0,-4.861,0.068,24
.598\H,0,-4.344,0.875,24.648\H,0,-4.594,-0.434,23.824\H,0,-5.793,0.288
,24.533\C,0,-6.09,-0.118,27.885\H,0,-6.336,-1.045,27.937\H,0,-6.021,0.
244,28.771\H,0,-6.759,0.364,27.393\C,0,-4.329,1.474,27.088\H,0,-3.484,
1.535,26.636\H,0,-4.99,1.969,26.598\H,0,-4.245,1.841,27.972\C,0,-5.435
,-2.061,25.804\H,0,-5.264,-2.567,26.601\H,0,-6.371,-1.853,25.752\H,0,-
5.178,-2.575,25.035\H,0,-2.330749,1.690866,22.437121\H,0,-1.807458,-1.
69114,27.509071\\Version=EM64L-G09RevB.01\State=1-A\HF=-1067.7993996\S
2=1.008811\S2-1=0.\S2A=0.221509\RMSD=2.270e-09\Dipole=0.0003016,-0.000
417,0.0005761\Quadrupole=22.6330028,2.1898651,-24.8228679,-1.1842575,2
.5466182,1.1059322\PG=C01 [X(C14H26N4O4)]\\@

Beta-PyrNN model dyad (replace pyrene and methyls by H) - triplet UB97D/6-31+G*

1\1\GINC-SKYNET\SP\UB97D\6-31+G(d)\C14H26N4O4(3)\LAHTI\29-Jul-2011\0\\
#P GFINPUT IOP(6/7=3) TEST SCF=DIRECT UB97D/6-31+G(d)\\NN-NN close con
tact, beta-PyrNN, no Pyr\\0,3\N,0,-0.45,0.685,21.965\O,0,-1.568,1.604,
25.078\N,0,-0.948,1.188,24.041\O,0,-0.468,0.656,20.688\C,0,0.614,-0.01
1,22.764\C,0,-1.398,1.22,22.768\C,0,0.487,0.76,24.104\C,0,0.722,-0.068
,25.347\H,0,0.206,-0.875,25.297\H,0,0.456,0.434,26.121\H,0,1.654,-0.28
8,25.412\C,0,1.951,0.118,22.061\H,0,2.197,1.045,22.008\H,0,1.883,-0.24
4,21.174\H,0,2.62,-0.364,22.553\C,0,0.19,-1.474,22.857\H,0,-0.655,-1.5
35,23.31\H,0,0.851,-1.969,23.347\H,0,0.107,-1.841,21.973\C,0,1.296,2.0
61,24.142\H,0,1.125,2.567,23.344\H,0,2.232,1.853,24.194\H,0,1.039,2.57
5,24.91\N,0,-3.688,-0.685,27.98\O,0,-2.57,-1.604,24.868\N,0,-3.19,-1.1
88,25.905\O,0,-3.671,-0.656,29.257\C,0,-4.753,0.011,27.182\C,0,-2.74,-
1.22,27.178\C,0,-4.626,-0.76,25.842\C,0,-4.861,0.068,24.598\H,0,-4.344
,0.875,24.648\H,0,-4.594,-0.434,23.824\H,0,-5.793,0.288,24.533\C,0,-6.
09,-0.118,27.885\H,0,-6.336,-1.045,27.937\H,0,-6.021,0.244,28.771\H,0,
-6.759,0.364,27.393\C,0,-4.329,1.474,27.088\H,0,-3.484,1.535,26.636\H,
0,-4.99,1.969,26.598\H,0,-4.245,1.841,27.972\C,0,-5.435,-2.061,25.804\
H,0,-5.264,-2.567,26.601\H,0,-6.371,-1.853,25.752\H,0,-5.178,-2.575,25
.035\H,0,-2.330749,1.690866,22.437121\H,0,-1.807458,-1.69114,27.509071
\\Version=EM64L-G09RevB.01\State=3-A\HF=-1067.7990203\S2=2.02913\S2-1=
0.\S2A=2.00042\RMSD=7.063e-09\Dipole=0.0003793,-0.0003779,0.0004844\Qu
adrupole=22.609546,2.1727677,-24.7823137,-1.1972674,2.5292104,1.109220
7\PG=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rail model dyad (replace pyrene by H) - singlet UB97D/6-31+G*

