Electronic Supporting Information for:

[*closo*-$B_{10}H_{10}$]$^{2-}$ as a Structural Element for Highly Quadrupolar Liquid Crystals: A new Class of Liquid Crystalline NLO Chromophores

Aleksandra Jankowiak,[a] Kristein Mason,[a] Andrzej Balinski,[a] James E. Harvey,[a] Adam Januszko,[a] Piotr Kaszynski,[a,b]* Victor G. Young Jr.,[c] and Andre Persoons[d]

[a] *Organic Materials Research Group, Department of Chemistry,Vanderbilt University, Nashville, TN 37235*

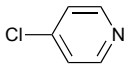
[b] *Faculty of Chemistry, University of Łódź, Tamka 12, 91403 Łódź, Poland*

[c] *X-ray Crystallographic Laboratory, Department of Chemistry, University of Minnesota, Twin Cities, MN 55455*

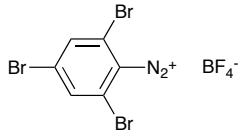
[d] *Department of Chemistry, University of Leuven, Celestijnenlaan 200D, 3001 Leuven, Belgium.*

Table of Content:

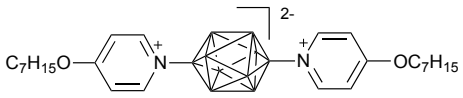
1. Additional synthetic details



4-Chloropyridine.[1] It was obtained according to a modified literature procedure.[1] 4-Chloropyridine hydrochloride (9.96 g, 64.2 mmol) was dissolved in cold water (60 mL) and a cold solution of 2M KOH (50 mL) was added in one portion. The resulting free pyridine was extracted into petroleum ether (3x), the combined extracts were dried (Na_2SO_4), solvent removed, and the resulting 4-chloropyridine was immediately used without further purification.

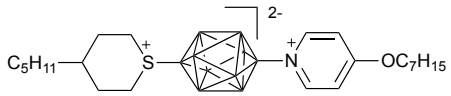


2,4,6-Tribromobenzenediazonium Tetrafluoroborate.[2] According to the literature procedure,[2] 2,4,6-tribromoaniline (20.05 g, 59.3 mmol) was dissolved in a mixture of acetic acid (135 mL) and tetrafluoroboric acid (20 mL) and cooled in a ice bath. *iso*-Amyl nitrite (12.5 mL, 94 mmol) was added dropwise at 10 ^{o}C causing precipitation. The solution was warmed up and the precipitate dissolved. After 30 min ether was added and the mixture was cooled in an ice bath. The resulting precipitation was filtered and the solid dried giving 24.00 g (94% yield) of the diazonium salt as a yellow solid: ^{1}H NMR (400 MHz, CD_3CN) δ 8.42 (s).



[*closo*-$B_{10}H_8$-1,10-bis(4-heptyloxypyridinyl)] (1).[3] Compound was obtained from bis-dinitrogen derivative **12** [4] and 4-heptyloxypyridine (**10b**) as described before: ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.92 (t, J = 6.8 Hz, 6H), 1.0-3.0 (m, 8H), 1.28-1.60 (m, 16H), 1.90 (quin, J = 7.2 Hz, 4H), 4.22 (t, J = 6.6 Hz, 4H), 7.12 (d, J = 7.2 Hz, 4H), 9.34 (d, J = 7.2 Hz, 4H); ^{1}H NMR

(300 MHz, C_6D_6) δ 0.91 (t, *J* = 6.8 Hz, 6H), 1.0-3.0 (m, 8H), 1.21 (brs, 16H), 1.46 (brs, 4H), 3.44 (brs, 4H), 6.14 (brs, 4H), 9.12 (d, *J* = 6.6 Hz, 4H); ^{13}C NMR (75 MHz, C_6D_6) δ 14.3, 23.0, 26.0, 28.7, 29.2, 32.0, 69.6, 111.3, 149.3, 168.0.

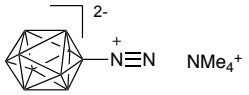


[*closo*-$B_{10}H_8$-1-(4-Heptyloxypyridinyl)-10-(4-pentyl-1-thiacyclohexyl)] (2b). NMR spectra in other solvents:

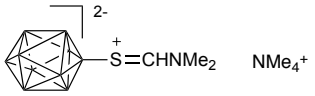
^{13}C NMR (100 MHz, toluene-d_8, –40 °C) δ 14.5, 23.2, 26.2, 26.5, 28.8, 29.6, 30.9. 32.3, 32.4, 35.6, 36.6, 41.8, 69.3, 110.9, 148.6, 167.7.

^{13}C NMR (75 MHz, C_6D_6) δ 14.3, 22.9, 23.0, 25.9, 26.2, 28.7, 29.2, 31.1, 32.0, 32.2, 35.8, 36.5, 42.0, 69.6, 111.3, 149.0, 168.1. Signals ascribed to the **2b-*cis*** isomer: 26.5, 35.9

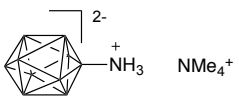
Decomposition product of 2b: An unidentified decomposition product was separated from an aged sample of **2b** as a less mobile fraction (Chromatotron, SiO_2, hexanes/CH_2Cl_2 2:1). It was obtained as a colorless solid and purity > 95% by NMR: ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.0-1.6 (br m, 8H), 0.86 (t, *J* = 7.2 Hz, 3H), 0.89 (t, *J* = 6.7 Hz, 3H), 1.02-1.48 (m, 16H), 1.62 (brs, 2H), 1.81 (quin. *J* = 7.0 Hz, 2H), 2.06 (br t, *J* = 13.8 Hz, 2H), 2.59 (dm, *J* = 12.8 Hz, 1H), 2.64 (dm, *J* = 13.1 Hz, 1H), 2.75-2.94 (m, 1H), 2.98 (dm, *J* = 12.4 Hz, 1H), 3.09 (dm, *J* = 12.7 Hz, 1H), 4.09 (t, *J* = 6.5 Hz, 2H), 6.84 (d, *J* = 7.3 Hz, 2H), 8.42 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 13.95, 14.00, 22.5, 25.6, 26.00, 28.4, 28.8, 31.0, 31.6, 31.7, 35.7, 36.3, 38.4, 38.8, 70.0, 111.2, 149.0, 168.5; ^{11}B NMR (128 MHz, $CDCl_3$) δ -31.3 (1B), -27.7 (2B), -22.6 (1B), -15.2 (1B), -6.4 (1B), -3.0 (d, 2B), -0.9 (d, 2B); IR 2499 (B–H), 1634, 1514, 1310, 1165 cm^{-1}; HRMS, calcd for $C_{22}H_{47}B_{10}NO_2S$: *m/z* 499.4258; found: *m/z* 499.4289.



Preparation of [*closo*-$B_{10}H_9$-1-N_2]$^-$ [NMe_4]$^+$ (6[NMe_4]).[5,6] It was prepared according to the literature procedure[5,6] from [*closo*-$B_{10}H_{10}$]$^{2-}$: ^{1}H NMR (400 MHz, CD_3CN) δ 0.0-1.6 (br m, 8H), 3.08 (s, 12H), 4.55 (br q, *J* = 151 Hz, 1H); ^{11}B NMR (128 MHz, CD_3CN) δ -25.0 (d, *J* = 135 Hz, 4B), -17.2 (d, *J* = 139 Hz, 4B), -13.0 (s, 1B), 21.3 (d, *J* = 150 Hz, 1B).

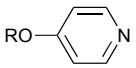


Preparation of [*closo*-$B_{10}H_9$-1-$SCHNMe_2$]$^-$ [NMe_4]$^+$ (7a[NMe_4]).[7] 1-Dinitrogen-*closo*-decaborate ([*closo*-$B_{10}H_9N_2$]$^-$ [NMe_4]$^+$, **6[NMe_4]**, 9.88 g, 45 mmol) was heated with *N*,*N*-dimethylthioformamide (100 mL) at 110 ºC for 24 hrs. Excess solvent was removed under reduced pressure and the viscous residue was dried under vacuum. The resulting crude product was dissolved in MeCN and quickly passed through a silica gel plug (5 cm). The plug was washed with a mixture of MeCN and CH_2Cl_2 (1:1) and the first 100 mL of the intense red solution was evaporated. The residue was treated with benzene/CH_2Cl_2 (1:1) and the resulting crystalline yellow mass was filtered and dried to give 9.00 g (71% yield) of **7a[NMe_4]** as a yellowish solid: ^{1}H NMR (400 MHz, CD_3CN) δ -0.6-1.3 (br m, 9H), 3.08 (s, 12H), 3.45 (s, 3H), 3.52 (s, 3H), 9.83 (s, 1H); ^{11}B NMR (128 MHz, CD_3CN) δ -28.0 (d, *J* = 132 Hz, 4B), -24.8 (d, *J* = 128 Hz, 4B), 2.6 (s, 1B), 4.4 (d, *J* = 137 Hz, 1B).

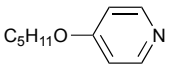


Preparation of [*closo*-$B_{10}H_9$-1-NH_3]$^-$ [NMe_4]$^+$ (7b[NMe_4]).[8] Tetramethylammonium 1-dinitrogen-*closo*-decaborate ([*closo*-$B_{10}H_9N_2$]$^-$ [NMe_4]$^+$, **6[NMe_4]**, 567 mg, 2.59 mmol) was

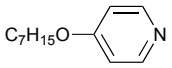
placed in a steel bomb. The bomb and its contents were cooled to –35 °C, liquid ammonia (50 mL) was added and the bomb was quickly sealed. The mixture was heated to 130–135 °C and the pressure rose slowly to about 1000 psi. After two hours at 135 °C, the bomb was cooled to –35°C and the remaining NH_3 gas was vented. A powdery pink and white material was collected using MeOH, and the solvent was evaporated to give 610 mg of crude amine **7b[NMe_4]** that was used without further purification: ^{11}B NMR (128 MHz, DMSO-d_6) δ -29.9 (d, J = 122 Hz, 4B), -27.8 (d, J = 120 Hz, 4B), -2.8 (d, J = 136 Hz, 1B), 7.0 (s, 1B).



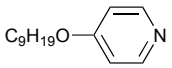
4-Alkoxypyridine 10. A general procedure.[1] To a suspension of NaH (0.63 g, mmol, 60% in oil, washed with hexane) in dry DMSO (10 mL), appropriate alcohol (15.40 mmol) was added dropwise. The mixture was stirred for 1 h, then crude 4-chloropyridine (3.00 g, 26.4 mmol) freshly liberated from its hydrochloride salt was added at once. A mixture was stirred overnight at rt, water was added, organic product was extracted into hexanes (**10a, 10d**, **10e**) or AcOEt (**10b**, **10c**), extracts dried (Na_2SO_4) and solvent was evaporated. The crude product was purified by short-path distillation (Kugel-rohr) yielding pyridine **10** as a colorless oil in a typical yield of 75-90%.



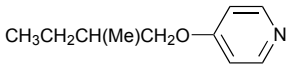
4-Pentyloxypyridine (10a).[9] Bp 100 °C/ 1 mm Hg (Kugel-Rohr); ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.93 (t, J = 7.1 Hz, 3H), 1.35-1.50 (m, 4H), 1.80 (quin. J = 7.0 Hz, 2H), 3.99 (t, J = 6.6 Hz, 2H), 6.78 (d, J = 6.4 Hz, 2H), 8.40 (d, J = 6.4 Hz, 2H).



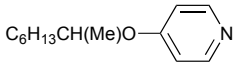
4-Heptyloxypyridine (10b).[3] Bp 96-98 °C/ 0.2 mm Hg;[3] ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.89 (t, *J* = 6.8 Hz, 3H), 1.25-1.38 (m, 6H), 1.42-148 (m, 2H), 1.79 (quin. *J* = 7.0 Hz, 2H), 3.99 (t, *J* = 6.6 Hz, 2H), 6.79 (d, *J* = 6.4 Hz, 2H), 8.40 (d, *J* = 6.4 Hz, 2H); ^{1}H NMR (300 MHz, C_6D_6) δ 0.87 (t, *J* = 6.9 Hz, 3H), 1.09-1.26 (m, 8H), 1.48 (quin. *J* = 6.9 Hz, 2H), 3.45 (t, *J* = 6.5 Hz, 2H), 6.47 (d, *J* = 6.1 Hz, 2H), 8.43 (d, *J* = 6.2 Hz, 2H).



4-Nonyloxypyridine (10c). Bp 125 °C/ 0.5 mm Hg; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.8 Hz, 3H), 1.25-1.38 (m, 10H), 1.42-1.48 (m, 2H) 1.79 (quin. *J* = 7.0 Hz, 2H), 4.00 (t, *J* = 6.6 Hz, 2H), 6.79 (d, *J* = 6.4 Hz, 2H), 8.41 (d, *J* = 6.4 Hz, 2H). Anal. Calcd for $C_{14}H_{23}NO$: C, 75.97; H, 10.47; N, 6.33. Found: C, 75.75; H, 10.69; N, 6.21.



(*S*)-4-(2-Methyl-1-butoxy)pyridine (10d). Yield 92%; bp 110-113 °C/0.1 mm Hg (Kugel-Rohr): ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.95 (t, *J* = 7.5 Hz, 3H), 1.01 (d, *J* = 6.8 Hz, 3H), 1.22-1.34 (m, 1H), 1.50-1.61 (m, 1H), 1.87 (pseudo-octet, *J* = 6.6 Hz, 1H), 3.78 (dd, J_1 = 9.1 Hz, J_2 = 6.6 Hz, 1H), 3.85 (dd, J_1 = 9.1 Hz, J_2 = 6.0 Hz, 1H), 6.79 (d, *J* = 6.4 Hz, 2H), 8.40 (d, *J* = 6.4 Hz, 2H).



(*S*)-2-Octyloxypyridine (10e).[1] Yield 73%; bp 150-160 °C/0.5 mm Hg (Kugel-Rohr): ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.7 Hz, 3H), 1.24-1.48 (m, 8H), 1.31 (d, *J* = 6.1 Hz, 3H), 1.54-1.64 (m, 1H), 1.69-1.82 (m, 1H), 4.44 (sext, *J* = 6.1 Hz, 1H), 6.76 (d, *J* = 6.4 Hz, 2H), 8.39

(d, J = 6.4 Hz, 2H). Anal. Calcd for $C_{13}H_{21}NO$: C, 75.32; H, 10.21; N, 6.76. Found: C, 75.19; H, 10.20; N, 6.79.

