Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1997, 36(21), 4772-4777, DOI:10.1021/ic970230n

TABLE S1. *EXPERIMENTAL DETAILS*

A. Crystal Data

Empirical Formula	$C_{17}H_{16}N_2SiS_2Cl_4$
Formula Weight	482.34
Crystal Color, Habit	colourless, block
Crystal Dimensions	0.32 x 0.20 x 0.23 mm
Crystal System	monoclinic
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (30.0 - 50.0°)
Omega Scan Peak Width at Half-height	0.36°
Lattice Parameters	a = 12.585(3) Å b = 12.211(2) Å c = 14.003(2) Å β = 101.86(2)° V = 2106.0(7) $Å^3$
Space Group	$P2_1/a$ (#14)
Z value	4
D_{calc}	1.521 g/cm^3
F_{000}	984
$\mu(MoK\alpha)$	8.22 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC6S
Radiation	$MoK\alpha$ (λ = 0.71069 Å) graphite monochromated
Temperature	23.0°C

Scan Type	ω-2θ
Scan Rate	4.0°/min (in ω) (up to 4 scans)
Scan Width	$(1.37 + 0.34 \tan\theta)°$
$2\theta_{max}$	50.1°
No. of Reflections Measured	Total: 4111 Unique: 3925 ($R_{int} = 0.064$)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.6795 - 0.9864) Decay (0.61%)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SAPI91)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$\frac{1}{\sigma^2(Fo)} = \frac{4Fo^2}{\sigma^2(Fo^2)}$
p-factor	0.020
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I>3.00\sigma(I)$)	1545
No. Variables	235
Reflection/Parameter Ratio	6.57
Residuals: R; Rw	0.050 ; 0.050
Goodness of Fit Indicator	1.92
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.40 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.31 $e^-/Å^3$

TABLE S2.

Atomic coordinates and B_{eq}

Atom	x	y	z	B_{eq}
Cl(1)	0.6530(2)	-0.0907(2)	0.6683(2)	4.57(6)
Cl(2)	0.7369(2)	-0.0086(2)	0.4889(2)	4.53(7)
Cl(3)	0.6541(2)	0.2124(2)	0.3903(2)	5.40(8)
Cl(4)	0.4782(2)	0.3440(2)	0.4656(2)	5.02(7)
S(1)	0.3894(2)	0.2669(2)	0.6473(2)	3.35(6)
S(2)	0.4879(2)	0.0302(2)	0.7531(2)	4.11(7)
Si(1)	0.5236(2)	0.4072(2)	0.8001(2)	3.40(6)
N(1)	0.4395(6)	0.2883(5)	0.7672(5)	3.0(2)
N(2)	0.4321(6)	0.1050(6)	0.8254(5)	3.5(2)
C(1)	0.4161(7)	0.2106(7)	0.8334(6)	3.1(2)
C(2)	0.4924(6)	0.1928(7)	0.6073(6)	2.8(2)
C(3)	0.5331(6)	0.0939(7)	0.6547(5)	2.5(2)
C(4)	0.6091(7)	0.0356(7)	0.6159(6)	3.0(2)
C(5)	0.6447(6)	0.0679(7)	0.5336(6)	2.8(2)
C(6)	0.6059(7)	0.1671(7)	0.4886(6)	3.4(2)
C(7)	0.5302(7)	0.2263(7)	0.5255(6)	2.9(2)
C(8)	0.3681(7)	0.2461(7)	0.9152(6)	3.2(2)
C(9)	0.3920(7)	0.1914(8)	1.0050(7)	4.1(3)
C(10)	0.3461(8)	0.2223(8)	1.0799(7)	4.6(3)
C(11)	0.2678(8)	0.3063(8)	1.0677(7)	4.4(3)

Atomic coordinates and B_{eq} (continued)

Atom	x	y	z	B_{eq}
C(12)	0.2443(7)	0.3582(7)	0.9801(7)	3.9(3)
C(13)	0.2939(8)	0.3303(7)	0.9045(6)	3.8(2)
C(14)	0.2122(9)	0.3349(9)	1.1499(8)	6.3(3)
C(15)	0.5818(8)	0.3979(8)	0.9315(7)	5.2(3)
C(16)	0.4428(8)	0.5318(7)	0.7732(7)	4.9(3)
C(17)	0.6314(8)	0.4022(9)	0.7275(7)	5.9(3)

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

TABLE S3.