1\1\GINC-SKYNET\SP\UB97D\6-31+G(d)\C14H26N4O4\LAHTI\06-Mar-2011\0\\#P
GFINPUT IOP(6/7=3) UB97D/6-31+G(d) TEST GUESS=(READ,MIX)\\Pyrene-NN co
C6F6 rail contact\\0,1\N,0,8.603,-7.075,2.422\O,0,8.241,-5.959,1.912\
H,0,7.494,-7.089,4.277\H,0,11.065,-10.428,2.052\H,0,11.033,-6.315,2.01
2\C,0,11.01,-7.227,2.31\H,0,11.762,-7.701,1.947\H,0,11.05,-7.251,3.269
\H,0,8.826,-8.297,0.043\C,0,8.426,-10.101,1.727\H,0,7.665,-9.559,1.504
\H,0,8.143,-10.839,2.273\H,0,8.827,-10.436,0.921\C,0,9.442,-9.261,2.49
2\H,0,7.494,0.428,4.277\H,0,10.393,-10.824,3.412\C,0,8.167,-7.604,3.58
3\N,0,8.739,-8.814,3.748\C,0,9.72,-7.885,1.838\O,0,8.628,-9.568,4.772\
H,0,11.291,-9.542,3.324\H,0,10.39,-8.329,-0.044\C,0,9.635,-7.865,0.323
\C,0,10.66,-10.09,2.853\H,0,9.636,-6.956,0.015\C,0,8.167,-0.087,3.583\
N,0,8.739,-1.297,3.748\O,0,8.628,-2.052,4.772\C,0,9.442,-1.745,2.492\C
,0,9.72,-0.368,1.838\N,0,8.603,0.441,2.422\O,0,8.241,1.557,1.912\C,0,8
.426,-2.585,1.727\H,0,7.665,-2.043,1.504\H,0,8.143,-3.322,2.273\H,0,8.
827,-2.919,0.921\C,0,10.66,-2.574,2.853\H,0,11.291,-2.026,3.324\H,0,11
.065,-2.912,2.052\H,0,10.393,-3.307,3.412\C,0,9.635,-0.349,0.323\H,0,8
.826,-0.781,0.043\H,0,10.39,-0.813,-0.044\H,0,9.636,0.56,0.015\C,0,11.
01,0.289,2.31\H,0,11.05,0.265,3.269\H,0,11.033,1.201,2.012\H,0,11.762,
-0.185,1.947\\Version=EM64L-G09RevB.01\State=1-A\HF=-1067.7886123\S2=1
.029076\S2-1=0.\S2A=0.23325\RMSD=3.071e-09\Dipole=1.6945342,-1.513231,
-1.7505637\Quadrupole=8.8620039,-6.5990905,-2.2629135,2.8301174,-1.908
3731,12.9400955\PG=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rail model dyad (replace pyrene by H) - triplet UB97D/6-31+G*

1\1\GINC-SKYNET\SP\UB97D\6-31+G(d)\C14H26N4O4(3)\LAHTI\06-Mar-2011\0\\
#P GFINPUT IOP(6/7=3) UB97D/6-31+G(d) TEST\\Pyrene-NN co C6F6 rail con
tact\\0,3\N,0,8.603,-7.075,2.422\O,0,8.241,-5.959,1.912\H,0,7.494,-7.0
89,4.277\H,0,11.065,-10.428,2.052\H,0,11.033,-6.315,2.012\C,0,11.01,-7
.227,2.31\H,0,11.762,-7.701,1.947\H,0,11.05,-7.251,3.269\H,0,8.826,-8.
297,0.043\C,0,8.426,-10.101,1.727\H,0,7.665,-9.559,1.504\H,0,8.143,-10
.839,2.273\H,0,8.827,-10.436,0.921\C,0,9.442,-9.261,2.492\H,0,7.494,0.
428,4.277\H,0,10.393,-10.824,3.412\C,0,8.167,-7.604,3.583\N,0,8.739,-8
.814,3.748\C,0,9.72,-7.885,1.838\O,0,8.628,-9.568,4.772\H,0,11.291,-9.
542,3.324\H,0,10.39,-8.329,-0.044\C,0,9.635,-7.865,0.323\C,0,10.66,-10
.09,2.853\H,0,9.636,-6.956,0.015\C,0,8.167,-0.087,3.583\N,0,8.739,-1.2
97,3.748\O,0,8.628,-2.052,4.772\C,0,9.442,-1.745,2.492\C,0,9.72,-0.368
,1.838\N,0,8.603,0.441,2.422\O,0,8.241,1.557,1.912\C,0,8.426,-2.585,1.
727\H,0,7.665,-2.043,1.504\H,0,8.143,-3.322,2.273\H,0,8.827,-2.919,0.9
21\C,0,10.66,-2.574,2.853\H,0,11.291,-2.026,3.324\H,0,11.065,-2.912,2.
052\H,0,10.393,-3.307,3.412\C,0,9.635,-0.349,0.323\H,0,8.826,-0.781,0.
043\H,0,10.39,-0.813,-0.044\H,0,9.636,0.56,0.015\C,0,11.01,0.289,2.31\
H,0,11.05,0.265,3.269\H,0,11.033,1.201,2.012\H,0,11.762,-0.185,1.947\\
Version=EM64L-G09RevB.01\State=3-A\HF=-1067.7886126\S2=2.029132\S2-1=0
.\S2A=2.00042\RMSD=5.142e-09\Dipole=1.6945407,-1.5133106,-1.7505907\Qu
adrupole=8.8624152,-6.5998097,-2.2626056,2.8304071,-1.9083149,12.94004
25\PG=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rung model dyad (replace pyrene by H) – singlet UB97D/6-31+G*

