

Electronic Supporting Information

Non-innocent pyridyl nitrogens: unprecedented interconversion of *N*-bridgehead-thiadiazolium salts and thiatriazine in the generation of thiatriazinyl

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General Procedures. The reagents 2-cyanopyridine (Alfa Aesar), ammonia (Linde), S₂Cl₂ (Aldrich), trimethylsilyl trifluorosulfonate (triflate, TCI America), carbon disulfide (Aldrich), triphenylantimony (Aldrich), 4-dimethylaminopyridine (Aldrich) and iodine (Aldrich) were obtained commercially and used as received. Acetonitrile was dried by distillation over P₂O₅ and stored over 4 Å molecular sieves. All other solvents were of reagent grade. Melting points were taken using a Mel-Temp apparatus and are uncorrected. NMR spectra were run in either CDCl₃ or CD₃CN solutions at room temperature on a Bruker Avance 400 MHz spectrometer. ¹⁹F NMR spectra were referenced to trifluoroacetic acid at -76.55 ppm. IR spectra of solid samples were recorded on an Agilent Technologies Cary 630 FT-IR spectrometer. Elemental analyses were performed by MHW Laboratories, Phoenix, AZ 85018.

Preparation of *N*-2-pyridylimidoyl-2-pyridylamidine 4: In a glass pressure vessel, gaseous ammonia was bubbled through a solution of 2-cyanopyridine (10.0 g, 0.0961 mol) in 100 mL MeCN for 20 min. The vessel was sealed and the contents were stirred and heated at 110 °C for 72 h, at which time the vessel was cooled to room temperature and vented carefully. The solvent was evaporated resulting in a sticky solid. Recrystallization from isopropyl alcohol afforded **4** as colourless crystals. Yield 7.0 g (0.0311 mol, 63 %) m.p. = 125-130 °C. ¹H NMR (δ, CDCl₃, RT, 400 MHz): 11.30 (br, s, 1H), 9.55 (br, s, 2H), 8.65 (d, 2H, *J* = 4.64 Hz), 8.56 (d, 2H, *J* = 7.89 Hz), 7.84 (dd, 2H, *J* = 3.42 Hz), 7.38 (dd, 2H, *J* = 1.88 Hz). ¹³C NMR (δ, CDCl₃, RT, 400 MHz): 165.08, 152.34, 148.72, 137.14, 125.23, 122.10. IR ν_{max} = 3360 (m), 3250 (m), 3058 (s), 1706 (w), 1615 (s), 1585 (m), 1561 (s), 1541 (s), 1498 (m), 1452 (m), 1429 (m), 1394 (s), 1368 (s), 1289 (m), 1251 (m), 1188 (m), 1136 (m), 1093 (m), 1047 (m), 993 (s), 914 (w), 878 (m), 816 (m), 777 (m), 747 (s), 702 (m), 684 (s) cm⁻¹. Anal. Calcd for C₁₂H₁₁N₅: C, 63.99; H, 4.92; N, 31.09. Found: C, 64.11; H, 5.11; N, 31.19.

Preparation of 3-*{(Z)-[amino(pyridinium-2-yl)methylidene]amino}*[1,2,5]thiadiazolo [2,3-*a*]pyridin-1-ium bis(trifluoromethanesulfonate) [5][OTf]·HOTf : Under an inert atmosphere, a solution of S₂Cl₂ (1.2 mL, 15.0 mmol) in 15 mL MeCN was added dropwise to a solution of **4** (1.15 g, 5.11 mmol) in 75 mL MeCN over 15 min. The