1,10-Diammonio-*closo*-decaborane (13).[4] It was obtained from bis-dinitrogen **12** [4] and NH_3 as described for the preparation of **6[NMe$_4$]** and used without further purification: ^{11}B NMR (128 MHz, DMSO-d_6) δ -29.1 (8B), 7.0 (2B).

2. Computational Details

Quantum-mechanical calculations were carried out with the B3LYP[10,11] method with 6-31G(d,p) basis set using Gaussian 09 package.[12] Geometry optimizations for unconstrained conformers of **1–3** in the most extended molecular shapes were undertaken using default convergence limits. The alkoxy and alkyl groups were set in all-*trans* conformation in the input structures. The former were set co-planar with the pyridine ring, while orientation of the pentyl substituent on the thiane and quinuclidine rings in the input structure was set according to conformational analysis of 1-ethyl derivatives of bicyclo[2.2.2]octane and cyclohexane. Vibrational frequencies were used to characterize the nature of the stationary points achieved with the DFT method, and to obtain thermodynamic parameters. Zero-point energy (ZPE) corrections were scaled by 0.9806.[13]

Electronic excitation energies were obtained at the B3LYP/6-31G(d,p)//B3LYP/6-31G(d,p) level using the time-dependent DFT calculations[14] supplied in the Gaussian package. Solvent effect on electronic excitations was included using the PCM model[15] [keywords: SCRF(PCM, Solvent=*name*)]. Frequency-dependent hyperpolarizabilities were obtained using Polar and

CPHF=RdFreq keywords.[16] The radius of the Onsager cavity a_0 for the Lippert-Mataga calculations was obtained using VOLUME keyword.

The transition state structure for *cis–trans* isomerization of **2b** was located using the STQN method[17] requested with the QST3 keyword and default convergence criteria at the B3LYP/6-31G(d,p) level of theory and default convergence criteria. Final energy for the optimized structure was calculated with the B3LYP/6-31G(d,p) method and inclusion of solvation effects with the PCM model[15] [keywords: SCRF(PCM, Solvent=*name*)].

3. Equilibrium and kinetic data for 2b.

In solution there are two conformers for each isomer **2b-*trans*** and **2b-*cis*** - a total of four species in equilibrium as shown in Figure S1. It is assumed that the higher intensity (lowfield) ^{1}H NMR signals (Figure 6 in the main text) are related to species **C'** and **T**, while low intensity signals (highfield) are ascribed to species **C** and **T'**.

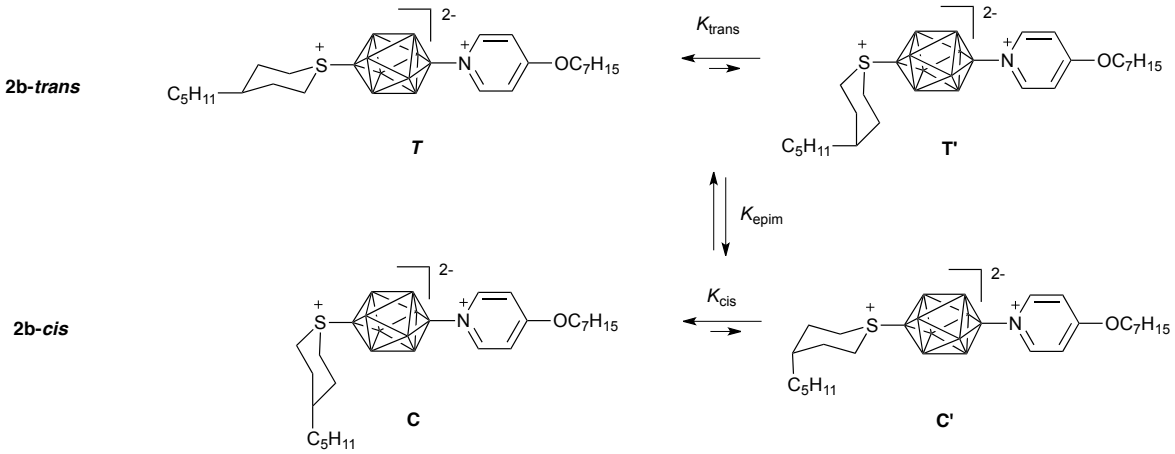
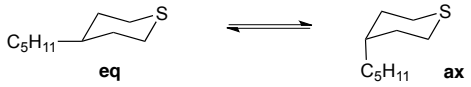


Figure S1. Isomer and conformer equilibrium for **2b**.

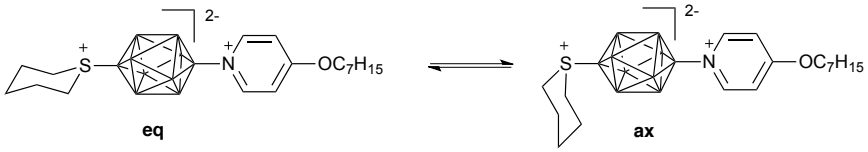
Therefore:

$$K_{obs} = \frac{\boldsymbol{C} + \boldsymbol{T'}}{\boldsymbol{C'} + \boldsymbol{T}}$$

It is assumed further that the C_5H_{11} and {*closo*-B_{10}} substituents are independent of each other do not affect each other's preference for either axial or equatorial position in **2b**. Consequently their preference can be described by equilibrium constant for monosubstituted thian:

$K_{C5} = \frac{ax}{eq}$ 

and

$K_{B10} = \frac{ax}{eq}$ 

With these assumptions, it can be demonstrated that the observed equilibrium describes the conformational preference of the {*closo*-B_{10}} cluster and is related to the steric parameter *A* of the cluster.

$$K_{obs} = K_{B10}$$

Equilibrium constant K_{epi} for the isomerization process can be calculated from:

$$K_{epi} = \frac{\boldsymbol{C} + \boldsymbol{C'}}{\boldsymbol{T} + \boldsymbol{T'}} = \frac{K_{B10} + K_{C5}}{1 + K_{B10} \times K_{C5}}$$

For these calculations K_{C5} can be assumed to be the same as in ethylcyclohexane ΔH = 1.60 kcal/mol, ΔS = -0.64 cal/molK.[18]

Table S1. Equilibrium constant measurement for **2b** in toluene-d_8

2b-*trans* ⇆ 2b-*cis*

T	323 K	333 K	343 K	353 K	363 K	373 K
K_{obs}	0.292	0.306	0.321	0.330	0.356	0.363

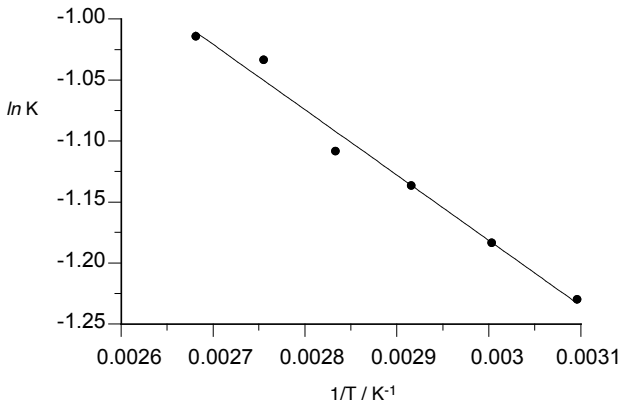


Figure S2. A plot of *ln* K vrs 1/T.

ΔH = +1.06±0.06 kcal/mol
ΔS = +0.8±0.2 cal/molK
ΔG_{298} = +0.82 kcal/mol
R^2 = 0.98

Table S2. Equilibrium constants K extrapolated from data in Table S1.

2b-*trans* ⇆ 2b-*cis*

T	273 K	278 K	283 K	288 K	293 K	298 K
K	0.219	0.225	0.231	0.237	0.243	0.249

Rate constants *k* in Table S3 were obtained from a plot of $ln(\alpha_\infty - \alpha)$ vrs t (Figure S3), where α is the observed mole fraction of the *cis* isomer, and α_∞ is the mole fraction of the *cis* isomer at infinite time. The latter was obtained from equilibrium constant K extrapolated from high temperature data shown in Table S1 to the given temperature T (Table S2).

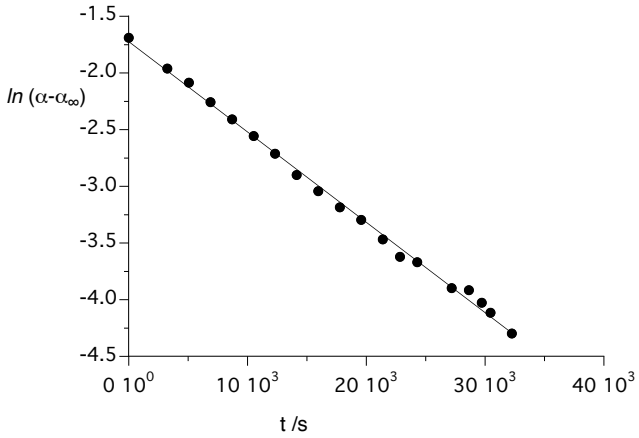


Figure S3. An example of first order kinetics for isomerization of **2b-*trans*** at 283 K. Rate k = 8.1x10-5 s^{-1}

Table S3. Kinetic data for isomerization of **2b-*trans*** obtained by integration of ^{1}H NMR signals and Arrhenius analysis

2b-*trans* → 2b-*cis*

$k \cdot 10^5$ s^{-1}						E_a	*ln*A	R^2
273 K	278 K	283 K	288 K	293 K	298 K	kcal/mol		
2.11±0.1	4.38±0.1	8.12±0.1	20.7±0.2	40.3±0.3	86.7±2	24.1±0.6	33.7±1.2	0.998

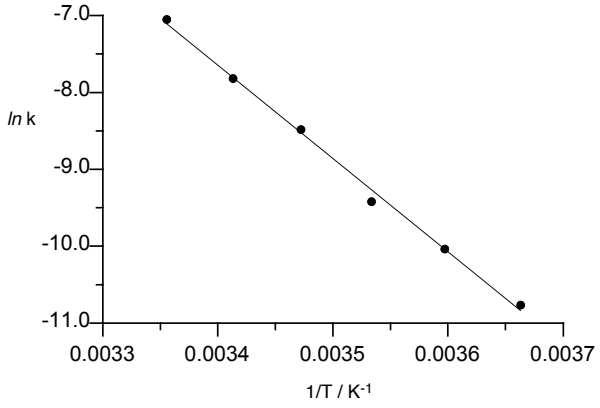


Figure S4. Arrhenius plot for interconversion of the {*closo*-B_{10}} cluster between axial and equatorial orientation in **2b**. Plot of data from Table S3.

Calculation of activation parameters: $\Delta S^{\ddagger} = R \cdot [lnA - ln(ekT/h)]$, $\Delta H^{\ddagger} = E_a - RT$

4. Fluorescence quantum yield

Quantum yield Φ_u for fluorescence of **2a** and **3b** was measured in MeCN and CH_2Cl_2 (**2a**) using aqueous solution of quinine bisulfate in 0.1 N H_2SO_4 as a reference. Both solutions, the unknown (**2a** and **3b**) and the reference were at concentrations so the optical density at around 325 nm did not exceed 0.1 (concentration of about 2×10^{-6} mol/L). A plot of the absorption spectra for the unknown and the reference in the same graph, gave the excitation wavelength as the crossing point for the two spectra (same optical density). Thus, the excitation wavelength for **2a** was λ_{ex} = 319 nm in MeCN and 331 nm in CH_2Cl_2. For **3b** λ_{ex} was 329 nm in MeCN.

The resulting emission for the reference and the unknown were integrated over a range of about 300 nm. The quantum yield was calculated from the formula:[19]

$$\Phi_u = \frac{F_u}{F_r}\frac{n_u^2}{n_r^2}\Phi_r$$

where Φ_u is area of emission peak for the unknown, Φ_r area of emission peak for a reference, n^2_u refractive index of the solvent for the unknown, n^2_u refractive index of the solvent for the reference; Φ_r quantum yield for the reference (quinine bisulfate $\Phi_r = 0.546$)

5. Solvatochromic data

Experimental data for the position of the long wavelength absorption peak for selected compounds in different solvents is shown in Table S4 and theoretical values are listed in Table S5. A plot of absorption energy for **2b** and **3b** *vrs* solvent parameter is shown in Figure S5, and contours of MOs involved in the cluster →N_2 excitation for **8a** are in Figure S6.

Table S4. Experimental solvent dependence of the cluster→pyridine or cluster →N_2 (π-π*) electronic excitation.

	λ_{max} /nm						
solvent compound	MeCN	Ether	CH_2Cl_2	$ClCH_2CH_2Cl$	THF	$(EtO)_3PO$	PrCN
2b	300.8	321.8	308.0	306.9	314.2	306.5	307.4
3b	310.0	332.4	316.2	317.3	325.5	316.5	315.9
8a	252.0	258.4	257.1	257.0	257.7	254.5	254.7
8b	255.3	262.5	259.5	259.4	261.7	–	258.0
$E_T(30)$ [a]	45.6	34.5	40.7	41.3	37.4	41.7	42.5
E_T^N [b]	0.460	0.117	0.309	0.327	0.207	0.324	0.370

[a] kcal/mol. [b] E_T^N normalized values (ref.[20])

Table S5. Theoretical solvent dependence of the cluster→pyridine or cluster→N_2 (π-π*) electronic excitation.[a]

	λ_{max} /nm					
solvent compound	MeCN	Ether	CH_2Cl_2	$ClCH_2CH_2C$	THF	vacuum
2b	324.9	342.2	332.5	331.5	334.3	386.1
3b	332.0	349.8	339.9	338.9	341.8	392.9
8a	264.8	266.6	266.0	266.0	266.1	268.4
8b	264.1	265.8	265.25	265.25	265.3	267.0

[a] TD-DFT data at the B3LYP/6-31G(d,p) // B3LYP/6-31G(d,p) level of theory using the PCM model.