1\1\GINC-SKYNET\SP\UB97D\6-31+G(d)\C14H26N4O4\LAHTI\06-Mar-2011\0\\#P
GFINPUT IOP(6/7=3) UB97D/6-31+G(d) TEST GUESS=(READ,MIX)\\Pyrene-NN co
C6F6 rung contact\\0,1\C,0,0.49,-0.087,2.377\C,0,-0.49,0.087,-4.79\C,
0,-1.765,1.745,-3.698\C,0,1.765,-1.745,1.285\C,0,-2.043,0.368,-3.045\C
,0,2.043,-0.368,0.631\C,0,0.749,-2.585,0.52\C,0,-0.749,2.585,-2.934\C,
0,-2.983,2.574,-4.059\C,0,2.983,-2.574,1.646\C,0,1.958,-0.349,-0.884\C
,0,-1.958,0.349,-1.53\C,0,3.333,0.289,1.103\C,0,-3.333,-0.289,-3.516\H
,0,0.183,-0.428,-5.484\H,0,-0.184,0.428,3.071\N,0,1.062,-1.297,2.542\N
,0,-1.062,1.297,-4.955\N,0,0.926,0.441,1.215\N,0,-0.926,-0.441,-3.628\
O,0,0.951,-2.052,3.566\O,0,-0.951,2.052,-5.979\O,0,-0.564,-1.557,-3.11
9\O,0,0.564,1.557,0.705\H,0,0.012,2.043,-2.711\H,0,-0.012,-2.043,0.297
\H,0,0.466,-3.322,1.067\H,0,-0.466,3.322,-3.48\H,0,1.15,-2.919,-0.286\
H,0,-1.15,2.919,-2.128\H,0,3.614,-2.026,2.117\H,0,-3.614,2.026,-4.53\H
,0,3.388,-2.912,0.845\H,0,-3.388,2.912,-3.258\H,0,2.716,-3.307,2.205\H
,0,-2.716,3.307,-4.618\H,0,1.149,-0.781,-1.164\H,0,-1.149,0.781,-1.25\
H,0,-2.713,0.813,-1.163\H,0,2.713,-0.813,-1.251\H,0,1.959,0.56,-1.192\
H,0,-1.959,-0.56,-1.222\H,0,-3.373,-0.265,-4.476\H,0,3.373,0.265,2.063
\H,0,-3.356,-1.201,-3.218\H,0,3.356,1.201,0.805\H,0,4.085,-0.185,0.74\
H,0,-4.085,0.185,-3.154\\Version=EM64L-G09RevB.01\State=1-A\HF=-1067.7
954087\S2=1.028666\S2-1=0.\S2A=0.230961\RMSD=6.063e-09\Dipole=-0.00035
02,-0.0000268,0.0000623\Quadrupole=20.1846342,-1.1324628,-19.0521713,-
4.3006087,1.1025746,9.4854012\PG=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rung model dyad (replace pyrene by H) - triplet UB97D/6-31+G*

1\1\GINC-SKYNET\SP\UB97D\6-31+G(d)\C14H26N4O4(3)\LAHTI\06-Mar-2011\0\\
#P GFINPUT IOP(6/7=3) UB97D/6-31+G(d) TEST\\Pyrene-NN co C6F6 rung con
tact\\0,3\C,0,0.49,-0.087,2.377\C,0,-0.49,0.087,-4.79\C,0,-1.765,1.745
,-3.698\C,0,1.765,-1.745,1.285\C,0,-2.043,0.368,-3.045\C,0,2.043,-0.36
8,0.631\C,0,0.749,-2.585,0.52\C,0,-0.749,2.585,-2.934\C,0,-2.983,2.574
,-4.059\C,0,2.983,-2.574,1.646\C,0,1.958,-0.349,-0.884\C,0,-1.958,0.34
9,-1.53\C,0,3.333,0.289,1.103\C,0,-3.333,-0.289,-3.516\H,0,0.183,-0.42
8,-5.484\H,0,-0.184,0.428,3.071\N,0,1.062,-1.297,2.542\N,0,-1.062,1.29
7,-4.955\N,0,0.926,0.441,1.215\N,0,-0.926,-0.441,-3.628\O,0,0.951,-2.0
52,3.566\O,0,-0.951,2.052,-5.979\O,0,-0.564,-1.557,-3.119\O,0,0.564,1.
557,0.705\H,0,0.012,2.043,-2.711\H,0,-0.012,-2.043,0.297\H,0,0.466,-3.
322,1.067\H,0,-0.466,3.322,-3.48\H,0,1.15,-2.919,-0.286\H,0,-1.15,2.91
9,-2.128\H,0,3.614,-2.026,2.117\H,0,-3.614,2.026,-4.53\H,0,3.388,-2.91
2,0.845\H,0,-3.388,2.912,-3.258\H,0,2.716,-3.307,2.205\H,0,-2.716,3.30
7,-4.618\H,0,1.149,-0.781,-1.164\H,0,-1.149,0.781,-1.25\H,0,-2.713,0.8
13,-1.163\H,0,2.713,-0.813,-1.251\H,0,1.959,0.56,-1.192\H,0,-1.959,-0.
56,-1.222\H,0,-3.373,-0.265,-4.476\H,0,3.373,0.265,2.063\H,0,-3.356,-1
.201,-3.218\H,0,3.356,1.201,0.805\H,0,4.085,-0.185,0.74\H,0,-4.085,0.1
85,-3.154\\Version=EM64L-G09RevB.01\State=3-A\HF=-1067.7954057\S2=2.02
8846\S2-1=0.\S2A=2.000413\RMSD=2.043e-09\Dipole=-0.0003494,-0.0000269,
0.0000638\Quadrupole=20.184151,-1.1322423,-19.0519087,-4.3007578,1.102
0654,9.485151\PG=C01 [X(C14H26N4O4)]\\@