resulting yellow precipitate was stirred at room temperature for 3 h before being filtered in vacuo, washed twice with MeCN and once with CS₂. Yield 1.23 g. IR ν_{\max} = 3483 (w), 3402 (m), 3283 (m), 3041 (s), 3000 (s), 1653 (s), 1607 (s), 1547 (s), 1524 (s), 1483 (m), 1459 (s), 1419 (s), 1361 (m), 1306 (m), 1213 (m), 1117 (m), 1098 (m), 1042 (m), 1004 (m), 962 (m), 915 (m), 799 (s), 761 (s), 747 (s), 701 (w) cm⁻¹. This air sensitive material (0.5 g) underwent a solid state thermolysis at 100 °C under reduced pressure (10⁻² mmHg) to afford the white solid of [5][Cl]·HCl. Yield 0.37 g (1.12 mmol, 69 % from 4). IR ν_{\max} = 3415 (m), 3287 (m), 3054 (w), 2997 (m), 1613 (s), 1583 (m), 1564 (m), 1523 (s), 1481 (m), 1459 (s), 1426 (s), 1351 (m), 1302 (w), 1164 (w), 1052 (w), 1033 (m), 995 (w), 906 (w), 807 (w), 778 (m), 755 (s), 703 (m), 688 (m) cm⁻¹. This material is essentially insoluble in organic solvents; its identity was determined by metathesis to the more soluble triflate salt by the following procedure: under an inert atmosphere, trimethylsilyl triflate (0.4 mL, 2.15 mmol) was added dropwise to a slurry of [5][Cl]·HCl (0.27 g, 0.822 mmol) in 5 mL MeCN. The white solid dissolves and a fine, white precipitate crashes out of solution. After 2 h the solvent was removed to give a light brown powder. Crude yield 0.32 g (0.576 mmol, 70 %). White crystals of [5][OTf]·HOTf were obtained by recrystallization from MeCN. dec > 275 °C. ¹H NMR (δ , CD₃CN, RT, 400 MHz): 9.50 (d, 1H, *J* = 1.67 Hz), 9.48 (br, s, 1H), 9.32 (d, 1H, *J* = 8.29 Hz), 9.06 (d, 1H, *J* = 2.22 Hz), 8.82 (dd, 1H, *J* = 3.50 Hz), 8.68 (d, 1H, *J* = 7.89 Hz), 8.59 (br, s, 1H), 8.57 (dd, 1H, *J* = 2.78 Hz), 8.30 (dd, 1H, *J* = 2.44 Hz), 8.12 (dd, 1H, *J* = 3.79 Hz). ¹³C NMR (δ , CD₃CN, RT, 400 MHz): 142.07, 138.81, 131.35, 127.17, 126.78, 126.72. ¹⁹F NMR (δ , CD₃CN, RT, 400 MHz): -79.03. IR ν_{\max} = 3355 (w), 3230 (w), 1655 (m), 1608 (w), 1563 (m), 1534 (w), 1488 (w), 1461 (m), 1438 (m), 1360 (w), 1312 (w), 1273 (s), 1249 (s), 1226 (s), 1173 (m), 1148 (s), 1025 (s), 961 (m), 912 (m), 814 (m), 785 (w), 757 (s), 732 (w), 691 (w) cm⁻¹. Anal. Calcd for C₁₄H₁₁F₆N₅O₆S₃: C, 30.27; H, 2.00; N, 12.61. Found: C, 30.44; H, 2.20; N, 12.86.

Preparation of 3,3'-iminobis[1,2,5]thiadiazolo[2,3-*a*]pyridin-1-ium bis(trifluoromethanesulfonate) [6][OTf]₂: Under an inert atmosphere, a solution of S₂Cl₂ (2.5 mL, 31.3 mmol) in 30 mL MeCN was added dropwise to a solution of 4 (2.25 g, 10.0 mmol) in 160 mL MeCN over 20 min. The resulting yellow slurry was heated at reflux for 16 h.