Anisotropic Displacement Parameters

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	0.068(2)	0.043(2)	0.065(2)	0.017(1)	0.018(1)	0.009(1)
Cl(2)	0.056(2)	0.051(2)	0.073(2)	0.005(1)	0.031(1)	-0.012(1)
Cl(3)	0.097(2)	0.056(2)	0.068(2)	-0.003(2)	0.054(2)	0.004(1)
Cl(4)	0.092(2)	0.044(2)	0.062(2)	0.016(1)	0.033(2)	0.019(1)
S(1)	0.046(1)	0.042(2)	0.040(1)	0.008(1)	0.011(1)	0.000(1)
S(2)	0.081(2)	0.031(1)	0.054(2)	0.003(1)	0.036(2)	0.005(1)
Si(1)	0.046(2)	0.033(2)	0.049(2)	-0.001(1)	0.009(1)	-0.002(1)
N(1)	0.055(5)	0.029(4)	0.035(4)	-0.002(4)	0.016(4)	-0.001(3)
N(2)	0.054(5)	0.039(5)	0.046(5)	-0.009(4)	0.023(4)	0.006(4)
C(1)	0.038(6)	0.043(6)	0.035(5)	-0.003(5)	0.007(4)	0.004(5)
C(2)	0.036(5)	0.035(5)	0.034(5)	-0.001(4)	0.005(4)	-0.003(4)
C(3)	0.027(5)	0.027(5)	0.041(5)	0.004(4)	0.008(4)	0.001(4)
C(4)	0.041(6)	0.031(5)	0.039(5)	0.003(4)	0.001(5)	0.001(4)
C(5)	0.036(5)	0.035(6)	0.039(5)	-0.005(4)	0.012(4)	-0.008(4)
C(6)	0.051(6)	0.039(6)	0.042(6)	-0.011(5)	0.017(5)	-0.005(5)
C(7)	0.046(6)	0.027(5)	0.043(6)	0.000(4)	0.018(5)	0.004(4)
C(8)	0.041(6)	0.037(6)	0.048(6)	-0.007(5)	0.015(5)	-0.009(5)
C(9)	0.054(7)	0.060(7)	0.046(6)	-0.002(5)	0.019(6)	0.005(5)
C(10)	0.063(7)	0.063(7)	0.051(7)	0.001(6)	0.018(6)	0.007(6)
C(11)	0.067(8)	0.061(8)	0.046(6)	-0.028(6)	0.026(6)	-0.017(6)
C(12)	0.049(6)	0.041(6)	0.065(7)	-0.006(5)	0.027(6)	-0.012(5)
C(13)	0.053(7)	0.038(6)	0.055(6)	-0.009(5)	0.018(5)	0.001(5)
C(14)	0.090(8)	0.080(9)	0.081(8)	-0.030(7)	0.049(7)	-0.027(7)
C(15)	0.079(8)	0.039(6)	0.071(7)	-0.002(6)	-0.001(6)	-0.006(5)

Anisotropic Displacement Parameters (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(16)	0.067(8)	0.039(6)	0.078(8)	0.003(5)	0.009(6)	0.008(5)
C(17)	0.063(7)	0.073(8)	0.098(8)	-0.024(7)	0.036(6)	-0.012(7)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

TABLE S4.

Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Cl(1)	C(4)	1.748(8)	Cl(2)	C(5)	1.706(8)
Cl(3)	C(6)	1.707(8)	Cl(4)	C(7)	1.724(8)
S(1)	N(1)	1.688(7)	S(1)	C(2)	1.763(8)
S(2)	N(2)	1.626(7)	S(2)	C(3)	1.774(8)
Si(1)	N(1)	1.800(7)	Si(1)	C(15)	1.839(9)
Si(1)	C(16)	1.826(9)	Si(1)	C(17)	1.856(9)
N(1)	C(1)	1.40(1)	N(2)	C(1)	1.31(1)
C(1)	C(8)	1.47(1)	C(2)	C(3)	1.42(1)
C(2)	C(7)	1.39(1)	C(3)	C(4)	1.39(1)
C(4)	C(5)	1.38(1)	C(5)	C(6)	1.40(1)
C(6)	C(7)	1.38(1)	C(8)	C(9)	1.40(1)
C(8)	C(13)	1.38(1)	C(9)	C(10)	1.35(1)
C(10)	C(11)	1.41(1)	C(11)	C(12)	1.36(1)
C(11)	C(14)	1.51(1)	C(12)	C(13)	1.38(1)

TABLE S5.

Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	S(1)	C(2)	104.3(4)	N(2)	S(2)	C(3)	119.1(4)
N(1)	Si(1)	C(15)	107.4(4)	N(1)	Si(1)	C(16)	110.3(4)
N(1)	Si(1)	C(17)	106.9(4)	C(15)	Si(1)	C(16)	110.4(4)
C(15)	Si(1)	C(17)	111.1(5)	C(16)	Si(1)	C(17)	110.7(5)
S(1)	N(1)	Si(1)	117.3(4)	S(1)	N(1)	C(1)	117.9(6)
Si(1)	N(1)	C(1)	124.7(6)	S(2)	N(2)	C(1)	134.3(6)
N(1)	C(1)	N(2)	123.5(8)	N(1)	C(1)	C(8)	119.6(8)
N(2)	C(1)	C(8)	116.9(7)	S(1)	C(2)	C(3)	120.4(6)
S(1)	C(2)	C(7)	120.6(7)	C(3)	C(2)	C(7)	118.9(7)
S(2)	C(3)	C(2)	126.3(6)	S(2)	C(3)	C(4)	115.8(6)
C(2)	C(3)	C(4)	117.6(7)	Cl(1)	C(4)	C(3)	118.1(6)
Cl(1)	C(4)	C(5)	118.4(6)	C(3)	C(4)	C(5)	123.3(8)
Cl(2)	C(5)	C(4)	120.9(7)	Cl(2)	C(5)	C(6)	120.5(6)
C(4)	C(5)	C(6)	118.7(8)	Cl(3)	C(6)	C(5)	119.5(7)
Cl(3)	C(6)	C(7)	121.3(7)	C(5)	C(6)	C(7)	119.2(8)
Cl(4)	C(7)	C(2)	119.1(6)	Cl(4)	C(7)	C(6)	118.6(6)
C(2)	C(7)	C(6)	122.3(8)	C(1)	C(8)	C(9)	120.9(8)
C(1)	C(8)	C(13)	121.0(8)	C(9)	C(8)	C(13)	118.0(8)
C(8)	C(9)	C(10)	121.1(9)	C(9)	C(10)	C(11)	120.6(9)
C(10)	C(11)	C(12)	117.9(9)	C(10)	C(11)	C(14)	120.0(9)
C(12)	C(11)	C(14)	122(1)	C(11)	C(12)	C(13)	121.9(9)
C(8)	C(13)	C(12)	120.4(8)				

TABLE S6.

Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Cl(1)	C(4)	C(3)	S(2)	-0.9(9)	Cl(1)	C(4)	C(3)	C(2)	-175.7(6)
Cl(1)	C(4)	C(5)	Cl(2)	-4(1)	Cl(1)	C(4)	C(5)	C(6)	177.2(6)
Cl(2)	C(5)	C(4)	C(3)	-179.1(6)	Cl(2)	C(5)	C(6)	Cl(3)	-1(1)
Cl(2)	C(5)	C(6)	C(7)	179.0(6)	Cl(3)	C(6)	C(5)	C(4)	176.6(6)
Cl(3)	C(6)	C(7)	Cl(4)	3(1)	Cl(3)	C(6)	C(7)	C(2)	-177.9(7)
Cl(4)	C(7)	C(2)	S(1)	2.0(10)	Cl(4)	C(7)	C(2)	C(3)	178.1(6)
Cl(4)	C(7)	C(6)	C(5)	-176.6(6)	S(1)	N(1)	Si(1)	C(15)	-171.8(4)
S(1)	N(1)	Si(1)	C(16)	67.9(5)	S(1)	N(1)	Si(1)	C(17)	-52.4(5)
S(1)	N(1)	C(1)	N(2)	51(1)	S(1)	N(1)	C(1)	C(8)	-127.0(7)
S(1)	C(2)	C(3)	S(2)	1(1)	S(1)	C(2)	C(3)	C(4)	176.0(6)
S(1)	C(2)	C(7)	C(6)	-176.1(7)	S(2)	N(2)	C(1)	N(1)	6(1)
S(2)	N(2)	C(1)	C(8)	-175.6(6)	S(2)	C(3)	C(2)	C(7)	-174.3(6)
S(2)	C(3)	C(4)	C(5)	173.4(7)	Si(1)	N(1)	S(1)	C(2)	86.7(5)
Si(1)	N(1)	C(1)	N(2)	-126.4(8)	Si(1)	N(1)	C(1)	C(8)	55(1)
N(1)	S(1)	C(2)	C(3)	54.7(7)	N(1)	S(1)	C(2)	C(7)	-129.2(7)
N(1)	C(1)	C(8)	C(9)	-147.5(8)	N(1)	C(1)	C(8)	C(13)	36(1)
N(2)	S(2)	C(3)	C(2)	-25.7(9)	N(2)	S(2)	C(3)	C(4)	160.0(6)
N(2)	C(1)	C(8)	C(9)	34(1)	N(2)	C(1)	C(8)	C(13)	-142.2(9)
C(1)	N(1)	S(1)	C(2)	-91.0(7)	C(1)	N(1)	Si(1)	C(15)	5.8(8)
C(1)	N(1)	Si(1)	C(16)	-114.6(7)	C(1)	N(1)	Si(1)	C(17)	125.1(7)
C(1)	N(2)	S(2)	C(3)	-5(1)	C(1)	C(8)	C(9)	C(10)	-178.5(9)
C(1)	C(8)	C(13)	C(12)	175.8(8)	C(2)	C(3)	C(4)	C(5)	-1(1)
C(2)	C(7)	C(6)	C(5)	1(1)	C(3)	C(2)	C(7)	C(6)	0(1)
C(3)	C(4)	C(5)	C(6)	2(1)	C(4)	C(3)	C(2)	C(7)	0(1)

Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(4)	C(5)	C(6)	C(7)	-2(1)	C(8)	C(9)	C(10)	C(11)	3(1)
C(8)	C(13)	C(12)	C(11)	1(1)	C(9)	C(8)	C(13)	C(12)	0(1)
C(9)	C(10)	C(11)	C(12)	-3(1)	C(9)	C(10)	C(11)	C(14)	176.1(9)
C(10)	C(9)	C(8)	C(13)	-1(1)	C(10)	C(11)	C(12)	C(13)	0(1)
C(13)	C(12)	C(11)	C(14)	-178.7(9)					

TABLE S7.