PyrNN*2 / C6F6 rung B model dyad (replace pyrene by H) - singlet UB97D/6-31+G*

1\1\GINC-SKYNET\Stability\UB97D\6-31+G(d)\C14H26N4O4\LAHTI\03-Nov-2011
\0\\#P GFINPUT IOP(6/7=3) UB97D/6-31+G(d) TEST STABLE=OPT GUESS=(READ,
MIX)\\Pyrene-NN Co-xtl Rung B model\\0,1\O,0,-2.267,5.818,4.34\O,0,-1.
929,2.154,7.161\N,0,-2.392,5.046,5.351\N,0,-2.275,3.285,6.666\C,0,-1.8
29,3.826,5.506\C,0,-3.076,5.492,6.622\C,0,-3.379,4.112,7.266\C,0,-2.04
4,6.317,7.393\H,0,-1.725,7.052,6.828\H,0,-1.288,5.745,7.641\H,0,-2.456
,6.682,8.203\C,0,-4.291,6.34,6.295\H,0,-4.787,6.531,7.119\H,0,-4.87,5.
854,5.672\H,0,-4.002,7.181,5.885\C,0,-4.692,3.479,6.794\H,0,-4.745,3.5
27,5.816\H,0,-5.448,3.964,7.186\H,0,-4.723,2.541,7.077\C,0,-3.286,4.07
1,8.782\H,0,-3.369,3.144,9.09\H,0,-4.008,4.61,9.168\H,0,-2.421,4.433,9
.065\O,0,-6.77,9.552,4.695\O,0,-7.107,5.888,1.873\N,0,-6.645,8.781,3.6
84\N,0,-6.761,7.02,2.368\C,0,-7.207,7.56,3.528\C,0,-5.96,9.227,2.412\C
,0,-5.657,7.846,1.768\C,0,-6.993,10.051,1.641\H,0,-7.311,10.786,2.206\
H,0,-7.748,9.479,1.393\H,0,-6.58,10.417,0.831\C,0,-4.745,10.074,2.739\
H,0,-4.249,10.266,1.915\H,0,-4.166,9.588,3.363\H,0,-5.034,10.916,3.149
\C,0,-4.344,7.213,2.24\H,0,-4.291,7.261,3.218\H,0,-3.588,7.698,1.848\H
,0,-4.313,6.275,1.957\C,0,-5.75,7.806,0.252\H,0,-5.667,6.879,-0.056\H,
0,-5.028,8.344,-0.134\H,0,-6.615,8.168,-0.031\H,0,-1.153,3.313,4.813\H
,0,-7.884,7.047,4.221\\Version=EM64L-G09RevB.01\State=1-A\HF=-1067.902
8414\S2=1.029521\S2-1=0.\S2A=0.239447\RMSD=1.951e-09\Dipole=0.1204994,
1.1605124,0.0518544\Quadrupole=-3.4758588,-8.1093115,11.5851703,6.3755
338,-3.1507423,-6.7885063\PG=C01 [X(C14H26N4O4)]\\@

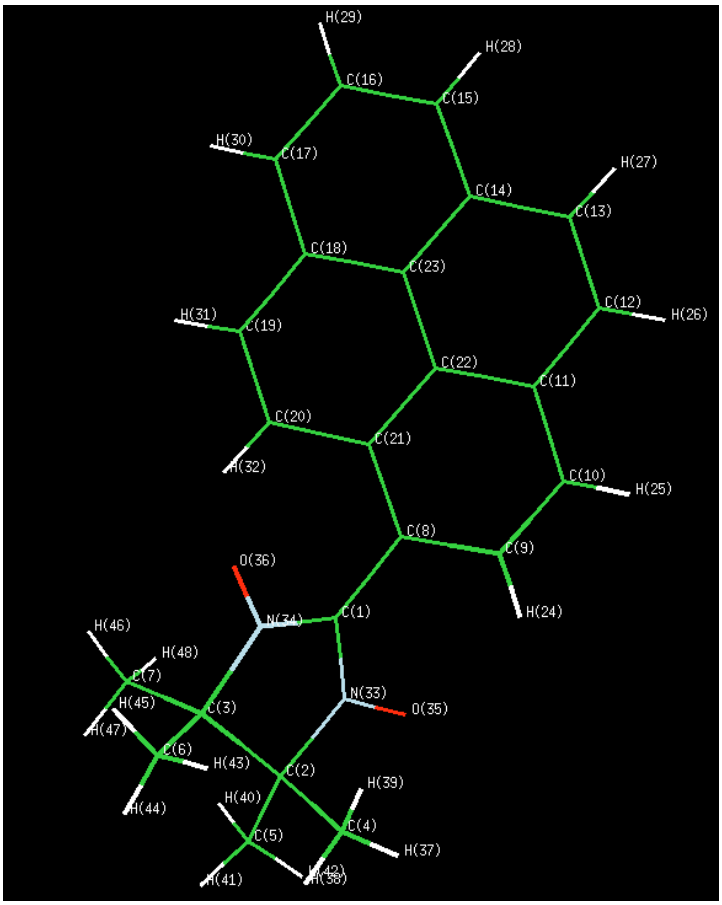
PyrNN*2 / C6F6 rung B model dyad (replace pyrene by H) - triplet UB97D/6-31+G*