After cooling to room temperature, the solid of [6][Cl]₂ was collected by filtration in vacuo, washed twice with MeCN and once with CS₂. Yield 3.44 g (9.60 mmol, 96 %) IR ν_{\max} = 3045 (w), 3003 (w), 2734 (br, w), 1606 (m), 1585 (w), 1555 (s), 1529 (w), 1505 (s), 1463 (s), 1424 (m), 1380 (s), 1354 (w), 1328 (w), 1300 (s), 1155 (w), 1098 (w), 1040 (w), 997 (w), 932 (w), 845 (m), 778 (s), 765 (s), 747 (s), 689 (m) cm⁻¹. This material is essentially insoluble in organic solvents; its identity was determined by metathesis to the more soluble triflate salt by the following procedure: under an inert atmosphere, trimethylsilyl triflate (0.64 mL, 3.54 mmol) was added dropwise to a slurry of [6][Cl]₂ (0.5 g, 1.40 mmol) in 5 mL MeCN over a few minutes. The yellow solid dissolves and the fine, white precipitate of [6][OTf]₂ crashes out of solution. After cooling to -20 °C for 1 h, the solid was filtered in vacuo. Yield 0.66 g (1.13 mol, 81 %). Colourless needles were obtained by recrystallization in MeCN. dec > 260 °C. ¹H NMR (δ , CD₃CN, RT, 400 MHz): 10.78 (br, s, 1H), 9.57 (2, 2H, *J* = 6.61 Hz), 9.17 (d, 2H, *J* = 8.61 Hz), 8.60 (dd, 2H, *J* = 2.81 Hz), 8.14 (dd, 2H, *J* = 3.75 Hz). ¹³C NMR (δ , CD₃CN, RT, 400 MHz): 143.89, 141.87, 140.92, 139.34, 127.04, 126.01. ¹⁹F NMR (δ , CD₃CN, RT, 400 MHz): -79.04. IR ν_{\max} = 3242 (w), 3116 (w), 1616 (w), 1573 (m), 1557 (m), 1507 (m), 1468 (s), 1436 (w), 1368 (w), 1328 (w), 1288 (m), 1257 (s), 1219 (s), 1165 (s), 1143 (s), 1023 (s), 870 (m), 781 (s), 746 (m) cm⁻¹. Anal. Calcd for C₁₄H₉F₆N₅O₆S₄: C, 28.72; H, 1.55; N, 11.96. Found: C, 29.02; H, 1.71; N, 12.09.

Preparation of 3,5-di(pyridin-2-yl)-4H-1,2,4,6-thiatriazine 7: Under an inert atmosphere, triphenylantimony (2.22 g, 6.29 mmol) was added to a thick slurry of [6][Cl]₂ (2.0 g, 5.58 mmol) in 14 mL MeCN. The reaction mixture was heated at reflux for 1 h at which time the solid dissolved and the solution turned red. The mixture was hot filtered in vacuo to remove any insoluble impurities and the filtrate was allowed to stand at room temperature. Dark red crystals of 7 were filtered and rinsed with hexanes. Crude yield 0.72 g (2.82 mol, 51 %). Recrystallization from toluene afforded pure material. Compound 7 can also be prepared via the sublimation of [5][Cl]·HCl at 140 °C and 10⁻² mmHg or by refluxing in chlorobenzene for 16 h. m.p. = 124 °C. ¹H NMR (δ , CDCl₃, RT, 400 MHz): 10.33 (br, s, 1H), 8.65 (d, 2H, *J* = 4.56 Hz), 8.09 (d, 2H, *J* = 7.93 Hz), 7.79 (dd, 2H, *J* = 5.15 Hz), 7.41 (dd, 2H, *J* = 4.08 Hz). ¹³C NMR (δ , CDCl₃, RT, 400 MHz):

151.86, 148.31, 147.55, 136.91, 125.76, 121.89. IR ν_{\max} = 3300 (m), 3049 (w), 3002 (w), 1665 (s), 1588 (s), 1566 (m), 1465 (m), 1437 (s), 1393 (s), 1365 (s), 1290 (w), 1268 (w), 1155 (m), 1090 (w), 1068 (w), 1040 (m), 993 (m), 893 (m), 790 (s), 737 (s), 725 (s), 660 (s) cm^{-1} . Anal. Calcd for $\text{C}_{12}\text{H}_9\text{N}_3\text{S}$: C, 56.45; H, 3.55; N, 27.43. Found: C, 56.42; H, 3.71; N, 27.17.

EPR Spectroscopy Compound **7** (19 mg, 0.0744 mmol), iodine (9 mg, 0.0355 mmol) and 4-dimethylaminopyridine (11 mg, 0.0900 mmol) were combined with 2 mL CH_2Cl_2 in an EPR cell and the mixture was sonicated.

Crystal Growth Single crystals of **[5][OTf]·HOTf** and **[6][OTf]₂** were grown by slow cooling of hot, saturated MeCN solutions in sealed glass vessels. Needles of **7** were obtained from layering pentane on a DCM solution of **7**.

X-ray Measurements A crystal of **[6][OTf]₂** was glued to a glass fiber with epoxy. X-ray data were collected using omega and phi scans with a Bruker Kappa APEX II CCD detector with Mo K_α ($\lambda = 0.71073 \text{ \AA}$) radiation. The data were scanned using Bruker's APEX II program and integrated using Bruker's SAINT software.¹ The structure was solved by direct methods using SHELXS-90² and refined by least-squares methods on F^2 using SHELXL-97³ incorporated in the SHELXTL⁴ suite of programs.

