

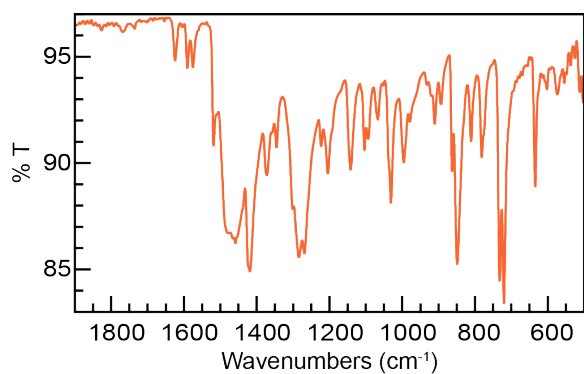
## Supplementary Information

### **A Series of Dithiocarbamates Americium, Curium, and Californium.**

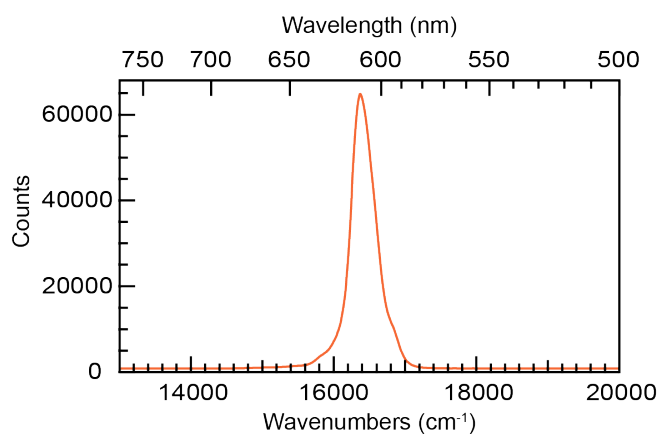
Samantha K. Cary,<sup>a‡</sup> Jing Su,<sup>a‡</sup> Shane S. Galley,<sup>b‡</sup> Thomas E. Albrecht-Schmitt,<sup>b\*</sup> Enrique R. Batista,<sup>a\*</sup>  
Maryline G. Ferrier,<sup>a</sup> Stosh A. Kozimor,<sup>a\*</sup> Veronika Mocko,<sup>a</sup> Brian L. Scott,<sup>a</sup> Cayla E. Van Alstine,<sup>b</sup>  
Frankie D. White,<sup>b</sup> Ping Yang<sup>a\*</sup>

#### **Table of Contents:**

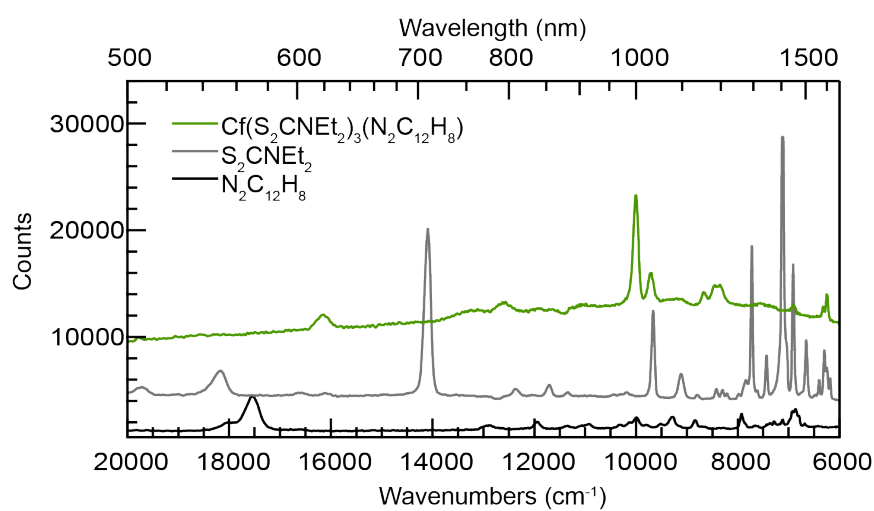
|                                 |          |
|---------------------------------|----------|
| <b>Figures and Tables .....</b> | <b>2</b> |
|---------------------------------|----------|



**Figure S1.** An FT-IR spectrum of a crystal of  $\text{Cm}(\text{S}_2\text{CNEt}_2)_3(\text{N}_2\text{C}_{12}\text{H}_8)$ .