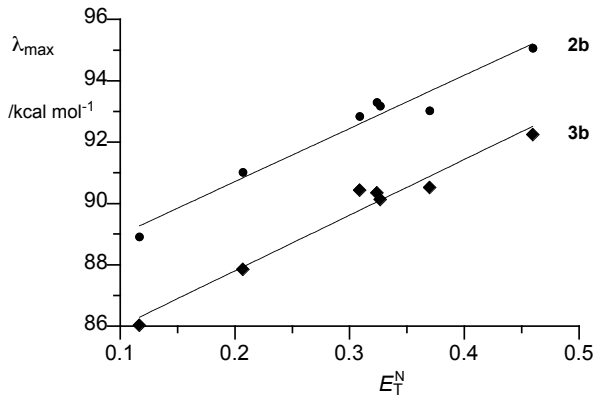
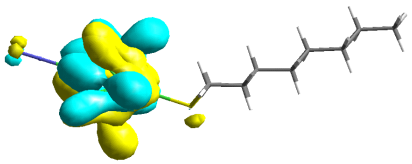
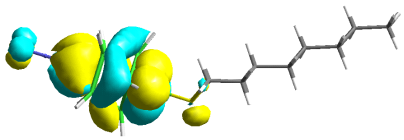


Figure S5. Dependence of absorption energy for **2b** and **3b** on solvent polarity E_T^N. Slope: 17.3±1.6 (**2b**) and 18.1±1.5 (**3b**), $r = 0.98$.



combined HOMO: -6.81 eV
HOMO-1: -6.92 eV



combined LUMO: -2.28 eV
LUMO+1:-2.25 eV

Figure S6. B3LYP/6-31G(d,p) derived contours and energies of frontier molecular orbitals for **8a** in MeCN dielectric medium.

6. Lippert-Mataga calculations

The change of the dipole moment upon excitation is calculated from the Lippert-Mataga relationship (eq 1):[21]

$$\left(\nu_{ab} - \nu_{fl}\right) = \frac{2(\mu_e - \mu_g)^2}{4\pi\varepsilon_0 hca_0^3}\Delta f + \text{const} \qquad \text{(eq 1)}$$

where

ν_{ab} – energy of maximum of absorption in cm^{-1}
ν_{fl} – energy of maximum of fluorescence in cm^{-1}

and solvent parameter Δf is given by equation 2:

$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{2n^2 - 1}{2n^2 + 1} \qquad \text{(eq 2)}$$

solvent	*n*	ε	Δf
MeCN	1.3441	36.00	0.3046
PrCN	1.3842	20.30	0.2744
Et_2O	1.3524	4.34	0.1669
THF	1.4072	7.58	0.2096
$(EtO)_3PO$	1.403	12.94	0.2480
CH_2Cl_2	1.424	9.08	0.2184
$ClCH_2CH_2Cl$	1.445	10.37	0.2208
DMSO	1.4793	46.45	0.2630

Thus, a plot of the difference between absorption and emission energies against solvent parameter Δf gives a slope expressed by eq 3 and in cm^{-1} units:

$$slope = \frac{2(\mu_e - \mu_g)^2}{4\pi\varepsilon_0 hca_0^3} \qquad \text{(eq 3)}$$

The change of the dipole moment Δμ is then calculated from eq 4 in which the slope is converted to m^{-1} units by multiplying by a factor of 100. The resulting Δμ value is in units Cm and is divided by 3.333564×10^{-30} to convert to Debye:

$$\Delta\mu = \mu_e - \mu_g = \sqrt{100\times slope\times 2\pi\varepsilon_0 hca_0^3} \qquad \text{(eq 4)}$$

$4\pi\varepsilon_0 = 1.114\times10^{-10}$ A s $(V\ m)^{-1}$

$h = 6.6261\times10^{-34}$ J s
$c = 2.997 \times10^{8}$ m s^{-1}
$a_0 = 6.26 \times10^{-10}$ m (cavity radius calculated for **2b** with the DFT method using VOLUME keyword)

7. Calculations for the nematic phase using the Maier-Meier relationship

For complete background and procedures of the calculations see ESI in ref. [22] The calculated values for the Krirkwood factor and order parameter were substituted into the original expressions for $\Delta\varepsilon$ and $\varepsilon_\perp$ to verify the correctness of the calculations.

Details of the calculations and assumptions:

Measurement temperature: T = 403 K

Ratio of **2b-*trans*** to **2b-*cis*** at 403 K: $K_{403} = 2.760$ (extrapolated from data in Table S1).

Assumptions:

• Only two forms of **2b** are present in the material designated as **2b-*trans*** and **2b-*cis*** (**T** and **C** in Figure S1).

• Density of the liquid is 1000 kg•m^{-3}.

• Static permittivity ε_s for calculations of field parameters *F* and *h* was obtained as $\varepsilon_s = (\varepsilon_{ll} + 2\,\varepsilon_\perp)/3$

Dipole moment and polarizability computational results for **2b**.

Dipole moments (D) and polarizability (au) at the B3LYP/6-31G(d,p) level of theory (full geometry optimization). 1Å^3 = 0.1482 au. Summary of results is given in Table S6

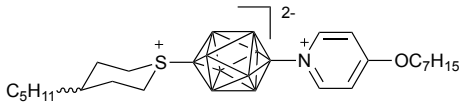
2b-*trans*:

```
Dipole moment (field-independent basis, Debye) in vacuum:
X= 3.7325    Y= 2.0669    Z= 0.7311  Tot= 4.3288
Dipole moment (field-independent basis, Debye) in CH2Cl2:
X= 4.1153    Y= 2.4065    Z= 0.9172  Tot= 4.8547
Exact polarizability: 657.085  12.240 317.015   0.029   6.547 288.440

Diagonalized: 657.53,  318.04,  286.99
```

2b-*cis*:

```
Dipole moment (field-independent basis, Debye) in vacuum:
X= -4.5006    Y= 4.3133    Z= 0.5000  Tot= 6.2538
Dipole moment (field-independent basis, Debye) in CH2Cl2:
X= -4.5096    Y= 5.1567    Z=  0.6792  Tot=  6.8840
Exact polarizability: 601.511  -8.726 354.392   9.003   7.757 289.190

Diagonalized: 600.84,  355.65,  288.60
```

Table S6. Calculated molecular parameters for **2b** in vacuum.[a]



	$\mu_{\parallel}$ /D	$\mu_{\perp}$ /D	μ /D	$\alpha_{\parallel}$/ Å^3	$\alpha_{\perp}$/ Å^3	$\Delta\alpha$/ Å^3	α_{avrg}/ Å^3
trans	3.73	2.19	4.33	97.42	44.83	52.58	62.36
cis	4.5	4.34	6.25	89.04	47.74	41.31	61.51
mix [b]	3.93	2.76	4.81	95.19	45.61	49.58	62.13

[a] Obtained at the B3LYP/6-31G(d,p) level of theory. Polarizability units were converted from au to Å^3 using the factor 0.1482. [b] **2b-*trans*** to **2b-*cis*** in a ratio of 2.760.

8. Crystal Structure Data

Table S7. Crystal Data and Summary of X-ray Data Collection

compound	**8b**	**8a**	**2b**
formula	$C_{12}H_{31}B_{10}N_3$	$C_{10}H_{28}B_{10}N_2S$	$C_{22}H_{47}B_{10}NOS$
fw	325.50	316.52	481.77
space group	$P2_1/c$	$P2_1/n$	P-1
a, Å	11.1832 (7)	10.7989 (2)	9.7645(12)
b, Å	11.4422 (7)	21.0221 (4)	15.716(2)
c, Å	16.2022 (10)	17.1320 (4)	20.148(3)
α, °	90	90	77.516(2)
β, °	109.272 (1)	99.468 (1)	83.823(2)
γ °	90	90	78.246(2)
V, $Å^3$	1957.1 (2)	3836.25 (14)	2948.9(6)
Z	4	8	4
D (calcd), g/cm^3	1.105	1.096	1.085
tot. reflcns	9435	25968	22591
unique reflcns	3414(R_{int} = 0.0312)	6707 (R_{int} = 0.0662)	10295 (R_{int} = 0.0293
no. with $I>2.0\sigma(I)$	2458	4514	6251
*R*1	0.0578	0.0594	0.0905
w*R*2	0.1296	0.1066	0.2374
goodness of fit on F^2	1.054	1.046	1.049
max Δ/σ in final cycle			
max/min peak (final diff peak) ($e^-/Å^3$)	0.514 and -0.209 $e^-/Å^3$	0.238 and -0.210 $e^-/Å^3$	0.865 and -0.406 $e^-/Å^3$

9. Archive files for DFT geometry optimizations

2a-trans

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C20H43B10N1O1S1\PIOTR\18-Sep-2
012\0\\#P B3LYP/6-31G(d,p) FOpt fcheck Geom(nodistance, noangle) #P fr
eq(noraman, readIso) Volume\\1-(4-C5H11O-Pyridine)-10-(4-C5H11-ThiaCyc
lohexane)decaborane, C1 symm\\0,1\B,-0.0359668761,-0.0108229403,0.0227
420263\B,0.0577032209,0.0336127611,1.6977977567\B,1.5445150585,-0.0486
815514,0.5917066939\B,-0.7385524321,-1.362783385,0.7335959394\B,1.5921
78655,-0.7179549975,2.2614223982\B,0.7472551288,-1.4423724313,-0.37335
12401\B,1.4686284446,-2.3929291134,2.2165891301\B,-0.0251128341,-1.648
9500673,2.3696188496\B,2.0896770839,-1.7657124366,0.7928955304\B,0.470
3002512,-2.6888427413,0.8969207584\N,-0.6801943509,1.0015380568,-0.923
2343997\O,-2.3730572924,3.8102088065,-3.4374302972\S,2.2689524103,-3.6
471640616,3.3578692282\C,-1.8488035764,2.8473174918,-2.6629041135\C,-1
.9408131342,1.4683540831,-2.9091959369\C,-1.3476220122,0.5876648672,-2
.0218677647\C,-0.5896842077,2.334276336,-0.6798162174\C,-1.1537801623,
3.2708460798,-1.5158877428\C,-3.0938438443,3.4441034799,-4.6289312757\
C,1.7407122965,-3.1514074299,5.0513076489\C,2.6181121905,-3.8055933159
,6.1199559321\C,4.1035687263,-3.3982918346,6.0490210666\C,4.7189154829
,-3.7566768641,4.6808615748\C,4.0236573229,-3.1023406413,3.4865739577\
C,-3.5608945996,4.7270976351,-5.2975371928\C,-4.3498374994,4.459008128
8,-6.5853720297\C,-4.8281504487,5.7443743936,-7.2726532711\C,-5.615782
3528,5.4802037389,-8.5587789375\C,4.93450384,-4.0256334874,7.184926470
3\C,4.5562596253,-3.5795039293,8.6041061225\C,5.4918163058,-4.14573783
27,9.6801387617\C,5.1165941535,-3.7176708117,11.1042398203\C,6.0553289
101,-4.2852451494,12.1729102605\H,-5.9432158819,6.4153903039,-9.023374
1401\H,-1.066897352,4.3285315783,-1.2993284935\H,-0.0466561772,2.60423
57756,0.2164090538\H,-1.3827407164,-0.4848105081,-2.1639261347\H,-2.45
9398437,1.0698282199,-3.7706184361\H,-2.4322487904,2.8710105375,-5.291
7278226\H,-3.9456945045,2.8073049331,-4.3564903443\H,-0.4271779238,0.9
444839146,2.3028750218\H,2.3210058959,0.7943746654,0.2521896575\H,-1.8
893430498,-1.6094960611,0.5245524386\H,0.8577567376,-1.7604555556,-1.5
213321419\H,2.2503418635,-0.1765877144,3.103193479\H,4.006468563,-2.01
12748898,3.5533604448\H,4.4806075507,-3.3790804219,2.5343340862\H,5.76
91385696,-3.43943655,4.6632097053\H,4.7235207761,-4.8477647805,4.55471
54494\H,4.1536328933,-2.3034835976,6.157920719\H,2.5344613722,-4.89882

31669,6.0505893623\H,2.2011867472,-3.5235172884,7.0929647843\H,0.69511
87752,-3.4562552211,5.1271955853\H,1.7805783098,-2.0592478007,5.085547
1042\H,-0.7397896359,-1.8787364619,3.2993251786\H,3.1653183707,-2.0929
064691,0.3879180904\H,0.1826936365,-3.8062511311,0.5927852107\H,-2.684
1630079,5.3490548545,-5.5142784785\H,-4.1785848952,5.2883769146,-4.586
2447273\H,-3.7274723041,3.8849952477,-7.2863316807\H,-5.2191312364,3.8
253132051,-6.3598863075\H,-5.449561222,6.3175735026,-6.5718993172\H,-3
.9595211899,6.3775989274,-7.4967820905\H,-5.0078356591,4.9396469238,-9
.2928835869\H,-6.5089494166,4.8770505574,-8.3608320945\H,5.99121466,-3
.7790508168,7.0125729599\H,4.8670084129,-5.1213647668,7.1163728632\H,4
.5684471616,-2.4813787244,8.6546177957\H,3.5274856383,-3.8839449651,8.
8362821913\H,5.4918494114,-5.2435819401,9.6205325908\H,6.5236827825,-3
.8317493641,9.4673785116\H,4.0861745732,-4.0334740159,11.316797959\H,5
.1150570535,-2.6208285306,11.163434452\H,5.7608254997,-3.9622604112,13
.1765838219\H,6.0519670631,-5.3811130371,12.1622050082\H,7.0879945986,
-3.9574297081,12.0081107638\\Version=EM64L-G09RevA.02\State=1-A\HF=-15
64.9416509\RMSD=3.924e-09\RMSF=3.220e-06\Dipole=-0.4825318,1.4192747,-
0.7319907\Quadrupole=-10.5679047,-10.7022689,21.2701737,-22.5376091,35
.7192929,-34.8271274\PG=C01 [X(C20H43B10N1O1S1)]\\