Atomic coordinates and B_{eq} for hydrogen atoms

Atom	x	y	z	B_{eq}
H(1)	0.4417	0.1319	1.0135	4.8781
H(2)	0.3671	0.1870	1.1417	5.4512
H(3)	0.1922	0.4150	0.9711	4.6181
H(4)	0.2768	0.3695	0.8448	4.4404
H(5)	0.2244	0.4099	1.1662	7.4082
H(6)	0.1365	0.3220	1.1296	7.4082
H(7)	0.2406	0.2908	1.2049	7.4082
H(8)	0.5250	0.3941	0.9667	6.1711
H(9)	0.6258	0.3342	0.9442	6.1711
H(10)	0.6251	0.4609	0.9516	6.1711
H(11)	0.4880	0.5940	0.7918	5.8855
H(12)	0.4125	0.5352	0.7054	5.8855
H(13)	0.3862	0.5315	0.8089	5.8855
H(14)	0.6728	0.3373	0.7431	7.1272
H(15)	0.5988	0.4024	0.6600	7.1272
H(16)	0.6771	0.4642	0.7425	7.1272

TABLE S8.

Optimized Cartesian Coordinates (Å)

$(HC)_2S_2N$ (2a)

N	.0000	.0000	.6643
S	-1.3993	.0000	-.2990
S	1.3993	.0000	-.2990
C	-.6733	.0000	-1.8884
C	.6733	.0000	-1.8884
H	-1.3207	.0000	-2.7656
H	1.3207	.0000	-2.7656

$(HC)_2S_2N^+$

N	.0000	.0000	.5914
S	-1.3592	.0000	-.3038
S	1.3592	.0000	-.3038
C	-.6854	.0000	-1.8674
C	.6854	.0000	-1.8674
H	-1.3383	.0000	-2.7453
H	1.3383	.0000	-2.7453

$(HC)_2S_2N^-$

N	.0000	.0000	.7712
S	-1.4485	.0000	-.3083
S	1.4485	.0000	-.3083
C	-.6725	.0000	-1.9022
C	.6725	.0000	-1.9022
H	-1.3022	.0000	-2.7960
H	1.3022	.0000	-2.7960

$((HC)_2S_2N)_2$

N	0.0000	1.2990	0.6057
S	-1.3953	1.5534	-0.3209
S	1.3953	1.5534	-0.3209
C	-0.6745	1.8866	-1.8737
C	0.6745	1.8866	-1.8737
H	-1.3215	2.0817	-2.7290
H	1.3215	2.0817	-2.7290
N	0.0000	-1.2990	0.6057
S	-1.3953	-1.5534	-0.3209
S	1.3953	-1.5534	-0.3209
C	-0.6745	-1.8866	-1.8737
C	0.6745	-1.8866	-1.8737
H	-1.3215	-2.0817	-2.7290
H	1.3215	-2.0817	-2.7290

$(HC)_2Se_2N$ (2b)

N	.0000	.0000	.8173
Se	-1.5090	.0000	-.2207
Se	1.5090	.0000	-.2207
C	-.6727	.0000	-1.9103
C	.6727	.0000	-1.9103
H	-1.2980	.0000	-2.8084
H	1.2980	.0000	-2.8084

$(HC)_2Se_2N^+$

N	.0000	.0000	.7277
Se	-1.4745	.0000	-.2226
Se	1.4745	.0000	-.2226
C	-.6828	.0000	-1.8840
C	.6828	.0000	-1.8840
H	-1.3042	.0000	-2.7880
H	1.3042	.0000	-2.7880

$(HC)_2Se_2N^-$

N	.0000	.0000	.9377
Se	-1.5457	.0000	-.2293
Se	1.5457	.0000	-.2293
C	-.6719	.0000	-1.9318
C	.6719	.0000	-1.9318
H	-1.2886	.0000	-2.8385
H	1.2886	.0000	-2.8385

$((HC)_2Se_2N)_2$

N	0.0000	1.2262	0.6821
Se	-1.5049	1.6775	-0.2644
Se	1.5049	1.6775	-0.2644
C	-0.6726	2.1925	-1.8787
C	0.6726	2.1925	-1.8787
H	-1.3007	2.4735	-2.7286
H	1.3007	2.4735	-2.7286
N	0.0000	-1.2262	0.6821
Se	-1.5049	-1.6775	-0.2644
Se	1.5049	-1.6775	-0.2644
C	-0.6726	-2.1925	-1.8787
C	0.6726	-2.1925	-1.8787
H	-1.3007	-2.4735	-2.7286
H	1.3007	-2.4735	-2.7286