**Figure S2.** The fluorescence spectrum of  $\text{Cm}(\text{S}_2\text{CNEt}_2)_3(\text{N}_2\text{C}_{12}\text{H}_8)$  when excited at 365 nm.



**Figure S3.** Raman Spectra of  $\text{An}(\text{S}_2\text{CNEt}_2)_3(\text{N}_2\text{C}_{12}\text{H}_8)$  shown in green,  $\text{S}_2\text{CNEt}_2$  shown in gray and  $\text{N}_2\text{C}_{12}\text{H}_8$  shown in black.

**Table S1.** Crystallographic Information for  $M(S_2CNEt_2)_3(N_2C_{12}H_8)$  ( $M = Am, Cm, \text{ and } Cf$ ).

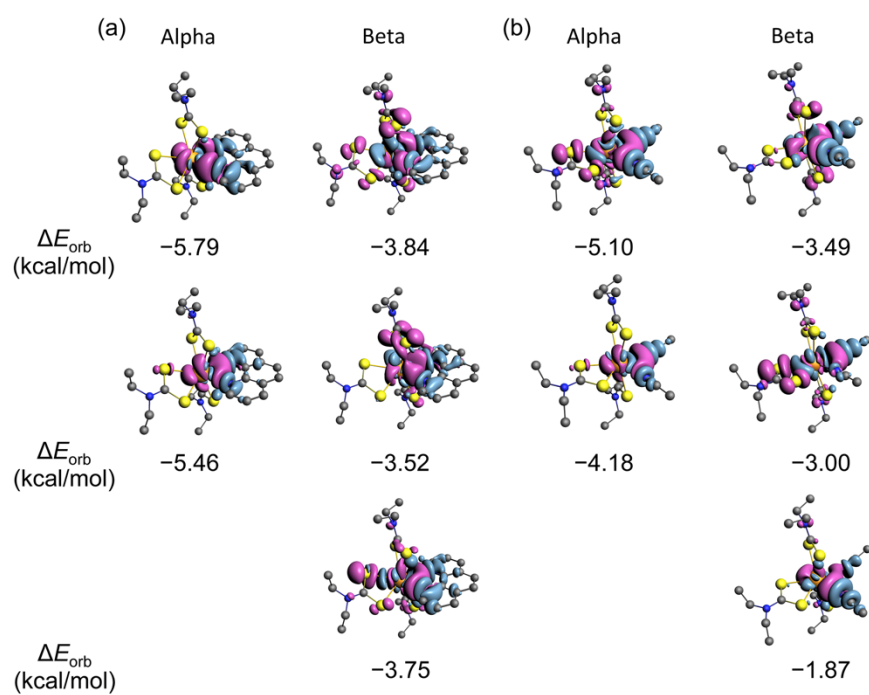
| Compound                                  | $Am(S_2CNEt_2)_3(N_2C_{12}H_8)$ | $Cm(S_2CNEt_2)_3(N_2C_{12}H_8)$ | $Cf(S_2CNEt_2)_3(N_2C_{12}H_8) \cdot C H_3CN$ |
|-------------------------------------------|---------------------------------|---------------------------------|-----------------------------------------------|
| Formula Mass                              | 867.98                          | 872.98                          | 916.10                                        |
| Space group                               | $P2_1/c$                        | $P2_1/c$                        | $P2_1/c$                                      |
| $a$ (Å)                                   | 16.9165(8)                      | 17.0129(11)                     | 10.4360(12)                                   |
| $b$ (Å)                                   | 10.5877(5)                      | 10.6573(7)                      | 34.561(4)                                     |
| $c$ (Å)                                   | 18.5943(9)                      | 18.7412(12)                     | 11.3259(14)                                   |
| $\alpha$ (°)                              | 90                              | 90                              | 90                                            |
| $\beta$ (°)                               | 96.9730(10)                     | 96.3710(13)                     | 117.142(3)                                    |
| $\gamma$ (°)                              | 90                              | 90                              | 90                                            |
| $V$ (Å <sup>3</sup> )                     | 3305.7(3)                       | 3377.0(4)                       | 3635.2(8)                                     |
| $Z$                                       | 4                               | 4                               | 4                                             |
| $T$ (K)                                   | 130(2)                          | 295(2)                          | 130(2)                                        |
| $\lambda$ (Å)                             | 0.71073                         | 0.71073                         | 0.71073                                       |
| Maximum $2\theta$ (°)                     | 26.372                          | 27.410                          | 27.601                                        |
| $\rho_{calc}$ (g/cm <sup>3</sup> )        | 1.744                           | 1.717                           | 1.668                                         |
| $\mu$ (Mo $K\alpha$ ) (cm <sup>-1</sup> ) | 27.25                           | 28.10                           | 27.03                                         |
| $R(F)$ for $F_o^2 >$                      |                                 |                                 |                                               |
| $2\sigma(F_o^2)^a$                        | 0.0199                          | 0.0207                          | 0.0525                                        |
| $R_w(F_o^2)^b$                            | 0.0443                          | 0.0600                          | 0.1231                                        |