2b-trans

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C22H47B10N1O1S1\PIOTR\18-Sep-2
012\0\\#P B3LYP/6-31G(d,p) FOpt fcheck Geom(nodistance, noangle) freq(
noraman, readIso)\\1-(4-C7H15O-Pyridine)-10-(4-C5H11-ThiaCyclohexane)d
ecaborane, C1 symm\\0,1\B,-0.047534559,-0.0161657663,0.026843241\B,0.0
484219587,0.029748338,1.7017566737\B,1.5338070143,-0.0501703059,0.5936
715605\B,-0.7461243848,-1.3691124726,0.7396625153\B,1.5854442853,-0.71
80000807,2.2638181603\B,0.738407831,-1.4462273663,-0.3692414673\B,1.46
54517474,-2.3932354646,2.2204464945\B,-0.0297774093,-1.6524628656,2.37
49532125\B,2.0830945724,-1.7657789173,0.7953508187\B,0.4659394593,-2.6
923351868,0.9023847851\N,-0.6949381202,0.9940314298,-0.919295186\O,-2.
3955557033,3.7970171226,-3.4344993753\S,2.2694034016,-3.6453703362,3.3
613063802\C,-1.868804507,2.835891225,-2.6596208705\C,-1.9593326168,1.4
564540281,-2.9039113135\C,-1.3635622916,0.5777834053,-2.0163228824\C,-
0.6057517635,2.3272194629,-0.6778822138\C,-1.1724107171,3.2618860602,-
1.5143283343\C,-3.1191878847,3.4286808937,-4.623709534\C,1.7455575162,

-3.1475676795,5.0554890952\C,2.6256160636,-3.8007314807,6.1225220324\C
,4.1109611779,-3.393642699,6.0475786281\C,4.7227533632,-3.7528693774,4
.6780332938\C,4.0242199606,-3.0997360956,3.4849647038\C,-3.5903752241,
4.7105568713,-5.2915968183\C,-4.3847209286,4.4406685394,-6.5759155584\
C,-4.8670016714,5.7256331138,-7.2608844856\C,-5.66564353,5.4701366433,
-8.5444048795\C,-6.1498205649,6.754633247,-9.2284237872\C,-6.946365348
,6.4932836155,-10.5099836328\C,4.9444237481,-4.0206084875,7.1818532838
\C,4.5694309858,-3.5734700624,8.6015910591\C,5.5047836038,-4.142295970
7,9.6764050483\C,5.1327846099,-3.7130009831,11.1009825565\C,6.07082491
24,-4.2838428557,12.1685128497\H,-1.0865399061,4.3199858018,-1.2993969
298\H,-0.0615290949,2.5991730072,0.2170145944\H,-1.397409232,-0.494924
2452,-2.1569179402\H,-2.4786128871,1.0561265579,-3.7640833281\H,-2.458
5161822,2.8562265315,-5.2879643953\H,-3.9691404194,2.790650076,-4.3482
426153\H,-0.4374986533,0.9401119242,2.3067686144\H,2.307802725,0.79448
0361,0.2523717907\H,-1.8966268171,-1.618736906,0.5324957934\H,0.848017
8384,-1.7649832261,-1.5171080811\H,2.2435399151,-0.1744266213,3.104215
488\H,4.0068137776,-2.008601752,3.5507489874\H,4.4788434142,-3.3771467
681,2.5318154271\H,5.7728464425,-3.4353963118,4.657380749\H,4.72727973
65,-4.8440451907,4.552684095\H,4.1614610881,-2.2987910423,6.1557733543
\H,2.5417496774,-4.8940245078,6.0543913522\H,2.2112078533,-3.517779508
3,7.0963375078\H,0.7001176482,-3.4521772787,5.1344163881\H,1.785641195
9,-2.0553733531,5.0883739567\H,-0.74274107,-1.8832283768,3.3057523973\
H,3.1588892429,-2.0910370571,0.3891497492\H,0.1803559357,-3.8106118364
,0.5995123469\H,-2.7152582492,5.3333082651,-5.5124390009\H,-4.20561348
18,5.271703311,-4.5781051547\H,-3.764464272,3.8665867598,-7.2784781307
\H,-5.2518232366,3.8060009748,-6.3453146468\H,-5.4841484956,6.30061161
89,-6.5564147657\H,-3.9995600529,6.3596457048,-7.4916790344\H,-5.04814
06849,4.8952520954,-9.2493403786\H,-6.5322824389,4.8343192812,-8.31343
33034\H,-5.2837095031,7.3898593322,-9.4583828713\H,-6.7671218616,7.328
2112155,-8.5237888602\H,-7.2778779638,7.4284746321,-10.9722930848\H,-6
.3433716491,5.9531135468,-11.2486213872\H,-7.8376887495,5.8889186574,-
10.3068277897\H,6.0008540362,-3.7746530372,7.0069298199\H,4.8761936114
,-5.1163425965,7.1140784561\H,4.5846551777,-2.4753786228,8.6520439039\
H,3.5400637835,-3.8750208551,8.835046408\H,5.5014783376,-5.2401401659,
9.6169248279\H,6.5373061165,-3.8314128803,9.462251555\H,4.1015618159,-
4.0253019791,11.3147954531\H,5.1350567124,-2.6161641655,11.1602347762\

H,5.7785386715,-3.9599821854,13.1725520838\H,6.0637653604,-5.3796938763,12.1576982486\H,7.1044277998,-3.959519851,12.0026305202\\Version=EM64L-G09RevA.02\State=1-A\HF=-1643.574709\RMSD=5.003e-09\RMSF=1.870e-06\Dipole=-0.5053525,1.4358893,-0.7637355\Quadrupole=-9.5525007,-11.749057 5,21.3015582,-21.3716196,35.0807403,-32.8396322\PG=C01 [X(C22H47B10N1O1S1)]\\@

2b-cis

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C22H47B10N1O1S1\PIOTR\20-Sep-2012\0\\#P B3LYP/6-31G(d,p) FOpt fcheck Geom(nodistance, noangle) freq(noraman, readIso)\\cis-1-(4-C7H15O-Pyridine)-10-(4-C5H11-ThiaCyclohexane)decaborane, C1 symm\\0,1\B,-0.1453344695,-0.0336417222,-0.1735978168\B,-0.1699188418,-0.1358288772,1.5011792644\B,1.3897828785,-0.0084617065,0.5087387689\B,-0.7863584962,-1.4911345403,0.3660684152\B,1.3752232784,-0.821861081,2.1119238275\B,0.7753656258,-1.3618845239,-0.6278699242\B,1.390198129,-2.4992826334,1.9191026107\B,-0.162609362,-1.8727933494,2.0234468131\B,2.0566961859,-1.6906725472,0.6094363277\B,0.5064205927,-2.7340532613,0.5053818109\N,-0.7968688312,1.0164054225,-1.0729886452\O,-2.4935480793,3.9388881299,-3.4509637321\S,2.2755273242,-3.6182603436,3.1410819463\C,-1.9604078498,2.9420653686,-2.727479171\C,-1.8856676809,1.5988825682,-3.1287592269\C,-1.301232637,0.6765847869,-2.278689136\C,-0.8710454816,2.3136694118,-0.6781794301\C,-1.4382370198,3.2876099867,-1.4680873391\C,-3.0243607193,3.657200654,-4.7596256033\C,1.0498397771,-4.8527724251,3.7537329532\C,0.5470686962,-5.8280277196,2.6906475295\C,1.660905366,-6.6505211045,2.0139378398\C,2.6496549707,-5.7274041703,1.275229931\C,3.3821211007,-4.7357039418,2.1762646833\C,-3.5272436735,4.9668576975,-5.345402645\C,-4.1008202742,4.7898008032,-6.7573001416\C,-4.6122212068,6.1026417473,-7.3636949445\C,-5.178423884,5.9398620252,-8.7792768746\C,-5.6906808588,7.2515048721,-9.3870650242\C,-6.2532431865,7.081926978,-10.8013181144\C,1.0925054738,-7.7010502591,1.0399941503\C,0.2748332203,-8.8257736365,1.6895902864\C,-0.1785360592,-9.894346871,0.6865654763\C,-0.9954051757,-11.0251798375,1.3235427689\C,-1.444003967,-12.0885207407,0.3167882715\H,-1.483328322,4.3157992655,-1.1305614312\H,-0.4556766443,2.5230057327,0.2988822312\H,-1.211314399,-0.3701914738,-2.5391133944\H,-2.268947868,1.2599353306,-4.0815924736\H,-2.2339551101,3.2227552467,-5.385660437\H,-3.8374831774,2.9246529105,

-4.6720172148\H,-0.7657518656,0.6783013827,2.1436785759\H,2.1176213731
,0.9157858364,0.3001341065\H,-1.8954560708,-1.8063914162,0.0508411725\
H,0.992440866,-1.5732465237,-1.7854709749\H,1.930561691,-0.3299236576,
3.0463815688\H,4.0017601191,-5.2423080924,2.9239696747\H,4.0152420131,
-4.054941086,1.6028471919\H,3.4167202032,-6.3365553161,0.7793758257\H,
2.1215198719,-5.1756758842,0.4914865012\H,2.2173814432,-7.187223928,2.
8010182999\H,-0.0119294523,-5.2730326415,1.9302450525\H,-0.1642749051,
-6.4959075905,3.1902495431\H,0.239717094,-4.2449801966,4.1625419764\H,
1.548947683,-5.3704569377,4.5799291895\H,-0.9240416187,-2.2389310617,2
.8694916901\H,3.1784947459,-1.903636028,0.2546978701\H,0.3060588127,-3
.8216307874,0.0532904655\H,-2.6979835015,5.6840637212,-5.3625814028\H,
-4.2904837918,5.3818694238,-4.6764431052\H,-3.3308068513,4.3630570945,
-7.4151928492\H,-4.9207359273,4.0583547553,-6.7326598746\H,-5.38563220
07,6.5268919826,-6.7083574475\H,-3.7937427692,6.8357716267,-7.38119684
13\H,-4.4039493649,5.51547384,-9.4340735639\H,-5.9959167494,5.20492292
18,-8.76216992\H,-4.8736551931,7.9854998718,-9.4031978937\H,-6.4647493
992,7.6747596718,-8.7326710031\H,-6.6101583012,8.0340259739,-11.206664
903\H,-5.4915869307,6.6935351863,-11.4868335911\H,-7.0946739418,6.3798
996805,-10.8118073891\H,1.9325458804,-8.1527410549,0.4941905409\H,0.48
0202981,-7.1911149648,0.2831466214\H,0.8751275141,-9.301725832,2.47868
71723\H,-0.611347259,-8.412613094,2.1883199946\H,-0.7743453959,-9.4189
231599,-0.1055143924\H,0.7025945366,-10.3213013382,0.1864364881\H,-1.8
764467715,-10.5982809561,1.8217723184\H,-0.3999984976,-11.4992124709,2
.1158929948\H,-2.0232422617,-12.880729317,0.8020704605\H,-2.0714899154
,-11.6512126196,-0.468072074\H,-0.5838042379,-12.5584591868,-0.1734772
557\\Version=EM64L-G09RevA.02\State=1-A\HF=-1643.5733478\RMSD=8.613e-0
9\RMSF=3.208e-06\Dipole=-1.2541606,0.2941829,-2.0962434\Quadrupole=-16
.4967481,19.9995364,-3.5027883,-23.9589024,14.0121515,-34.3110367\PG=C
01 [X(C22H47B10N1O1S1)]\\@

2b-TS

1\1\GINC-OCTOPUS\FTS\RB3LYP\6-31G(d,p)\C22H47B10N1O1S1\PIOTR\31-Aug-20
11\0\\#P B3LYP/6-31G(d,p) FOpt(QST3, CalcFC) fcheck Geom(nodistance, n
oangle) #P freq(noraman, readIso)\\TS 1-(4-C7H15O-Pyridine)-10-(4-C5H1
1-ThiaCyclohexane)decaborane\\0,1\B,0.8507801191,0.2418277792,0.147498
5473\B,-0.163730319,0.9875667066,1.263897722\B,0.0344745063,-0.8498759

802,1.125836235\B,-0.388768008,1.0960118874,-0.5956296584\B,-1.4803396
316,-0.1255328285,1.7530525814\B,-0.1925359071,-0.7412876755,-0.734624
2701\B,-2.6644549228,-0.1664345305,0.5513341092\B,-1.8063598617,1.2582
738887,0.5321365303\B,-1.5249117544,-1.3591981585,0.3388709402\B,-1.80
10958243,0.0317709333,-0.8862630078\N,2.3595477792,0.4219679234,-0.024
1949155\O,6.4212818506,1.0205461236,-0.5073292039\S,-4.5219984481,-0.3
794193143,0.7610578512\C,5.1162743486,0.7582327153,-0.3312244775\C,4.5
838919514,-0.468747452,0.0943801379\C,3.2124912321,-0.5929976514,0.234
1364936\C,2.8703945141,1.610618041,-0.4380490588\C,4.2223972437,1.8101
696149,-0.5993642721\C,7.3945968869,-0.00093355,-0.2218770947\C,-5.765
6233446,0.9437100062,0.9229493401\C,-6.9700179503,0.6777940997,0.01443
68717\C,-7.6459123482,-0.6943148194,0.2308895156\C,-6.6892367337,-1.86
08567541,-0.1036403242\C,-5.4501743446,-1.9483004347,0.7912309519\C,8.
76918365,0.586497482,-0.4997078803\C,9.9021487797,-0.3998889764,-0.189
7298251\C,11.2926101381,0.1803172386,-0.4777587339\C,12.4381816719,-0.
7820954017,-0.1435202896\C,13.8275347862,-0.2031394728,-0.4379363949\C
,14.9687174277,-1.1635731609,-0.091042757\C,-8.9412095936,-0.828406202
9,-0.5953749889\C,-10.0883231043,0.1057489519,-0.1863953907\C,-11.3750
779135,-0.1461249309,-0.9834563777\C,-12.5350863571,0.7734536736,-0.58
28768312\C,-13.8145209134,0.5136873108,-1.3836839759\H,4.6032601865,2.
7687974719,-0.9297806621\H,2.1381228737,2.382295898,-0.6367335867\H,2.
7475843726,-1.5119681165,0.5677529381\H,5.2096343646,-1.3218497349,0.3
190938507\H,7.3004791912,-0.3080282907,0.8281202483\H,7.2019678863,-0.
8761796991,-0.8561634173\H,0.2879642875,1.7735769536,2.0416678317\H,0.
64213693,-1.6320475598,1.7981144227\H,-0.1389343097,1.9784156294,-1.36
50539202\H,0.2387956157,-1.4245422751,-1.6145531759\H,-1.7893713568,-0
.243810576,2.8990184797\H,-5.7140017066,-2.17300221,1.8289756157\H,-4.
7372524155,-2.6987936133,0.4427041549\H,-7.2318107533,-2.8095647141,-0
.0022759908\H,-6.3708568782,-1.7836692777,-1.1503093429\H,-7.916183128
6,-0.7759545013,1.2965509025\H,-6.6574372997,0.7645857629,-1.033438665
4\H,-7.6931745214,1.4796038386,0.2017537716\H,-5.2332663886,1.85714597
79,0.6487295862\H,-6.0588564799,1.0137556237,1.9746350032\H,-2.3408950
663,2.3196026968,0.6599486562\H,-1.8191503381,-2.5171593935,0.30566009
78\H,-2.3778875802,0.0472358829,-1.9303442526\H,8.8872035435,1.4958787
467,0.1016269878\H,8.8130450194,0.8956069279,-1.5509350201\H,9.8468585
728,-0.7013047295,0.8657269491\H,9.7639994304,-1.3184741321,-0.7771547