1\1\GINC-SKYNET\Stability\UB3LYP\6-31G(d)\C14H26N4O4(3)\LAHTI\02-Nov-2
011\0\\#P GFINPUT IOP(6/7=3) TEST UB3LYP/6-31G* STABLE=OPT\\Pyrene-NN
Co-xtl Rung B model\\0,3\O,0,-2.267,5.818,4.34\O,0,-1.929,2.154,7.161\
N,0,-2.392,5.046,5.351\N,0,-2.275,3.285,6.666\C,0,-1.829,3.826,5.506\C
,0,-3.076,5.492,6.622\C,0,-3.379,4.112,7.266\C,0,-2.044,6.317,7.393\H,
0,-1.725,7.052,6.828\H,0,-1.288,5.745,7.641\H,0,-2.456,6.682,8.203\C,0
,-4.291,6.34,6.295\H,0,-4.787,6.531,7.119\H,0,-4.87,5.854,5.672\H,0,-4
.002,7.181,5.885\C,0,-4.692,3.479,6.794\H,0,-4.745,3.527,5.816\H,0,-5.
448,3.964,7.186\H,0,-4.723,2.541,7.077\C,0,-3.286,4.071,8.782\H,0,-3.3
69,3.144,9.09\H,0,-4.008,4.61,9.168\H,0,-2.421,4.433,9.065\O,0,-6.77,9
.552,4.695\O,0,-7.107,5.888,1.873\N,0,-6.645,8.781,3.684\N,0,-6.761,7.
02,2.368\C,0,-7.207,7.56,3.528\C,0,-5.96,9.227,2.412\C,0,-5.657,7.846,
1.768\C,0,-6.993,10.051,1.641\H,0,-7.311,10.786,2.206\H,0,-7.748,9.479
,1.393\H,0,-6.58,10.417,0.831\C,0,-4.745,10.074,2.739\H,0,-4.249,10.26
6,1.915\H,0,-4.166,9.588,3.363\H,0,-5.034,10.916,3.149\C,0,-4.344,7.21
3,2.24\H,0,-4.291,7.261,3.218\H,0,-3.588,7.698,1.848\H,0,-4.313,6.275,
1.957\C,0,-5.75,7.806,0.252\H,0,-5.667,6.879,-0.056\H,0,-5.028,8.344,-
0.134\H,0,-6.615,8.168,-0.031\H,0,-1.153,3.313,4.813\H,0,-7.884,7.047,
4.221\\Version=EM64L-G09RevB.01\State=3-A\HF=-1068.545048\S2=2.109194\
S2-1=0.\S2A=2.005089\RMSD=9.840e-09\Dipole=0.1259893,1.0249854,0.08749
09\Quadrupole=-2.7835724,-7.5628624,10.3464349,5.6587351,-3.1294121,-6
.1829461\PG=C01 [X(C14H26N4O4)]\\@

Spin Density – PyrNN, EPR-II method

Mulliken atomic spin densities:

		1
1	C	-0.224814
2	C	-0.013570
3	C	-0.011896
4	C	0.018679
5	C	-0.000379
6	C	-0.000509
7	C	0.016773
8	C	0.027645
9	C	-0.015133
10	C	0.009337
11	C	-0.013253
12	C	0.006957
13	C	-0.011083
14	C	0.003317
15	C	-0.006377
16	C	0.003516
17	C	-0.006660
18	C	0.003609
19	C	-0.007572
20	C	0.011422
21	C	-0.022408
22	C	0.006267
23	C	-0.002625
24	H	0.000519
25	H	-0.000583
26	H	-0.000280
27	H	0.000526
28	H	0.000281
29	H	-0.000154
30	H	0.000302
31	H	0.000272
32	H	-0.000829
33	N	0.285112
34	N	0.266781
35	O	0.351403
36	O	0.327934
37	H	-0.000667
38	H	0.000262
39	H	-0.000312
40	H	0.000056
41	H	-0.000582
42	H	-0.000169
43	H	0.000143
44	H	-0.000559
45	H	-0.000183
46	H	-0.000780
47	H	0.000463
48	H	-0.000197