$$^a R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$$

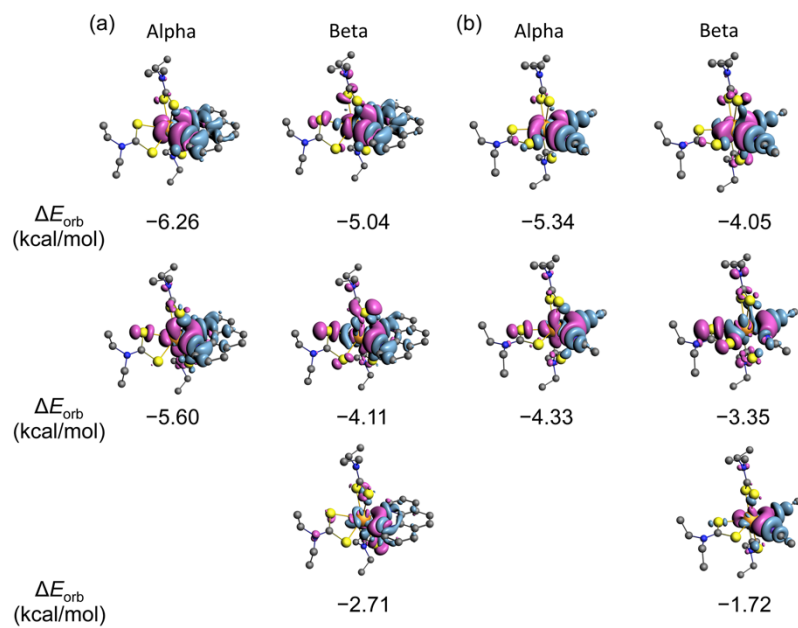
$$^b R_w(F_o^2) = \left[ \sum \left[ w(F_o^2 - F_c^2)^2 \right] / \sum wF_o^4 \right]^{1/2}$$

**Table S2.** Selected Bond Lengths for  $M(S_2CNEt_2)_3(N_2C_{12}H_8)$  ( $M = Am, Cm, \text{ and } Cf$ ) in Å, error is calculated standard deviation.