371\H,11.3528857079,0.4650064396,-1.5374968291\H,11.4210514427,1.11028
55354,0.0936615609\H,12.3799036918,-1.0613066366,0.9182714519\H,12.307
6495946,-1.7157552123,-0.7092320916\H,13.9542698817,0.7336089173,0.121
5797087\H,13.8878410258,0.0687106932,-1.5004759189\H,15.9449386566,-0.
7214077349,-0.3140298637\H,14.9577208167,-1.4248580794,0.9732031717\H,
14.8889943081,-2.0967659123,-0.6601103691\H,-9.2942141025,-1.865397350
2,-0.5128139893\H,-8.7046266116,-0.6757532705,-1.6582638161\H,-10.2953
946705,-0.022461609,0.885733443\H,-9.7930533331,1.1549031662,-0.316825
8752\H,-11.1676243768,-0.0214481828,-2.0557914457\H,-11.6826659841,-1.
1937678504,-0.8551941141\H,-12.2282778027,1.8202670914,-0.7121029558\H
,-12.7421863839,0.6485788922,0.4886622743\H,-14.6230075744,1.184098255
2,-1.0750804758\H,-13.6484347798,0.6650244685,-2.4562530116\H,-14.1655
83163,-0.5154172888,-1.2468136786\\Version=EM64L-G09RevA.02\State=1-A\
HF=-1643.5393698\RMSD=4.594e-09\RMSF=1.905e-06\Dipole=1.0449802,-0.338
2812,-0.1650651\Quadrupole=69.4291286,-29.8751832,-39.5539454,2.467891
5,-4.994366,-2.1196944\PG=C01 [X(C22H47B10N1O1S1)]\\@

3b

#P B3LYP/6-31G(d,p) FOpt fcheck Geom(nodistance, noangle) freq(no
raman, readIso)\\1-(4-C7H15O-Pyridine)-10-(4-C5H11-Quinuclidine)decabo
rane, C1 symm\\0,1\B,0.1063968775,-0.1846631547,5.6826715874\B,-0.6112
378732,0.8399755647,6.8027206068\B,-0.7930170835,-1.0061434477,6.83898
97508\B,1.0531091114,-1.1922315806,6.6327055236\B,1.2362385977,0.65775
06968,6.5974491035\B,1.6904607575,-0.2878991405,8.0619399674\B,0.51703
12335,1.147968935,8.1807295357\B,-0.9110811804,-0.0275574723,8.3513071
705\B,0.2605253095,-1.4686777396,8.2314445491\B,0.506615006,-0.1547097
828,9.249204651\N,-0.0643649208,-0.194704274,4.1651287412\N,0.68019757
81,-0.1878598128,10.8196884545\O,-0.4271696997,-0.2458874986,0.0473599
565\C,-1.271439534,0.0351231646,3.605025529\C,-1.470196776,0.034597333
7,2.2353320656\C,-0.3781266091,-0.2145688241,1.3895314623\C,0.87585274
39,-0.452914991,1.9794950932\C,0.9952308998,-0.4355545622,3.3507013552
\C,-0.5894431901,-0.6650223432,11.4870939784\C,-0.3681400216,-0.870004
1809,13.0019242926\C,0.9814590292,-0.2576262687,13.4425541388\C,2.0955
122252,-1.0491909198,12.7220006068\C,1.017157249,1.1898164707,12.90343
08131\C,1.0122418116,1.1839605248,11.357065086\C,1.7954052151,-1.13408
37669,11.2079942179\C,1.1011056926,-0.3226328747,14.9782463828\C,2.426

4635596,0.1414002149,15.5993910829\C,-1.6796791823,0.0003558429,-0.617
1442086\C,-1.4392423243,-0.1067035409,-2.1145921415\C,-2.7146772765,0.
1543426313,-2.9260860396\C,-2.4972231242,0.0382268127,-4.4400526641\C,
-3.7659723401,0.3049636318,-5.2584989339\C,-3.5544837536,0.1848231367,
-6.7727793252\C,-4.8264363997,0.4528624805,-7.5825568702\C,2.416941133
1,0.0595219696,17.131952663\C,3.7300076105,0.5177370919,17.7782053888\
C,3.7129290727,0.4301069844,19.3071084852\H,1.4665518086,-2.1268508514
,10.8974507921\H,2.655099269,-0.8704619147,10.5934347795\H,2.170283512
3,-2.0587654433,13.1419004642\H,3.0635558915,-0.5650150858,12.88601314
31\H,0.2812334664,1.8731643948,10.9358010519\H,1.9828090809,1.44733716
45,10.9332420072\H,-2.4635933503,0.2263493136,1.8529521393\H,0.1509354
574,1.7416635913,13.2868937539\H,-2.0757916464,0.2235053589,4.30437629
17\H,1.9089801078,1.7137628466,13.2599822071\H,-0.3801658464,-1.937427
3606,13.2508538059\H,-1.1880186486,-0.4062995791,13.5615475761\H,-0.88
40613117,-1.5810559036,10.9750730692\H,-1.3493565006,0.0858256316,11.2
695027486\H,0.1960105074,-2.5782488926,8.6780082061\H,0.6726363527,2.2
67015805,8.5712201017\H,-1.971123615,0.0862205546,8.8932269269\H,2.846
060249,-0.3945819077,8.35518507\H,2.0391285816,1.3593358101,6.05600329
66\H,1.7050910349,-2.0589036067,6.1273765612\H,-1.6956336566,-1.714698
7643,6.5018298509\H,-1.359877371,1.6985950048,6.435642968\H,1.93462175
92,-0.6140714284,3.857272688\H,1.7372848441,-0.6477828925,1.3524825115
\H,0.9144680711,-1.3605680369,15.288993382\H,0.2813827363,0.2700824366
,15.4090020553\H,3.2545715605,-0.4686613601,15.2161396908\H,2.64470425
97,1.1752667897,15.301325443\H,-2.0437680661,1.0002063657,-0.34610348\
H,-2.4204503341,-0.7381673532,-0.2833010176\H,-0.658456274,0.609467312
6,-2.3972108979\H,-1.0473354361,-1.1063118541,-2.3372451272\H,-3.49744
17593,-0.5531038552,-2.6182296948\H,-3.0999224053,1.1565422007,-2.6914
945652\H,-1.710545122,0.7411357881,-4.7478725279\H,-2.116356613,-0.965
5164147,-4.6748048214\H,-4.1449481613,1.3101212627,-5.0245717815\H,-4.
5539707231,-0.3954032696,-4.9465787719\H,-2.7672755005,0.8846183895,-7
.0844201683\H,-3.1761817437,-0.8196538601,-7.006151246\H,-4.6429088483
,0.3608158782,-8.6577664505\H,-5.6204936441,-0.2549689074,-7.319138711
3\H,-5.2096419975,1.4624572441,-7.3959785681\H,2.2030752024,-0.9741527
322,17.4392648184\H,1.5890413224,0.66789674,17.5233760161\H,4.55744359
13,-0.0888735216,17.3857102514\H,3.9415738426,1.5515329494,17.47297033
39\H,4.6623133609,0.7641183679,19.7377338404\H,2.9179108542,1.05397460

67,19.7311428535\H,3.5390294266,-0.5983353233,19.6433540781\\Version=E
M64L-G09RevA.02\State=1-A\HF=-1378.1629593\RMSD=9.062e-09\RMSF=2.219e-
06\Dipole=-0.6102359,0.0643528,-0.9636907\Quadrupole=-24.9107445,-34.4
887731,59.3995176,-1.4883266,19.1189824,-0.9756406\PG=C01 [X(C24H50B10
N2O1)]\\@

8a-trans

#P B3LYP/6-31G(d,p) FOpt fcheck Geom(nodistance, noangle) freq(no
raman, readIso)\\1-Dinitrogen-10-(4-C5-ThiaCyclohexane)decaborane\\0,1
\B,0.8799597442,1.0316969913,1.5971909906\B,0.9264248787,-0.849826563,
1.6154148984\B,-0.9601655166,-0.8982379344,1.5322251607\B,-1.007956971
,0.9833047706,1.512302488\B,1.3515083654,0.0870651157,0.1399903139\B,0
.061307965,-1.2684863518,0.0893286473\B,-1.2964429517,0.0180290094,0.0
239515847\B,-0.0047776085,1.3761926437,0.0623089084\B,-0.08701114,0.07
63650361,2.5940417187\B,0.0729163862,0.0448878245,-0.9537649094\N,-0.1
512818564,0.0894155474,4.0347584953\N,-0.2007785759,0.0998872776,5.151
4225546\S,0.1748293992,0.0313310686,-2.8315052314\C,-1.0199342858,1.32
64169436,-3.3708279909\C,-0.8072730658,-1.443078327,-3.3401478725\C,-1
.3609503744,1.1654851887,-4.8525639601\C,-1.1666889414,-1.3745612579,-
4.8255549779\C,-2.0499124518,-0.1687787525,-5.2054752716\C,-2.44361091
59,-0.1828466275,-6.6952876383\C,-3.3275615483,-1.3588739279,-7.132838
3703\C,-3.7898941848,-1.249060646,-8.5916496939\C,-4.6652069339,-2.423
2916619,-9.0464098958\C,-5.1290270983,-2.3018923078,-10.5008770863\H,-
2.9744981921,-0.232558568,-4.6106386481\H,1.6153679256,1.8348923859,2.
0745291462\H,1.7005650285,-1.6055826927,2.1088815333\H,-1.7371288233,-
1.6938440466,1.9540814333\H,-1.8245851337,1.7470610675,1.9177603347\H,
2.4761836963,0.1108503408,-0.2502913347\H,0.1040708814,-2.385296585,-0
.3266845542\H,-2.3883804309,-0.0151130568,-0.4597314708\H,-0.018872366
,2.485195097,-0.3760171639\H,-1.8969895404,1.2362905139,-2.724529595\H
,-0.5294282681,2.2779277872,-3.1558550943\H,-1.6896126094,-1.472639773
6,-2.6952275819\H,-0.1788209552,-2.3036255084,-3.102581478\H,-2.021551
4051,1.9974116073,-5.125741792\H,-0.4510037383,1.2814650946,-5.4562691
719\H,-1.6863709712,-2.3073399339,-5.0693462894\H,-0.2491471038,-1.362
2150396,-5.4291837325\H,-1.5309386879,-0.1628990917,-7.3086339112\H,-2
.9745546659,0.7529788234,-6.9167525996\H,-2.7900781333,-2.3073893034,-
7.0038281566\H,-4.2080571768,-1.4145378878,-6.476957726\H,-2.910664169

8,-1.1775693035,-9.247796615\H,-4.3449856511,-0.3098561076,-8.72673767
87\H,-4.1081502385,-3.3611496729,-8.9168105281\H,-5.540764796,-2.49765
1763,-8.3873347446\H,-5.7502171156,-3.1538968901,-10.7946784536\H,-5.7
196570968,-1.3916140914,-10.6540840601\H,-4.2756415808,-2.2604584611,-
11.1871839299\\Version=EM64L-G09RevA.02\State=1-A\HF=-1154.3248004\RMS
D=8.417e-09\RMSF=6.224e-06\Dipole=-1.0360653,-0.1639728,-2.9542329\Qua
drupole=-4.5013617,1.1339848,3.3673768,-0.8888771,-3.3495903,-1.069366
\PG=C01 [X(C10H28B10N2S1)]\\

8b

#P B3LYP/6-31G(d,p) FOpt fcheck Geom(nodistance, noangle) freq(nora
man, readIso)\\1-Dinitrogen-10-(4-C5-Quinuclidinedecaborane\\0,1\B,2.5
660359404,0.9408782572,-1.0485382313\B,2.5660069459,-0.9409777603,-1.0
485286091\B,2.6079704623,-0.9425300883,0.8355337837\B,2.6079994521,0.9
424570466,0.8355156644\B,1.0699866357,-0.0000277448,-1.3903391561\B,1.
100197657,-1.317145288,-0.076423654\B,1.1287227782,-0.000009377,1.2435
653118\B,1.1002326241,1.3171031139,-0.0764429477\B,3.6196822924,-0.000
0644501,-0.1280191968\B,0.0476692104,-0.0000055464,-0.0466685849\N,5.0
589437604,-0.0001231148,-0.161381906\N,6.1771217116,0.0003005582,-0.18
70178817\N,-1.526421489,0.0000119211,0.030416871\C,-4.1636732251,0.000
0382479,0.1883579017\C,-2.1344672873,0.0000052384,-1.3533620123\C,-3.6
789012938,0.0000116545,-1.2797344894\C,-2.0164640335,-1.2281502502,0.7
689012386\C,-2.016439645,1.2281970258,0.7688781677\C,-3.5599820391,-1.
2461704183,0.8706285263\C,-3.5599582967,1.246256024,0.8705917904\C,-5.
7061857688,0.0000509639,0.2183139472\C,-6.3815602588,0.0000366929,1.59
76611391\C,-7.9136575795,0.0000585505,1.5021637345\C,-8.6092974678,0.0
000382778,2.8690271424\C,-10.1374706214,0.0000617482,2.7686373303\H,2.
995038146,1.7205066739,-1.8378937582\H,2.9949832333,-1.7206303112,-1.8
378743174\H,3.0700746612,-1.7232236239,1.6048806161\H,3.0701295118,1.7
231483863,1.6048492653\H,0.622678158,-0.0000293098,-2.4958065353\H,0.6
801878456,-2.434145325,-0.0678679212\H,0.7220838267,0.0000048062,2.367
1199373\H,0.6802533791,2.4341146781,-0.0679038845\H,-1.7381697236,-0.8
774774037,-1.8651332576\H,-1.7381637488,0.8774786976,-1.8651444879\H,-
4.0784837704,-0.8792312503,-1.7967419298\H,-4.0784771865,0.8792398765,
-1.7967717578\H,-1.6217417237,-2.0878254022,0.2283423969\H,-1.53156527
84,-1.2075534583,1.7455425835\H,-1.6216912933,2.0878547592,0.228311041