$(HC)N_2S_2$ (3a)

C	.0000	.0000	.0781
N	-1.1829	.0000	-.5323
N	1.1829	.0000	-.5323
S	-1.0732	.0000	-2.1952
S	1.0732	.0000	-2.1952
H	.0000	.0000	1.1704

$(HC)N_2S_2^+$

C	.0000	.0000	.0909
N	-1.1608	.0000	-.5731
N	1.1608	.0000	-.5731
S	-1.0373	.0000	-2.1674
S	1.0373	.0000	-2.1674
H	.0000	.0000	1.1836

$(HC)N_2S_2^-$

C	.0000	.0000	.0645
N	-1.2105	.0000	-.4813
N	1.2105	.0000	-.4813
S	-1.1183	.0000	-2.2368
S	1.1183	.0000	-2.2368
H	.0000	.0000	1.1654

$((HC)N_2S_2)_2$

C	.0000	1.5952	.0736
N	-1.1832	1.5738	-.5323
N	1.1832	1.5738	-.5323
S	-1.0697	1.5328	-2.1907
S	1.0697	1.5328	-2.1907
H	.0000	1.6257	1.1660
C	.0000	-1.5952	.0736
N	-1.1832	-1.5738	-.5323
N	1.1832	-1.5738	-.5323
S	-1.0697	-1.5328	-2.1907
S	1.0697	-1.5328	-2.1907
H	.0000	-1.6257	1.1660

$(HC)N_2Se_2$ (3b)

C	.0000	.0000	.0650
N	-1.2024	.0000	-.5066
N	1.2024	.0000	-.5066
Se	-1.1812	.0000	-2.3108
Se	1.1812	.0000	-2.3108
H	.0000	.0000	1.1634

$(HC)N_2Se_2^+$

C	.0000	.0000	.0651
N	-1.2023	.0000	-.5064
N	1.2023	.0000	-.5064
Se	-1.1811	.0000	-2.3108
Se	1.1811	.0000	-2.3108
H	.0000	.0000	1.1630

$(HC)N_2Se_2^-$

C	.0000	.0000	.0513
N	-1.2276	.0000	-.4552
N	1.2276	.0000	-.4552
Se	-1.2215	.0000	-2.3527
Se	1.2215	.0000	-2.3527
H	.0000	.0000	1.1582

$((HC)N_2Se_2)_2$

C	.0000	1.6259	.0610
N	-1.2028	1.6267	-.5068
N	1.2028	1.6267	-.5068
Se	-1.1777	1.6524	-2.3064
Se	1.1777	1.6524	-2.3064
H	.0000	1.6119	1.1592
C	.0000	-1.6259	.0610
N	-1.2028	-1.6267	-.5068
N	1.2028	-1.6267	-.5068
Se	-1.1777	-1.6524	-2.3064
Se	1.1777	-1.6524	-2.3064
H	.0000	-1.6119	1.1592

$(HC)_2S_2N_2(CH)$ (4a)

C	.0000	.0000	-.0524
N	-1.2229	.0000	-.5627
N	1.2229	.0000	-.5627
S	-1.8230	.0000	-2.0779
S	1.8230	.0000	-2.0779
C	-.6670	.0000	-3.4360
C	.6670	.0000	-3.4360
H	-1.2271	.0000	-4.3811
H	1.2271	.0000	-4.3811
H	.0000	.0000	1.0466

$(HC)_2S_2N_2(CH)^+$

C	.0000	.0000	-.0890
N	-1.2368	.0000	-.5747
N	1.2368	.0000	-.5747
S	-1.7627	.0000	-2.1213
S	1.7627	.0000	-2.1213
C	-.7270	.0000	-3.3805
C	.7270	.0000	-3.3805
H	-1.2557	.0000	-4.3469
H	1.2557	.0000	-4.3469
H	.0000	.0000	1.0150