Sum of Mulliken atomic spin densities = 1.00000

Isotropic Fermi Contact Couplings

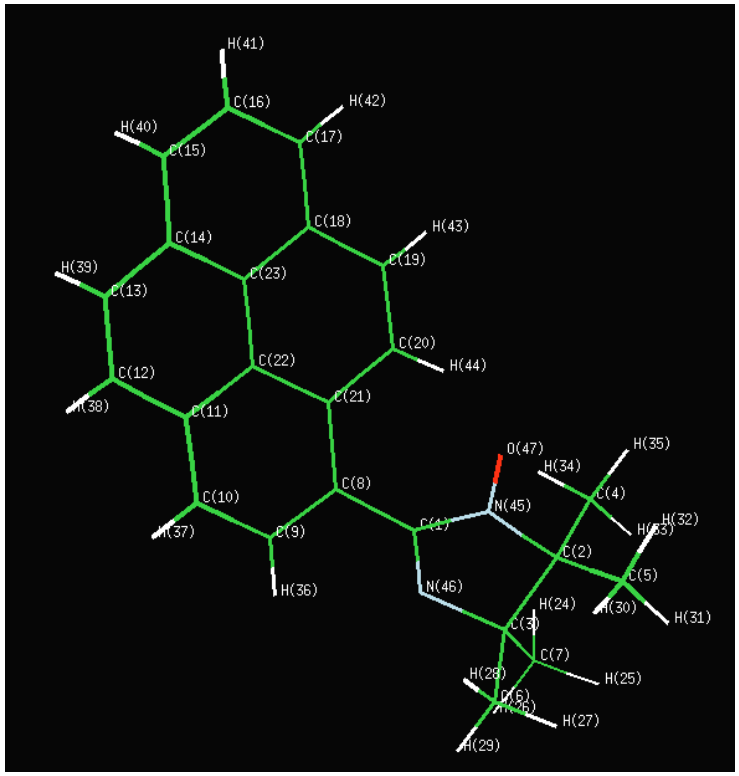
	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.03674	-41.30081	-14.73716	-13.77647
2	C(13)	-0.00488	-5.48054	-1.95559	-1.82811
3	C(13)	-0.00456	-5.12489	-1.82869	-1.70948
4	C(13)	0.00888	9.98765	3.56384	3.33152
5	C(13)	0.00174	1.95318	0.69694	0.65151
6	C(13)	0.00135	1.52116	0.54279	0.50740
7	C(13)	0.00780	8.76989	3.12932	2.92532
8	C(13)	0.00841	9.44979	3.37192	3.15211
9	C(13)	-0.00648	-7.28766	-2.60042	-2.43090
10	C(13)	0.00071	0.79606	0.28405	0.26554
11	C(13)	-0.00145	-1.62884	-0.58121	-0.54332
12	C(13)	0.00097	1.08612	0.38755	0.36229
13	C(13)	-0.00083	-0.93343	-0.33307	-0.31136
14	C(13)	0.00072	0.80530	0.28735	0.26862
15	C(13)	-0.00052	-0.58006	-0.20698	-0.19349
16	C(13)	0.00048	0.53684	0.19156	0.17907
17	C(13)	-0.00052	-0.58917	-0.21023	-0.19653
18	C(13)	0.00055	0.62141	0.22173	0.20728

19	C(13)	-0.00048	-0.53678	-0.19154	-0.17905
20	C(13)	0.00041	0.45792	0.16340	0.15274
21	C(13)	-0.00642	-7.21729	-2.57531	-2.40743
22	C(13)	0.00093	1.04227	0.37191	0.34766
23	C(13)	-0.00060	-0.66982	-0.23901	-0.22343
24	H(1)	0.00026	1.17814	0.42039	0.39298
25	H(1)	-0.00022	-0.96597	-0.34468	-0.32221
26	H(1)	-0.00009	-0.38293	-0.13664	-0.12773
27	H(1)	0.00016	0.70951	0.25317	0.23667
28	H(1)	0.00009	0.40239	0.14358	0.13422
29	H(1)	-0.00004	-0.19774	-0.07056	-0.06596
30	H(1)	0.00009	0.42439	0.15143	0.14156
31	H(1)	0.00008	0.34068	0.12156	0.11364
32	H(1)	-0.00010	-0.43478	-0.15514	-0.14503
33	N(14)	0.04708	15.21196	5.42801	5.07416
34	N(14)	0.04387	14.17403	5.05765	4.72795
35	O(17)	0.04483	-27.17361	-9.69622	-9.06414
36	O(17)	0.04199	-25.45127	-9.08165	-8.48963
37	H(1)	-0.00041	-1.83312	-0.65410	-0.61146
38	H(1)	0.00041	1.83605	0.65515	0.61244
39	H(1)	-0.00023	-1.03648	-0.36984	-0.34573
40	H(1)	-0.00012	-0.53177	-0.18975	-0.17738
41	H(1)	-0.00014	-0.64563	-0.23038	-0.21536
42	H(1)	-0.00011	-0.49373	-0.17617	-0.16469
43	H(1)	-0.00010	-0.45795	-0.16341	-0.15275
44	H(1)	-0.00015	-0.66060	-0.23572	-0.22035
45	H(1)	-0.00011	-0.48489	-0.17302	-0.16174
46	H(1)	-0.00037	-1.66727	-0.59492	-0.55614
47	H(1)	0.00033	1.46630	0.52321	0.48910
48	H(1)	-0.00021	-0.92985	-0.33179	-0.31016

Spin Density – PyrIN, syn conformer, EPR-II method

Mulliken atomic spin densities:

		1
1	C	-0.106245
2	C	-0.005477
3	C	-0.009257
4	C	0.025204
5	C	-0.000006
6	C	0.014363
7	C	0.001630
8	C	0.018846
9	C	-0.009216
10	C	0.005248
11	C	-0.006399
12	C	0.003235
13	C	-0.004753
14	C	0.001638
15	C	-0.003323
16	C	0.001832
17	C	-0.003490
18	C	0.002301
19	C	-0.005851
20	C	0.011154
21	C	-0.016950
22	C	0.004441
23	C	-0.001658
24	H	-0.000093
25	H	0.000701
26	H	-0.000005
27	H	0.002172
28	H	-0.000887
29	H	-0.000774
30	H	-0.000067
31	H	-0.000905
32	H	-0.000333
33	H	0.001115
34	H	-0.000749
35	H	-0.000931
36	H	0.000263