3\H,-1.5315489933,1.2076009077,1.7455235762\H,-3.9566495028,-2.1515132
457,0.397812108\H,-3.8576070167,-1.2815170973,1.9225641749\H,-3.956601
7502,2.1515915386,0.3977412364\H,-3.8575893763,1.2816459804,1.92252401
51\H,-6.0559940777,-0.8766213745,-0.3448408068\H,-6.0559812731,0.87674
1708,-0.3448201264\H,-6.0631248751,-0.8779197167,2.1744043436\H,-6.063
1020125,0.8779637052,2.1744360838\H,-8.2426406461,-0.877625909,0.92785
16008\H,-8.242617823,0.8777758091,0.9278886661\H,-8.2796051276,-0.8772
450929,3.4418732483\H,-8.2795809605,0.8772874105,3.4419118631\H,-10.60
30053838,0.0000460293,3.7592529323\H,-10.4997435266,0.8837992856,2.231
4398979\H,-10.4997681569,-0.8836416187,2.2314003165\\Version=EM64L-G09
RevA.02\State=1-A\HF=-888.9155097\RMSD=8.361e-09\RMSF=3.332e-05\Dipole
=-3.3943496,-0.000001,0.2187898\Quadrupole=-1.5230411,0.9501275,0.5729
135,-0.0009225,1.6974167,0.00003\PG=C01 [X(C12H31B10N3)]\\

8c

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C5H18B10N2S1\PIOTR\01-Sep-2011
\0\\#P B3LYP/6-31G(d,p) FOpt freq(noraman, ReadIso) fcheck #P Geom(NoD
istance, NoAngle)\\1-Dinitrogen-10-ThiaCyclohexanedecaborane, Cs symme
try eclipsed\\0,1\B,-0.9304852946,2.6066145201,0.9403709431\B,-0.93048
52946,2.6066145243,-0.9403709315\B,0.9234284338,2.2337062519,-0.941975
5991\B,0.9234284338,2.2337062477,0.941975609\B,-1.596945015,1.22550383
36,0.0000000027\B,-0.3000061014,0.9600201775,-1.3219845485\B,1.0018454
626,0.7047482346,0.0000000016\B,-0.3000061014,0.9600201716,1.321984552
8\B,0.2008686194,3.4295506705,0.0000000076\N,0.4850825994,4.8438549841
,0.0000000108\N,0.7051772978,5.9396972061,0.0000000132\B,-0.500641679,
-0.0520919675,-0.0000000001\S,-0.8870100988,-1.8923529782,-0.000000004
2\C,0.1108935559,-2.5722909718,1.3958498523\C,0.1108935559,-2.57229096
55,-1.3958498638\C,0.2344865892,-4.0929275035,1.282934624\C,0.23448658
92,-4.0929274978,-1.2829346422\C,0.9471259026,-4.5498870561,-0.0000000
101\H,1.0238911184,-5.642241207,-0.0000000126\H,1.9753348535,-4.164102
3547,-0.0000000093\H,-1.6022719424,3.2020950098,1.7200011878\H,-1.6022
719424,3.2020950174,-1.7200011735\H,1.774109313,2.5195666748,-1.722380
6405\H,1.774109313,2.5195666671,1.7223806518\H,-2.7681735163,1.0112322
649,0.0000000023\H,-0.380606641,0.540049137,-2.4352217635\H,2.00730849
09,0.059272808,0.0000000001\H,-0.380606641,0.5400491261,2.4352217659\H
,1.0808178397,-2.0688004213,1.36433906\H,-0.4122976202,-2.2584479168,2

.3011790181\H,1.0808178397,-2.0688004152,-1.3643390692\H,-0.4122976202
,-2.2584479066,-2.3011790282\H,0.7898151734,-4.4440226867,2.1604426085
\H,-0.7617892808,-4.5490211353,1.3412506395\H,0.7898151734,-4.44402267
71,-2.1604426283\H,-0.7617892808,-4.5490211293,-1.3412506598\\Version=
EM64L-G09RevA.02\State=1-A'\HF=-957.7424404\RMSD=5.822e-09\RMSF=4.874e
-05\Dipole=0.4870566,-2.8903756,0.\Quadrupole=-9.4512483,14.8221725,-5
.3709242,0.5833171,0.,0.\PG=CS [SG(C1H4B4N2S1),X(C4H14B6)]\\@

8d

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C7H21B10N3\PIOTR\02-Sep-2011\0
\\#P B3LYP/6-31G(d,p) FOpt(CalcFC) freq(noraman, ReadIso) fcheck #P Ge
om(NoDistance, NoAngle)\\1-Dinitrogen-10-Quinuclidinedecaborane, C1 sy
mmetry free\\0,1\B,3.5496881326,-0.0091223048,0.0088926491\B,-0.022351
6245,0.0398693275,-0.0137188204\B,1.0094937967,-1.2620854453,0.2570639
904\B,1.0486035498,1.3185334825,-0.2738858656\B,1.025833646,0.29677119
96,1.2815562537\B,1.0345216315,-0.2352404093,-1.2990882345\B,2.5279438
153,1.1191598877,0.7335160866\B,2.5061536514,-1.107040373,-0.729388517
6\B,2.5342896607,0.7376900401,-1.1107993238\B,2.4998004073,-0.72581977
86,1.115030953\N,-1.5980610121,0.0186145432,-0.0087795907\C,-2.1190870
522,-0.8261592817,-1.1556478171\C,-2.154716211,1.4206076502,-0.1508331
188\C,-2.1110644456,-0.5755007983,1.2909165989\C,-3.6583886399,-0.9665
083124,-1.0850956826\C,-3.6977727737,1.3947893379,-0.2668928398\C,-3.6
540415661,-0.4933328631,1.3666439933\C,-4.2037178716,-0.0316019384,0.0
073346275\N,4.9892761641,-0.0276394949,0.0176619896\N,6.1076304676,-0.
0425596098,0.0246743911\H,-1.8066436733,1.9742165529,0.7226150154\H,-1
.674327374,1.861022392,-1.0240576901\H,-4.1358162332,2.0986999217,0.44
77295905\H,-4.0099030414,1.7180708955,-1.2655087739\H,-1.743010511,-1.
6019483971,1.3165071259\H,-1.6192744194,-0.0314233467,2.0962380703\H,-
4.0654437669,-1.4724319158,1.6315570948\H,-3.961359969,0.2056395054,2.
1515732724\H,-5.2975979628,-0.0514903083,0.0128224207\H,-4.0984888268,
-0.7172697342,-2.0557828491\H,-3.9375818393,-2.0020819018,-0.864105250
3\H,-1.7833364484,-0.3375347212,-2.0703795114\H,-1.6042298064,-1.78495
85072,-1.0913418185\H,2.9956156134,1.3373865391,-2.0286382593\H,2.9298
416048,-1.3377441392,2.0399149094\H,2.9835122815,2.0338500746,1.342321
3574\H,2.9418425001,-2.0344625805,-1.3334479353\H,0.6168009531,-0.4554
282613,-2.3945871371\H,0.6448829308,2.417594383,-0.5001898425\H,0.6000

350659,0.5286148253,2.3725951598\H,0.5606764741,-2.3472280789,0.477446
4804\\Version=EM64L-G09RevA.02\State=1-A\HF=-692.3333972\RMSD=4.612e-0
9\RMSF=1.441e-06\Dipole=-3.1984561,-0.0207201,0.0002209\Quadrupole=11.
8128113,-5.899894,-5.9129173,-0.2384504,0.1376805,0.0026089\PG=C01 [X(
C7H21B10N3)]\\

8e

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C5H13B10N3\PIOTR\02-Sep-2011\0
\\#P B3LYP/6-31G(d,p) FOpt freq(noraman, ReadIso) fcheck #P Geom(NoDis
tance, NoAngle)\\1-Dinitrogen-10-Pyridinedecaborane, C2v symmetry stag
gered\\0,1\B,0.,0.,-0.5131220143\B,0.,0.,3.0454239495\B,0.,-1.33413501
85,2.0151945397\B,1.3337620591,0.,2.0120017497\B,0.,1.3341350185,2.015
1945397\B,-1.3337620591,0.,2.0120017497\B,-0.9312667882,-0.9371344829,
0.5279792826\B,0.9312667882,-0.9371344829,0.5279792826\B,0.9312667882,
0.9371344829,0.5279792826\B,-0.9312667882,0.9371344829,0.5279792826\C,
0.,-1.2010824643,-4.1048618277\C,0.,1.2010824643,-4.1048618277\C,0.,-1
.1703305754,-2.7196702434\C,0.,1.1703305754,-2.7196702434\C,0.,0.,-4.8
143875602\N,0.,0.,-2.0389801006\N,0.,0.,4.4860393181\N,0.,0.,5.6043291
087\H,0.,-2.4347278417,2.4659932021\H,2.4356805356,0.,2.4589751214\H,0
.,2.4347278417,2.4659932021\H,-2.4356805356,0.,2.4589751214\H,0.,-2.15
84370951,-4.6127421928\H,0.,2.1584370951,-4.6127421928\H,-1.7145603187
,-1.7169556252,0.0782338304\H,1.7145603187,-1.7169556252,0.0782338304\
H,1.7145603187,1.7169556252,0.0782338304\H,-1.7145603187,1.7169556252,
0.0782338304\H,0.,-2.063324402,-2.1083852799\H,0.,2.063324402,-2.10838
52799\H,0.,0.,-5.8993762754\\Version=EM64L-G09RevA.02\State=1-A1\HF=-6
11.2966012\RMSD=3.195e-09\RMSF=5.807e-05\Dipole=0.,0.,-3.3746001\Quadr
upole=-15.0392928,-6.8617711,21.9010639,0.,0.,0.\PG=C02V [C2(H1C1N1B1B
1N1N1),SGV(C4H6B2),SGV'(H2B2),X(H4B4)]\\

8f

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C6H15B10N3O1\PIOTR\20-Sep-2012
\0\\#P B3LYP/6-31G(d,p) FOpt freq(noraman, ReadIso) fcheck #P Geom(NoD
istance, NoAngle)\\1-Dinitrogen-10-(4MeO-Pyridine)decaborane, Cs symme
try staggered\\0,1\B,-0.0213292769,0.,0.0414086863\B,0.0081158294,0.,3
.6019915771\B,1.3330858406,0.,2.5590314452\B,-0.0001633608,1.332915335
4,2.5684336211\B,-1.3341154374,0.,2.5808073846\B,-0.0001633608,-1.3329

153354,2.5684336211\B,0.923132213,-0.9317296087,1.0754480729\B,0.92313
2213,0.9317296087,1.0754480729\B,-0.948172498,0.9325663668,1.090337627
3\B,-0.948172498,-0.9325663668,1.0903376273\C,1.1860857696,0.,-3.55452
11382\C,-1.2268766167,0.,-3.5522566046\C,1.1397903242,0.,-2.1723369049
\C,-1.1926625955,0.,-2.1770272514\C,-0.0194615193,0.,-4.274148368\N,-0
.0234432758,0.,-1.485519685\N,0.0183311152,0.,5.0413390851\N,0.0257309
552,0.,6.1600205364\C,1.0724000687,0.,-6.3990542346\O,-0.1222295146,0.
,-5.6109176856\H,2.4377285963,0.,3.0006807652\H,0.0035300566,2.4349710
442,3.0158737586\H,-2.4314556793,0.,3.0400494706\H,0.0035300566,-2.434
9710442,3.0158737586\H,2.1505431696,0.,-4.0441645806\H,-2.1713918413,0
.,-4.0821934272\H,1.7011554812,-1.7147086586,0.621045759\H,1.701155481
2,1.7147086586,0.621045759\H,-1.7330804398,1.7164268943,0.6501365744\H
,-1.7330804398,-1.7164268943,0.6501365744\H,2.0372524616,0.,-1.5671713
536\H,-2.0902727754,0.,-1.5726213194\H,1.6708911387,-0.8966510461,-6.2
06350901\H,0.7386152306,0.,-7.4359204483\H,1.6708911387,0.8966510461,-
6.206350901\\Version=EM64L-G09RevA.02\State=1-A'\HF=-725.8280959\RMSD=
8.156e-09\RMSF=1.476e-05\Dipole=0.5653295,0.,-4.1956535\Quadrupole=-6.
2519497,-14.7797172,21.0316669,0.,-6.3397274,0.\PG=CS [SG(C6H7B4N3O1),
X(H8B6)]\\

16-trans

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C11H25B10N1O1S1\PIOTR\20-Sep-2
012\0\\#P B3LYP/6-31G(d,p) FOpt freq(noraman, ReadIso) fcheck #P Geom(
NoDistance, NoAngle)\\1-Pyridine-10-ThiaCyclohexanedecaborane, Cs symm
etry eclipsed\\0,1\B,0.,-0.0126254158,0.0056341592\B,0.,0.0087541598,3
.5763858147\B,1.3198297985,-0.0024874411,1.0378262976\B,-1.3198297985,
-0.0024874411,1.0378262976\B,0.9284009926,-0.9333445332,2.5424518347\B
,-0.9262349586,0.9405696082,2.5297528821\B,-0.9284009926,-0.9333445332
,2.5424518347\B,0.9262349586,0.9405696082,2.5297528821\B,0.,1.31896375
94,1.032437778\B,0.,-1.3275772982,1.0510963912\S,0.,-0.0131583357,-1.8
68514238\C,-1.3904506621,-1.1300270633,-2.3368471238\C,1.3904506621,-1
.1300270633,-2.3368471238\C,0.,-2.3417137307,-4.1126035113\C,-1.282985
3588,-1.5534717962,-3.8031430358\C,1.2829853588,-1.5534717962,-3.80314
30358\C,0.,1.1931039435,5.7798914545\C,0.,1.2530392759,7.1626840888\C,
0.,0.0555611052,7.8938648697\C,0.,-1.1578861634,7.1841773663\C,0.,-1.1
366849127,5.8078510445\C,0.,1.1678497049,10.0067214219\N,0.,0.02431191