$(HC)_2S_2N_2(CH)^-$

C	.0000	.0000	-.0647
N	-1.2464	.0000	-.5193
N	1.2464	.0000	-.5193
S	-1.8143	.0000	-2.1060
S	1.8143	.0000	-2.1060
C	-.6792	.0000	-3.4374
C	.6792	.0000	-3.4374
H	-1.2332	.0000	-4.3871
H	1.2332	.0000	-4.3871
H	.0000	.0000	1.0431

$((HC)_2S_2N_2(CH))_2$

C	0.0000	1.4741	-0.0579
N	-1.2227	1.5008	-0.5627
N	1.2227	1.5008	-0.5627
S	-1.8169	1.6272	-2.0684
S	1.8169	1.6272	-2.0684
C	-0.6660	1.6317	-3.4390
C	0.6660	1.6317	-3.4390
H	-1.2303	1.6671	-4.3811
H	1.2303	1.6671	-4.3811
H	0.0000	1.4055	1.0391
C	0.0000	-1.4741	-0.0579
N	-1.2227	-1.5008	-0.5627
N	1.2227	-1.5008	-0.5627
S	-1.8169	-1.6272	-2.0684
S	1.8169	-1.6272	-2.0684
C	-0.6660	-1.6317	-3.4390
C	0.6660	-1.6317	-3.4390
H	-1.2303	-1.6671	-4.3811
H	1.2303	-1.6671	-4.3811
H	0.0000	-1.4055	1.0391

$(HC)_2Se_2N_2(CH)$ (4b)

C	.0000	.0000	.0457
N	-1.2341	.0000	-.4372
N	1.2341	.0000	-.4372
Se	-1.9128	.0000	-2.0793
Se	1.9128	.0000	-2.0793
C	-.6662	.0000	-3.5429
C	.6662	.0000	-3.5429
H	-1.2263	.0000	-4.4910
H	1.2263	.0000	-4.4910
H	.0000	.0000	1.1501

$(HC)_2Se_2N_2(CH)^+$

C	.0000	.0000	.0574
N	-1.2136	.0000	-.4791
N	1.2136	.0000	-.4791
Se	-1.9296	.0000	-2.0305
Se	1.9296	.0000	-2.0305
C	-.6591	.0000	-3.5531
C	.6591	.0000	-3.5531
H	-1.2284	.0000	-4.4974
H	1.2284	.0000	-4.4974
H	.0000	.0000	1.1582

$(HC)_2Se_2N_2(CH)^-$

C	.0000	.0000	.0406
N	-1.2567	.0000	-.3795
N	1.2567	.0000	-.3795
Se	-1.9003	.0000	-2.1098
Se	1.9003	.0000	-2.1098
C	-.6762	.0000	-3.5549
C	.6762	.0000	-3.5549
H	-1.2331	.0000	-4.5060
H	1.2331	.0000	-4.5060
H	.0000	.0000	1.1549

$((HC)_2Se_2N_2(CH))_2$

C	0.0000	1.4772	0.0374
N	-1.2338	1.5175	-0.4349
N	1.2338	1.5175	-0.4349
Se	-1.9041	1.7351	-2.0634
Se	1.9041	1.7351	-2.0634
C	-0.6645	1.6763	-3.5492
C	0.6645	1.6763	-3.5492
H	-1.2309	1.6525	-4.4928
H	1.2309	1.6525	-4.4928
H	0.0000	1.3826	1.1380
C	0.0000	-1.4772	0.0374
N	-1.2338	-1.5175	-0.4349
N	1.2338	-1.5175	-0.4349
Se	-1.9041	-1.7351	-2.0634
Se	1.9041	-1.7351	-2.0634
C	-0.6645	-1.6763	-3.5492
C	0.6645	-1.6763	-3.5492
H	-1.2309	-1.6525	-4.4928
H	1.2309	-1.6525	-4.4928
H	0.0000	-1.3826	1.1380