37	H	-0.000303
38	H	-0.000126
39	H	0.000226
40	H	0.000144
41	H	-0.000080
42	H	0.000155
43	H	0.000165
44	H	-0.001124
45	N	0.329826
46	N	0.258098
47	O	0.496246

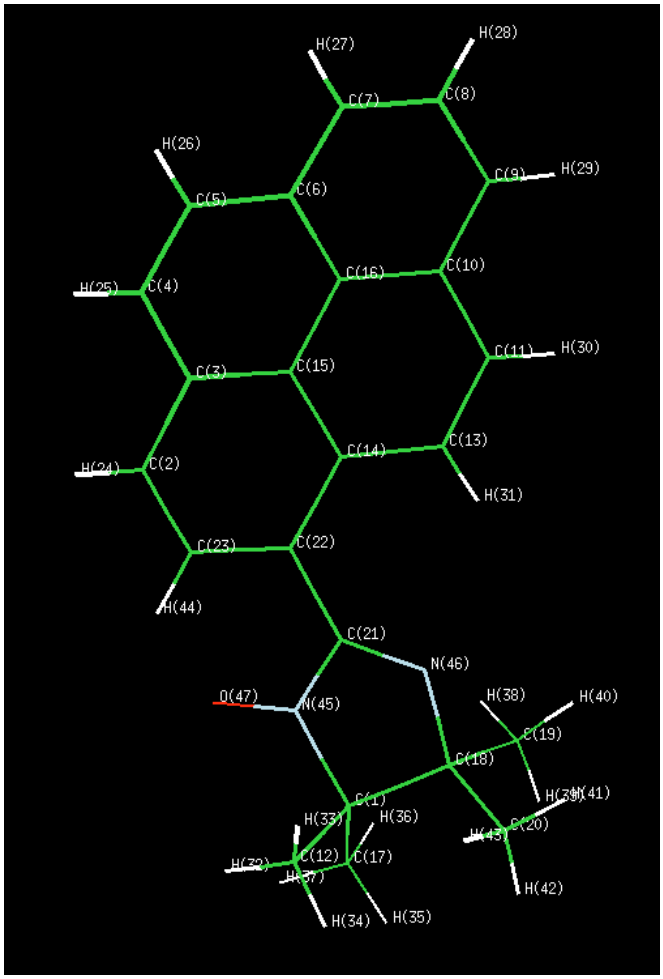
Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.02339	-26.29593	-9.38304	-8.77138
2	C(13)	-0.00708	-7.95879	-2.83989	-2.65477
3	C(13)	-0.00447	-5.02948	-1.79464	-1.67765
4	C(13)	0.01678	18.86339	6.73093	6.29215
5	C(13)	0.00350	3.93569	1.40435	1.31280
6	C(13)	0.00933	10.48962	3.74296	3.49896
7	C(13)	0.00314	3.52740	1.25866	1.17661
8	C(13)	0.00357	4.01264	1.43181	1.33847
9	C(13)	-0.00444	-4.99020	-1.78063	-1.66455
10	C(13)	0.00012	0.13634	0.04865	0.04548
11	C(13)	-0.00063	-0.71298	-0.25441	-0.23782
12	C(13)	0.00043	0.48780	0.17406	0.16271
13	C(13)	-0.00037	-0.41581	-0.14837	-0.13870
14	C(13)	0.00033	0.37238	0.13287	0.12421
15	C(13)	-0.00026	-0.29695	-0.10596	-0.09905
16	C(13)	0.00025	0.28141	0.10041	0.09387
17	C(13)	-0.00027	-0.30593	-0.10916	-0.10205
18	C(13)	0.00028	0.31248	0.11150	0.10423
19	C(13)	-0.00027	-0.30373	-0.10838	-0.10131
20	C(13)	-0.00007	-0.07738	-0.02761	-0.02581
21	C(13)	-0.00301	-3.38670	-1.20846	-1.12968
22	C(13)	0.00043	0.48108	0.17166	0.16047
23	C(13)	-0.00028	-0.31013	-0.11066	-0.10345
24	H(1)	-0.00009	-0.38701	-0.13810	-0.12909
25	H(1)	0.00038	1.68283	0.60047	0.56133
26	H(1)	-0.00003	-0.11620	-0.04146	-0.03876
27	H(1)	0.00088	3.92844	1.40177	1.31039
28	H(1)	-0.00023	-1.04639	-0.37338	-0.34904
29	H(1)	-0.00017	-0.76419	-0.27268	-0.25491
30	H(1)	-0.00012	-0.51504	-0.18378	-0.17180
31	H(1)	-0.00015	-0.66224	-0.23630	-0.22090
32	H(1)	-0.00015	-0.64954	-0.23177	-0.21666
33	H(1)	0.00059	2.64567	0.94404	0.88250
34	H(1)	-0.00024	-1.08820	-0.38830	-0.36298
35	H(1)	-0.00034	-1.52843	-0.54538	-0.50983
36	H(1)	0.00017	0.74243	0.26492	0.24765
37	H(1)	-0.00008	-0.37691	-0.13449	-0.12572
38	H(1)	-0.00004	-0.17863	-0.06374	-0.05958
39	H(1)	0.00007	0.30562	0.10905	0.10194
40	H(1)	0.00005	0.20719	0.07393	0.06911
41	H(1)	-0.00002	-0.10162	-0.03626	-0.03390
42	H(1)	0.00005	0.22149	0.07903	0.07388
43	H(1)	0.00005	0.21192	0.07562	0.07069
44	H(1)	-0.00006	-0.28925	-0.10321	-0.09648
45	N(14)	0.05550	17.93187	6.39854	5.98143
46	N(14)	0.03161	10.21388	3.64457	3.40699
47	O(17)	0.05964	-36.15201	-12.89994	-12.05901