58,5.1039741713\O,0.,-0.0346077466,9.2351433453\H,0.,-2.0386255942,5.2
100697549\H,0.,-2.0974753014,7.7229229193\H,0.,2.22269919,7.642073784\
H,0.,2.0830835685,5.1638161041\H,0.,2.4262633254,0.5878870066\H,0.,0.8
487716982,11.0484421253\H,0.,-2.4469438032,0.6249716741\H,0.,-3.273426
0439,-3.5310950684\H,0.,-2.6327459225,-5.1685932035\H,1.7126569462,1.7
247928147,2.973021822\H,-1.7168274506,-1.713751961,2.9888392983\H,1.35
35339091,-1.979915503,-1.6497333438\H,-1.3535339091,-1.979915503,-1.64
97333438\H,1.3408932395,-0.6668975296,-4.4474019383\H,-1.3408932395,-0
.6668975296,-4.4474019383\H,2.1602335811,-2.1677442108,-4.0382165742\H
,-2.1602335811,-2.1677442108,-4.0382165742\H,-2.297894583,-0.560046465
3,-2.1284104504\H,2.297894583,-0.5600464653,-2.1284104504\H,-2.4377080
362,-0.008462565,0.6157375804\H,2.4377080362,-0.008462565,0.6157375804
\H,-1.7126569462,1.7247928147,2.973021822\H,1.7168274506,-1.713751961,
2.9888392983\H,-0.896013674,1.7658099618,9.8074996273\H,0.896013674,1.
7658099618,9.8074996273\\Version=EM64L-G09RevA.02\State=1-A'\HF=-1211.
0872263\RMSD=8.160e-09\RMSF=3.301e-05\Dipole=0.,-0.3757164,1.3525992\Q
uadrupole=-29.6943216,-22.903056,52.5973776,0.,0.,19.6045092\PG=CS [SG
(C7H9B4N1O1S1),X(C4H16B6)]\\@

17

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C19H31B10N1O1S1\PIOTR\07-Oct-2
012\0\\#P B3LYP/6-31G(d,p) FOpt fcheck Geom(nodistance, noangle) freq(
noraman, readIso)\\4-MeO-Stilbazole-B10-thian\\0,1\B,0.0282853297,-0.0
149079667,-0.2087567294\B,-0.3077253375,-0.1172678215,3.3474012309\B,1
.2415012508,0.051554284,0.9461160205\B,-1.3798381013,-0.1334135545,0.6
930580515\B,0.7786469424,-0.9572913669,2.3780197006\B,-1.1961309083,0.
7848860229,2.2406126722\B,-1.0621442856,-1.0871979379,2.2003300273\B,0
.6407276998,0.9145743447,2.4178758219\B,-0.1650601973,1.2770906672,0.8
491713537\B,0.0266229721,-1.362359171,0.7941021458\S,0.2034673752,0.04
88859636,-2.0736199011\C,-1.0515244817,-1.146612192,-2.702877463\C,1.7
095795744,-0.9510827267,-2.4367341276\C,0.5838015139,-2.1971760676,-4.
3691767412\C,-0.7766871694,-1.5118169682,-4.1629624481\C,1.7710280747,
-1.3314353743,-3.9173687921\C,-0.6027333827,0.9879246466,5.5736348816\
C,-0.7351055979,0.9885561244,6.9452217625\C,-0.717167988,-0.2231561263
,7.6698479317\C,-0.5583641858,-1.3959869935,6.9034657265\C,-0.43027965
43,-1.3353509109,5.5306703452\C,-1.0050626442,0.7131677615,9.972706312

8\C,-1.1401527734,0.651954322,11.4215335166\C,-1.2933504298,1.84900031
65,12.1412734717\C,-1.4279899706,1.8683929373,13.5274906134\C,-1.41143
04091,0.660810413,14.2362546037\C,-1.6899732707,1.7360542532,16.352109
3061\C,-1.259189889,-0.5510883477,13.536973062\C,-1.1268412749,-0.5526
025884,12.1615111689\C,-0.849309727,-0.3220088222,9.1151901903\O,-1.53
31009374,0.5493654371,15.5840726659\N,-0.4510416797,-0.1578460501,4.86
22229559\H,-0.8149094416,-1.3362500208,9.5057699609\H,-0.8254299405,2.
4021370403,16.243377018\H,-2.6018343541,2.2777609809,16.0728441795\H,-
1.7669711487,1.4121089615,17.3903570744\H,-1.0111487303,-1.503140877,1
1.6509577708\H,-1.2489866721,-1.4752471368,14.1049153917\H,-1.54362951
88,2.816182962,14.0386903368\H,-1.3075431082,2.7920111731,11.601026404
8\H,-1.036994312,1.7221527779,9.5649665217\H,-0.3069107953,-2.21550176
25,4.91321121\H,-0.5347790089,-2.3665519576,7.3875004015\H,-0.85263195
06,1.9423292856,7.4453171592\H,-0.6118611878,1.8960555367,4.9850854494
\H,-0.2042019089,2.3960766463,0.4368254099\H,0.1484542311,-2.463098122
4,0.3376415175\H,0.5975922909,-3.1456160296,-3.8156482272\H,0.70389203
68,-2.4517779561,-5.4278854795\H,1.324042405,1.7349556162,2.955331732\
H,-1.8307459397,-1.9340968126,2.5486173402\H,1.6709367162,-1.824079601
3,-1.7793675621\H,-1.0169891059,-2.014455637,-2.0384922963\H,1.8237876
307,-0.4219125946,-4.5292350201\H,-0.8386248435,-0.6103980217,-4.78586
21921\H,2.709140316,-1.874191231,-4.0837548009\H,-1.580934723,-2.17791
7593,-4.497352205\H,-2.0137728683,-0.64918538,-2.5669222666\H,2.549387
445,-0.3260222177,-2.1271059839\H,-2.4502151748,-0.2035112591,0.166613
6914\H,2.3916170011,0.1382395702,0.6338734714\H,-2.0767166894,1.494853
735,2.6270829349\H,1.5772159122,-1.6936965826,2.8773337208\\Version=EM
64L-G09RevC.01\State=1-A\HF=-1519.5579347\RMSD=3.591e-09\RMSF=7.114e-0
6\Dipole=-0.2093292,-0.2653421,2.3716892\Quadrupole=-38.829217,-25.564
7913,64.3940084,-3.6942662,-12.0216281,27.4851398\PG=C01 [X(C19H31B10N
1O1S1)]\\

18

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C12H22B1N1O1\PIOTR\18-Oct-2012
\0\\#P B3LYP/6-31G(d,p) FOpt fcheck Geom(nodistance, noangle) freq(nor
aman, readIso)\\4-C7H15O-Pyridine-BH3, Cs\\0,1\B,0.0150702934,0.,-0.00
1346906\N,0.0068506595,0.,1.6185649387\O,0.1723076399,0.,5.7560836301\
C,-1.1334568076,0.,2.3258809294\C,-1.1662213599,0.,3.7152307489\C,0.04

60170109,0.,4.4166876884\C,1.240511432,0.,3.673387966\C,1.1771487704,0
.,2.297189576\C,-1.0109184919,0.,6.5732964743\C,-0.5663825162,0.,8.027
4118706\C,-1.7516561629,0.,9.0014947354\C,-1.315389144,0.,10.472019436
4\C,-2.4897630617,0.,11.4579467845\C,-2.0522793717,0.,12.9279398171\C,
-3.2285668881,0.,13.9086575935\H,-1.146698033,0.,-0.3431755054\H,0.609
6903143,-1.0059818481,-0.32769095\H,0.6096903143,1.0059818481,-0.32769
095\H,-2.0408885324,0.,1.7346753305\H,-2.1241362904,0.,4.2177940532\H,
2.1939054085,0.,4.187892329\H,2.0671707737,0.,1.6795387515\H,-1.612550
1046,-0.8897871755,6.3446763747\H,-1.6125501046,0.8897871755,6.3446763
747\H,0.0645812208,-0.8799278861,8.200828236\H,0.0645812208,0.87992788
61,8.200828236\H,-2.3841092612,0.8784920383,8.8114447358\H,-2.38410926
12,-0.8784920383,8.8114447358\H,-0.6817134964,-0.8777987449,10.6606668
505\H,-0.6817134964,0.8777987449,10.6606668505\H,-3.1240245622,-0.8778
758213,11.2689795787\H,-3.1240245622,0.8778758213,11.2689795787\H,-1.4
18499433,-0.8772283235,13.1157702513\H,-1.418499433,0.8772283235,13.11
57702513\H,-2.8831821135,0.,14.9473905669\H,-3.8614492857,0.8837209794
,13.7691620179\H,-3.8614492857,-0.8837209794,13.7691620179\\Version=EM
64L-G09RevC.01\State=1-A'\HF=-625.3958222\RMSD=7.054e-09\RMSF=8.669e-0
6\Dipole=-0.5094714,0.,3.4519901\Quadrupole=20.049443,14.8143936,-34.8
638367,0.,4.814401,0.\PG=CS [SG(C12H6B1N1O1),X(H16)]\\

19

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C14H16B1N1O1\PIOTR\17-Oct-2012
\0\\#P B3LYP/6-31G(d,p) FOpt fcheck Geom(nodistance, noangle) freq(nor
aman, readIso)\\4-MeO-Stilbazole-BH3\\0,1\B,6.0803195135,-0.1845620504
,-0.0793196037\N,4.4817844207,0.0367814451,-0.0903634374\C,3.648207667
8,-1.0265489848,-0.0798963582\C,2.2741634099,-0.8996930302,-0.04945947
3\C,1.6774881745,0.3792876018,-0.0318594353\C,0.239785034,0.6190746193
,-0.0016855458\C,-0.7242766202,-0.3281402412,0.0258607725\C,2.56548402
92,1.4703925589,-0.0480916554\C,3.9356446713,1.2665725722,-0.078217470
3\C,-2.1676565809,-0.1256761881,0.0582318933\C,-3.0113919461,-1.248208
4837,0.0923009836\C,-4.3994137785,-1.1319848328,0.12548723\C,-4.982460
4946,0.1408820278,0.1248050186\C,-7.2094083264,-0.7236386164,0.1918121
717\C,-4.1574356227,1.2803245818,0.0902966283\C,-2.7821388614,1.147090
9671,0.057784734\O,-6.3186364053,0.3841390435,0.1553482664\H,6.3544101
495,-0.5288798274,1.0532559994\H,6.30136566,-1.065086847,-0.8833474214

\H,6.5739242835,0.8800943786,-0.3768831372\H,4.1382661171,-1.992593216
7,-0.0990241345\H,1.6735465079,-1.8016522172,-0.0443298508\H,-0.044607
6765,1.6687377262,0.000232937\H,-0.4219048864,-1.3740928203,0.02615734
27\H,2.1847943867,2.4865439509,-0.0403624109\H,4.6442228523,2.08540599
34,-0.0947561523\H,-2.5695220584,-2.2412962889,0.0933031968\H,-5.00866
26386,-2.0270592687,0.1513657168\H,-7.101307597,-1.3561483036,-0.69776
54621\H,-7.0557650049,-1.3337716273,1.0902696829\H,-8.2136345405,-0.29
93436731,0.2120583848\H,-4.6287968316,2.2573587022,0.0898411878\H,-2.1
728530078,2.0447313491,0.0311074016\\Version=EM64L-G09RevC.01\State=1-
A\HF=-697.9607594\RMSD=8.076e-09\RMSF=2.437e-06\Dipole=-4.1611961,-0.2
011532,0.0629551\Quadrupole=-27.6841659,20.7974208,6.8867451,9.6613585
,0.2367651,-0.2693408\PG=C01 [X(C14H16B1N1O1)]\\

20c

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C5H18B10S1\PIOTR\06-Oct-2012\0
\\#P B3LYP/6-31G(d,p) FOpt freq(noraman, ReadIso) fcheck #P Geom(NoDis
tance, NoAngle)\\1-ylide-10-ThiaCyclohexanedecaborane, Cs symmetry ecl
ipsed\\0,1\B,-0.9573886604,2.6103641785,0.9661262127\B,-0.9573886604,2
.6103641785,-0.9661262127\B,0.9532142355,2.2379218099,-0.9656189065\B,
0.9532142355,2.2379218099,0.9656189065\B,-1.6007500719,1.2185028774,0.
\B,-0.292298777,0.9586872592,-1.3313716214\B,1.0216126955,0.7092662009
,0.\B,-0.292298777,0.9586872592,1.3313716214\B,0.1645003185,3.27990177
5,0.\B,-0.4827712941,-0.0359488469,0.\S,-0.8641579287,-1.8705158407,0.
\C,0.1277751407,-2.56308214,1.3929710739\C,0.1277751407,-2.56308214,-1
.3929710739\C,0.2247099756,-4.0862776315,1.2828793247\C,0.2247099756,-
4.0862776315,-1.2828793247\C,0.9281010905,-4.5577310441,0.\H,0.9837554
674,-5.6513542086,0.\H,1.9635400113,-4.1920509705,0.\H,-1.6313936387,3
.2002337463,1.7470791029\H,-1.6313936387,3.2002337463,-1.7470791029\H,
1.8008315368,2.5275768937,-1.7467342052\H,1.8008315368,2.5275768937,1.
7467342052\H,-2.7675406205,0.9836244111,0.\H,-0.3722283674,0.528698750
8,-2.4401885535\H,2.0221369545,0.0570706303,0.\H,-0.3722283674,0.52869
87508,2.4401885535\H,1.1060561492,-2.0762685348,1.3559732458\H,-0.3858
697736,-2.2382962636,2.2998555107\H,1.1060561492,-2.0762685348,-1.3559
732458\H,-0.3858697736,-2.2382962636,-2.2998555107\H,0.7738385179,-4.4
460457394,2.1607005608\H,-0.7797926527,-4.5236703251,1.3421977894\H,0.
7738385179,-4.4460457394,-2.1607005608\H,-0.7797926527,-4.5236703251,-