Data collection results for compounds **[5][OTf]·HOTf** and **7** represent the best data sets obtained in several trials for each sample. The crystals were mounted on thin glass fibers using paraffin oil. Prior to data collection crystals were cooled to 200.15 °K. Data were collected on a Bruker AXS KAPPA single crystal diffractometer equipped with a sealed Mo tube source (wavelength 0.71073 Å) and APEX II CCD detector. Raw data collection and processing were performed with APEX II software package from

¹ SAINT, version 6.22 Bruker Advanced X-ray Solutions, Inc., Madison, WI, 2001.

² Sheldrick, G. M. SHELXS-90. *Acta Crystallogr. A* 1990, **46**, 467.

³ Sheldrick, G. M. SHELXL-97. Program for the Refinement of Crystal Structures, University of Gottingen, Gottingen, Germany, 1997.

⁴ SHELXTL, VERSION 6.12 Program Library for Structure Solution and Molecular Graphics, Bruker Advanced X-ray Solutions, Inc., Madison, WI, 2001.

BRUKER AXS.⁵ Diffraction data for **7** were collected with a sequence of 0.5° ω scans at 0, 120, and 240° in φ . Due to lower unit cell symmetry in order to ensure adequate data redundancy, diffraction data for **[5][OTf]·HOTf** were collected with a sequence of 0.5° ω scans at 0, 90, 180 and 270° in φ . Initial unit cell parameters for both compounds were determined from 60 data frames with 0.3° ω scan each, collected at the different sections of the Ewald sphere. Semi-empirical absorption corrections based on equivalent reflections were applied to the full data sets.⁶ Systematic absences in the diffraction data set and unit-cell parameters were consistent with triclinic $P\bar{1}$ (№2) for compounds **[5][OTf]·HOTf** and monoclinic $P2_1/c$ (№14) for **7**. Solutions in the centrosymmetric space groups for both compounds yielded chemically reasonable and computationally stable results of refinement. The structures were solved by direct methods, completed with difference Fourier synthesis, and refined with full-matrix least-squares procedures based on F^2 . For both compounds all hydrogen atom positions were located as residual electron density peaks from the Fourier maps difference. However, after initial positioning all hydrogen atoms were restrained to a riding model and were treated as idealized contributions during consequent refinement. All scattering factors are contained in several versions of the SHELXTL 2013 program library.⁷

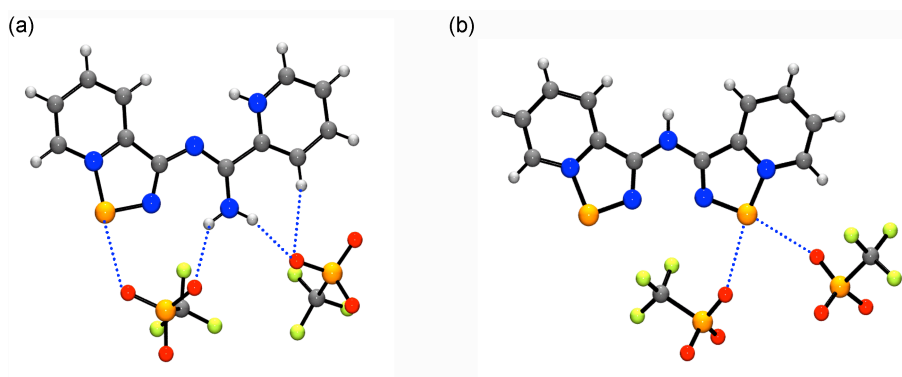


Figure S1 PLUTO drawings of (a) **[5][OTf]·HOTf** and (b) **[6][OTf]₂**.

⁵ APEX Software Suite v.2010; Bruker AXS: Madison, WI, 2005.

⁶ Sheldrick, G. M.: SADABS ver. 2008/1, University of Göttingen, Germany, 2008.

⁷ Sheldrick, G.M. *Acta Cryst.* 2008, *A64*, 112.