Spin Density – PyrIN, anti conformer, EPR-II method

Mulliken atomic spin densities:

		1
1	C	-0.006990
2	C	0.005085
3	C	-0.007100
4	C	0.004011
5	C	-0.005964
6	C	0.002078
7	C	-0.004279
8	C	0.002372
9	C	-0.004609
10	C	0.002272
11	C	-0.004931
12	C	0.026835
13	C	0.005049
14	C	-0.006945
15	C	0.002517
16	C	-0.001101
17	C	0.000401
18	C	-0.010985
19	C	0.015131
20	C	0.001964
21	C	-0.097412
22	C	0.004858
23	C	-0.006259
24	H	-0.000338
25	H	-0.000163
26	H	0.000280
27	H	0.000192
28	H	-0.000103
29	H	0.000204
30	H	0.000244
31	H	0.000177
32	H	-0.000968
33	H	-0.000791
34	H	0.000440
35	H	-0.000729
36	H	0.000068
37	H	-0.000269
38	H	-0.000493
39	H	0.000761
40	H	-0.000661
41	H	0.000001
42	H	0.000551
43	H	0.000068
44	H	0.000319
45	N	0.334842
46	N	0.262262
47	O	0.488110



Sum of Mulliken atomic spin densities = 1.00000

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.00751	-8.44373	-3.01293	-2.81652
2	C(13)	0.00048	0.53484	0.19085	0.17840
3	C(13)	-0.00088	-0.98473	-0.35138	-0.32847
4	C(13)	0.00054	0.60687	0.21655	0.20243
5	C(13)	-0.00047	-0.52302	-0.18663	-0.17446
6	C(13)	0.00044	0.49403	0.17628	0.16479
7	C(13)	-0.00034	-0.37846	-0.13504	-0.12624
8	C(13)	0.00033	0.36764	0.13118	0.12263
9	C(13)	-0.00035	-0.38906	-0.13883	-0.12978
10	C(13)	0.00044	0.49816	0.17775	0.16617
11	C(13)	-0.00026	-0.28915	-0.10318	-0.09645
12	C(13)	0.01372	15.41957	5.50209	5.14342
13	C(13)	0.00136	1.52529	0.54426	0.50878
14	C(13)	-0.00226	-2.54050	-0.90651	-0.84742
15	C(13)	0.00070	0.78139	0.27882	0.26064
16	C(13)	-0.00033	-0.37075	-0.13229	-0.12367
17	C(13)	0.00360	4.04728	1.44417	1.35003
18	C(13)	-0.00486	-5.46038	-1.94840	-1.82139
19	C(13)	0.00857	9.63199	3.43693	3.21288
20	C(13)	0.00307	3.44674	1.22988	1.14971
21	C(13)	-0.02417	-27.16806	-9.69424	-9.06229

22	C(13)	0.00347	3.90366	1.39292	1.30212
23	C(13)	-0.00339	-3.80803	-1.35880	-1.27022
24	H(1)	-0.00011	-0.51039	-0.18212	-0.17025
25	H(1)	-0.00005	-0.22258	-0.07942	-0.07424
26	H(1)	0.00009	0.38112	0.13599	0.12713
27	H(1)	0.00006	0.27388	0.09773	0.09136
28	H(1)	-0.00003	-0.12787	-0.04563	-0.04265
29	H(1)	0.00007	0.29243	0.10435	0.09754
30	H(1)	0.00007	0.32291	0.11522	0.10771
31	H(1)	0.00007	0.31714	0.11316	0.10579
32	H(1)	-0.00050	-2.22382	-0.79351	-0.74179
33	H(1)	-0.00029	-1.30738	-0.46651	-0.43609
34	H(1)	0.00050	2.23885	0.79888	0.74680
35	H(1)	-0.00017	-0.76290	-0.27222	-0.25448
36	H(1)	-0.00012	-0.54976	-0.19617	-0.18338
37	H(1)	-0.00014	-0.63607	-0.22697	-0.21217
38	H(1)	-0.00022	-0.99688	-0.35571	-0.33252
39	H(1)	0.00047	2.12190	0.75715	0.70779
40	H(1)	-0.00006	-0.28760	-0.10262	-0.09593
41	H(1)	-0.00003	-0.12788	-0.04563	-0.04266
42	H(1)	0.00028	1.27235	0.45401	0.42441
43	H(1)	-0.00007	-0.29581	-0.10555	-0.09867
44	H(1)	0.00017	0.74474	0.26574	0.24842
45	N(14)	0.05592	18.06715	6.44681	6.02655
46	N(14)	0.03238	10.46171	3.73300	3.48965
47	O(17)	0.05953	-36.08386	-12.87562	-12.03628