1.3421977894\\Version=EM64L-G09RevC.01\State=1-A'\HF=-848.1537886\RMSD
=5.259e-09\RMSF=4.061e-05\Dipole=0.4433682,-3.0593084,0.\Quadrupole=-5
.8874757,7.7864228,-1.8989471,0.2967842,0.,0.\PG=CS [SG(C1H4B4S1),X(C4
H14B6)]\\@

21-trans

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C23H43B9O2S1\PIOTR\01-May-2010
\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck freq(nor
aman)\\C5-C5S-CB9-COO-PhC5 start at the HF/6-31G* geom\\0,1\B,-0.11096
61673,0.0065589271,0.6406172951\B,-0.4054918217,-0.1196476622,2.484218
8462\B,1.4161431303,-0.1750336982,2.7715773652\B,1.7110293492,-0.04917
11152,0.9285783835\C,0.6697797444,0.8397529434,1.7714268997\C,0.712124
5528,2.331218494,1.8252193342\O,0.5569656609,2.7628129814,3.110901641\
C,0.574024728,4.1245940388,3.4232751495\C,1.5299121911,5.0087850931,2.
9250994644\C,1.5113749115,6.3325272544,3.3623982533\C,0.5656847172,6.7
910697835,4.2892791534\C,0.592066389,8.2204862334,4.7853016\C,1.514742
2655,8.4229362014,6.0038504231\C,1.5514876077,9.8725315818,6.500557218
5\C,2.4730989562,10.0816586166,7.7087479306\C,2.5093149557,11.53264624
14,8.1975858721\H,1.5126524734,11.874465839,8.4992368975\H,3.175015401
3,11.6491699187,9.0589937113\H,2.863836019,12.2072125651,7.40988418\H,
2.148598764,9.4265596666,8.5285491409\H,3.4895048007,9.7575355461,7.44
73542685\H,1.8749561631,10.5299880583,5.6806114451\H,0.5331376553,10.1
94935264,6.7615069866\H,1.1851089989,7.7611881759,6.816012152\H,2.5299
366605,8.0964974089,5.7414545038\H,0.9208559629,8.8843634177,3.9756219
482\H,-0.424567713,8.5367821323,5.0508828513\C,-0.3779715473,5.8749977
599,4.7716994058\C,-0.3797637781,4.5483027236,4.3451627915\H,-1.108614
3564,3.8354290156,4.7159668282\H,-1.1260936746,6.2033092531,5.48895621
48\H,2.2511770086,7.0252805656,2.9688420988\H,2.2607753556,4.674463111
6,2.2007436963\O,0.863365165,3.051591638,0.8690542783\H,-0.7345846641,
0.5880908319,-0.1801456061\H,-1.2671689399,0.3596656048,3.1397900388\H
,2.0617583134,0.2576612568,3.6644734095\H,2.5900649708,0.4882245732,0.
3456546139\B,0.833020172,-1.4856381646,0.2995433887\B,-0.6776742096,-1
.536732486,1.3968785609\B,0.4159102083,-1.6664906025,2.905143238\B,1.9
249093765,-1.61589133,1.8074486287\B,0.6037271404,-2.6096932336,1.5265
653511\S,0.5604682284,-4.4889116731,1.4020537355\C,2.1215807915,-4.928
8287055,0.5266721128\C,2.048935066,-6.3540615003,-0.0226035658\C,0.938

5084225,-6.5780822274,-1.0696257943\C,-0.4542717689,-6.2649335348,-0.4
861234214\C,-0.6116086123,-4.8301858606,0.0204124512\C,1.0235336038,-8
.0101807206,-1.6323147786\C,0.1197054853,-8.2993408806,-2.8388852963\C
,0.336014556,-9.7007470772,-3.4245748918\C,-0.5662152383,-10.0081234,-
4.6261011779\C,-0.3396019965,-11.406668279,-5.2074250485\H,1.001667591
3,-1.8360688032,-0.8287508031\H,-1.78830213,-1.914269606,1.1888777514\
H,0.2327254902,-2.1705108099,3.9669877927\H,3.0205084392,-2.0619186918
,1.9485666106\H,2.2662682296,-4.1816690142,-0.2581214219\H,2.912752487
8,-4.8076860584,1.2693272907\H,1.9237045001,-7.0636846793,0.8059928837
\H,3.0231168504,-6.5758108042,-0.4749557628\H,1.1179428021,-5.87703783
21,-1.8997161918\H,-1.2214645499,-6.414864732,-1.2531268708\H,-0.68111
39679,-6.9715293465,0.3235337382\H,-0.4111368343,-4.0869933921,-0.7557
0492\H,-1.604642992,-4.6400691407,0.4326425702\H,2.065178366,-8.201131
3036,-1.9238595802\H,0.8005202291,-8.72602381,-0.8277714173\H,-0.93618
18279,-8.1939159343,-2.5573644451\H,0.3047518535,-7.5476114718,-3.6193
33922\H,1.3879674525,-9.8106179392,-3.7241141858\H,0.1645812442,-10.45
27786579,-2.6411891285\H,-1.6174425594,-9.9022342962,-4.3255886982\H,-
0.3970897184,-9.2545243664,-5.4070860896\H,-0.9963125574,-11.595087243
8,-6.0625534572\H,0.6942644808,-11.5314649201,-5.5486515106\H,-0.53608
13147,-12.1835047118,-4.4598654097\\Version=EM64L-G09RevA.02\State=1-A
\HF=-1674.8865527\RMSD=5.656e-09\RMSF=3.075e-06\Dipole=0.0800887,-3.79
04274,-0.8804738\Quadrupole=-15.8960307,30.5974084,-14.7013776,1.05823
45,-1.2109348,24.9424581\PG=C01 [X(C23H43B9O2S1)]\\

21-cis

1\1\GINC-OCTOPUS\FOpt\RB3LYP\6-31G(d,p)\C23H43B9O2S1\PIOTR\02-May-2010
\0\\#P B3LYP/6-31G(d,p) FOpt Geom(NoAngle, noDistance) fcheck freq(nor
aman)\\C5-C5S-CB9-COO-PhC5, cis, CB9 axial, at HF/6-31G* geom\\0,1\B,-
0.4724630517,0.4732894816,0.9271714499\B,-0.6533286663,-0.1836305709,2
.6392003576\B,-1.283931448,-1.8050148968,1.9514622759\B,-1.1049296039,
-1.1455649217,0.2375248343\C,-0.0106417213,-0.9892668358,1.4058549675\
C,1.3684013987,-1.558207763,1.338004037\O,2.2769451588,-0.6386311487,1
.7740105384\C,3.6420799902,-0.9284720078,1.839182071\C,4.3080956401,-0
.4231535666,2.9537671557\C,5.6851117695,-0.5983477605,3.0673263364\C,6
.4144617242,-1.2743870713,2.0800892356\C,7.9161672129,-1.4268868332,2.
1891033616\C,8.6926376514,-0.242659167,1.5795674935\C,10.2136918951,-0

.3905849378,1.6986336923\C,10.9914783214,0.7856986966,1.0955447403\C,1
2.5104180354,0.6341324258,1.2205931328\C,5.7152137878,-1.7686289191,0.
9714766205\C,4.3368581533,-1.6020757123,0.8356019013\O,1.6375016241,-2
.6710082358,0.9563685367\H,0.3263883689,1.2197285642,0.4734587825\H,-0
.0032386449,0.0153416901,3.6084463162\H,-1.1324107047,-2.9043034864,2.
3630377924\H,-0.8047572729,-1.7021460219,-0.7632507173\H,3.7389399527,
0.0990008874,3.7155727892\H,6.1999046363,-0.2060447121,3.9408305166\H,
8.1990495718,-1.532634184,3.2442375252\H,8.2287739037,-2.3532968341,1.
6910010462\H,8.4124253004,-0.1373900816,0.5229561133\H,8.3723109689,0.
6857963215,2.0710266184\H,10.4872419563,-0.500050972,2.7580728139\H,10
.528883936,-1.3228347108,1.2080223113\H,10.7197755875,0.8935812264,0.0
367624816\H,10.6750358223,1.7167513086,1.5850468394\H,12.8620121948,-0
.2703088445,0.7111354541\H,13.0360260983,1.4881875638,0.7812023613\H,1
2.8161652329,0.5601748592,2.2704667824\H,6.2573471846,-2.3008148174,0.
1936908168\H,3.8123131153,-2.0017189766,-0.0216363887\B,-2.1551455237,
0.3258207971,0.2690857795\B,-1.8335537015,0.9955401222,1.9768961773\B,
-2.4127118769,-0.615902003,2.713811561\B,-2.7248305176,-1.2945835245,1
.002908996\B,-3.2599736304,0.2135511258,1.5267092159\S,-4.9371475328,1
.0618393934,1.6788802677\C,-5.7981462166,0.8982380756,0.0545082694\C,-
6.2049543892,-0.527997255,-0.3100279527\C,-7.1092204561,-1.2199544685,
0.7287970938\C,-6.3842830243,-1.3552544585,2.0820138024\C,-6.001562908
6,-0.0234228484,2.7247007327\C,-7.5871340015,-2.5836582286,0.191876258
6\C,-8.65987542,-3.2806840108,1.0396397535\C,-9.1898243283,-4.57037731
41,0.3988438088\C,-10.2491048543,-5.2816820459,1.2491509863\C,-10.7793
300193,-6.5656659202,0.6042368293\H,-2.4298649245,0.869664391,-0.75515
2989\H,-1.8749708344,2.1066491574,2.3999419081\H,-2.9056854068,-0.8719
348952,3.7685025944\H,-3.4734559523,-2.1292739032,0.6029620403\H,-6.66
44699191,1.5630730382,0.1320598722\H,-5.0989551349,1.3251924957,-0.668
0608974\H,-5.3064739376,-1.1302313792,-0.478015239\H,-6.7317569133,-0.
4689656705,-1.2709798732\H,-7.9998133305,-0.5873555226,0.8799449262\H,
-7.0289401217,-1.8690287443,2.8038547948\H,-5.4892143687,-1.9741388191
,1.9593303823\H,-6.8812073002,0.586352241,2.9546595475\H,-5.4261013156
,-0.1602851616,3.6428659572\H,-7.985447703,-2.4317301178,-0.8205859343
\H,-6.7190376531,-3.24801532,0.0783568991\H,-8.2614814835,-3.521771400
6,2.0336292189\H,-9.4982089143,-2.5885481979,1.2057347591\H,-9.6122505
69,-4.338963539,-0.5893111694\H,-8.3509898179,-5.2567578465,0.21610882

39\H,-9.8236007943,-5.5159009472,2.2343799622\H,-11.0848059272,-4.5934
938199,1.436123335\H,-11.5325644443,-7.0483219088,1.2350347338\H,-11.2
4214075,-6.3594890597,-0.3674877531\H,-9.972490163,-7.288323543,0.4382
125279\\Version=EM64L-G09RevA.02\State=1-A\HF=-1674.8849855\RMSD=6.377
e-09\RMSF=2.668e-06\Dipole=-3.4721305,0.7239292,-0.026613\Quadrupole=3
8.7791475,-22.6087429,-16.1704046,-4.6800127,2.6951157,-0.2597175\PG=C
01 [X(C23H43B9O2S1)]\\

10. References

1 G. H. Schmid, A. W. Wolkoff *Can. J. Chem.* 1972, **50**, 1181.

2 T. Nozaki, Y. Tanaka *Int. J. Appl. Rad. Isotopes* 1967, **18**, 111.

3 P. Kaszynski, J. Huang, G. S. Jenkins, K. A. Bairamov, D. Lipiak *Mol. Cryst. Liq. Cryst.* 1995, **260**, 315.

4 W. H. Knoth *J. Am. Chem. Soc.* 1966, **88**, 935.

5 R. N. Leyden, M. F. Hawthorne *Inorg. Chem.* 1975, **14**, 2444.

6 D. Naoufal, B. Gruner, B. Bonnetot, H. Mongeot *Polyhedron* 1999, **18**, 931.

7 M. Komura, H. Nakai, M. Shiro *J. Chem. Soc., Dalton Trans.* 1987, 1953.

8 M. F. Hawthorne, F. P. Olsen *J. Am. Chem. Soc.* 1965, **87**, 2366.

9 J. L. Born, W. M. Hadley *J. Pharm. Sci.* 1980, **69**, 465.

10 A. D. Becke *J. Chem. Phys.* 1993, **98**, 5648.

11 C. Lee, W. Yang, R. G. Parr *Phys. Rev. B,* 1988, **37**, 785.

12 Frisch, M. J. *et al* Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2011.

13 A. P. Scott, L. Radom *J. Phys. Chem.* 1996, **100**, 16502.

14 R. E. Stratmann, G. E. Scuseria, M. J. Frisch *J. Chem. Phys.* 1998, **109**, 8218.

15 M. Cossi, G. Scalmani, N. Rega, V. Barone *J. Chem. Phys.* 2002, **117**, 43.

16 J. E. Rice, N. C. Handy *Int. J. Quantum Chem.* 1992, **43**, 91.

17 C. Peng, P. Y. Ayala, H. B. Schlegel, M. J. Frisch *J. Comp. Chem.* 1996, **17**, 49.

18 H. Booth, J. R. Everett *J. Chem. Soc., Perkin Trans. 2* 1980, 255.

19 D. F. Eaton *Pure Appl. Chem.* 1988, **60**, 1107.

20 C. Reichardt *Chem. Rev.* 1994, **94**, 2319.

21 Lippert, E. V. *Z. Elektrochem.* **1957**, *61*, 962–975. Mataga, K. N.; Kaifu, Y.; Koizumi, M. *Bull. Chem. Soc. Jpn.* **1956**, *29*, 465–470.

22 B. Ringstrand, P. Kaszynski *J. Mater. Chem.* 2011, **21**, 90.