Computational Chemistry and Archival Files Molecular geometry optimizations were performed on **3** at the DFT (UB3LYP) level of theory with the 6-311+G(d,p) basis set, using the Gaussian 09W program package.⁸ The exo and endo conformations were initially calculated within the constraints of C_{2V} geometry, but further optimized without any symmetry restrictions. Hyperfine coupling constants a_N (in mT) were taken from single-point (U)B3LYP/EPR-II/6-31G(d) calculations on the 6-311G(d,p)-optimized geometries. The exo conformation is 0.08 eV lower in energy than the endo arrangement, and the coupling constants associated with this structure were compared to the derived values obtained from EPR measurements.

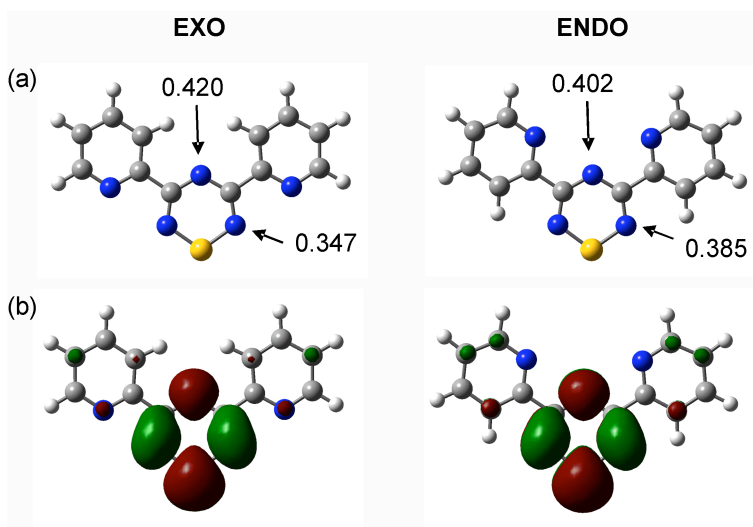


Figure S2 The exo and endo conformations of **3** with (a) optimized geometries and derived coupling constants a_N (in mT) and (b) singly occupied molecular orbitals.

⁸ 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. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, 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, D. J. Fox, *Gaussian 09*, Revision A.02; Gaussian, Inc.: Wallingford, CT, 2009.

Archive file (geometry optimization) for **3** (exo):

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Archive file (geometry optimization) for **3** (endo):

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Archive file (EPR-II) for 3 (exo):

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Archive file (EPR-II) for 3 (endo):

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1|1|UNPC-CHMSTAFF-187065|SP|UB3LYP|GenECP|C12H8N5S1(2)|ALICEA|03-Feb-2014|0||# ub3lyp/genecp prop=EPR scf=tight||UB3LYP/EPR-II/6-31G(d)//ub3lyp/6-311g(d,p) Calc of EPR properties on Endo PyTTA||0,2|C,0,0.,0.,0.|N,0,0.001686,0.,1.34609|C,0,1.168785,0.,2.016773|N,0,2.397872,0.,1.514201|S,0,2.560261,0.,-0.136776|N,0,1.047123,0.,-0.81662|C,0,1.096662,0.,3.518227|N,0,-0.119944,0.,4.072418|C,0,-0.202095,0.,5.401436|C,0,0.910007,0.,6.243872|C,0,2.174508,0.,5.662724|C,0,2.274649,0.,4.276813|H,0,3.234345,0.,3.778919|H,0,3.067955,0.,6.276829|H,0,0.782449,0.,7.320021|H,0,-1.206583,0.,5.816008|C,0,-1.338607,0.,-0.683932|N,0,-2.424315,0.,0.096111|C,0,-3.61827,0.,-0.49336|C,0,-3.796335,0.,-1.877101|C,0,-2.663462,0.,-2.68531|C,0,-1.411066,0.,-2.083144|H,0,-0.501894,0.,-2.668262|H,0,-2.752073,0.,-3.765823|H,0,-4.793527,0.,-2.301316|H,0,-4.47737,0.,0.172102||Version=IA32W-G09RevA.02|State=2-A"|HF=-1134.0761482|S2=0.769556|S2-1=0.|S2A=0.750244|RMSD=5.889e-009|Dipole=0.1561072,0.,-0.0905022|Quadrupole=0.3574424,-11.6867541,11.3293117,0.,9.5737719,0.|PG=CS [SG(C12H8N5S1)]||@
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