| $Am(S_2CNEt_2)_3(N_2C_{12}H_8)$ |               | $Cm(S_2CNEt_2)_3(N_2C_{12}H_8)$ |               | $Cf(S_2CNEt_2)_3(N_2C_{12}H_8)$ |               |
|---------------------------------|---------------|---------------------------------|---------------|---------------------------------|---------------|
| Am-S1                           | 2.8015 ± 0.05 | Cm-S1                           | 2.8420 ± 0.04 | Cf-S1                           | 2.8370 ± 0.04 |
| Am-S2                           | 2.9304 ± 0.05 | Cm-S2                           | 2.8607 ± 0.04 | Cf-S2                           | 2.8050 ± 0.04 |
| Am-S3                           | 2.8757 ± 0.05 | Cm-S3                           | 2.8998 ± 0.04 | Cf-S3                           | 2.7950 ± 0.04 |
| Am-S4                           | 2.8530 ± 0.05 | Cm-S4                           | 2.8594 ± 0.04 | Cf-S4                           | 2.8186 ± 0.04 |
| Am-S5                           | 2.8673 ± 0.05 | Cm-S5                           | 2.7942 ± 0.04 | Cf-S5                           | 2.8508 ± 0.04 |
| Am-S6                           | 2.9193 ± 0.05 | Cm-S6                           | 2.9156 ± 0.04 | Cf-S6                           | 2.9066 ± 0.04 |
| Am-N1                           | 2.609 ± 0.008 | Cm-N1                           | 2.596 ± 0.006 | Cf-N1                           | 2.572 ± 0.02  |
| Am-N2                           | 2.598 ± 0.008 | Cm-N2                           | 2.605 ± 0.006 | Cf-N2                           | 2.540 ± 0.02  |



**Figure S4.** The NOCV deformation densities of alpha and beta spin and associated energy contributions representing Cm-N  $\sigma$  bonding in (a)  $\text{Cm}(\text{S}_2\text{CNET}_2)_3(\text{N}_2\text{C}_{12}\text{H}_8)$  and (b)  $\text{Cm}(\text{S}_2\text{CNET}_2)_2(\text{MeCN})$ . The contour values are 0.0001 au. Light blue represents positive and pink negative.



**Figure S5.** The NOCV deformation densities of alpha and beta spin and associated energy contributions representing Gd-N  $\sigma$  bonding in (a)  $\text{Gd}(\text{S}_2\text{CNEt}_2)_3(\text{N}_2\text{C}_{12}\text{H}_8)$  and (b)  $\text{Gd}(\text{S}_2\text{CNEt}_2)_2(\text{MeCN})$ . The contour values are 0.0001 au. Light blue represents positive and pink negative.

**Table S3.** Cartesian coordinates of optimized geometries of  $M(S_2CNEt_2)_3(N_2C_{12}H_8)$  and  $M(S_2CNEt_2)_3((MeCN)_2)$  ( $M = Am, Cm, Cf, Eu, Gd$ ).

| $Am(S_2CNEt_2)_3(N_2C_{12}H_8)$ |             |             |             | $Cm(S_2CNEt_2)_3(N_2C_{12}H_8)$ |             |             |             |
|---------------------------------|-------------|-------------|-------------|---------------------------------|-------------|-------------|-------------|
| Am                              | 0.07443300  | 0.08103000  | -0.06325600 | Cm                              | -0.07339400 | -0.13765700 | -0.07448600 |
| S                               | -1.02594600 | 1.42851300  | -2.33398600 | S                               | 1.22362700  | -1.33817200 | -2.31042800 |
| S                               | 1.32468000  | 1.91307900  | 1.79878600  | S                               | 2.32558500  | -1.68740100 | 0.43154100  |
| S                               | -2.12731400 | 1.90945200  | 0.38441900  | N                               | 3.21005400  | -3.00871200 | -1.70563100 |
| S                               | 0.78185900  | -1.58715500 | -2.31216000 | C                               | 2.34286000  | -2.09827300 | -1.23757100 |
| S                               | 1.32074500  | -2.44864100 | 0.47820900  | C                               | 4.17490500  | -3.67721100 | -0.83799400 |
| S                               | 2.69161100  | 1.07333900  | -0.68881300 | H                               | 4.46869100  | -2.98343600 | -0.04985200 |
| N                               | -2.79335400 | 3.34082600  | -1.76082600 | H                               | 5.06401500  | -3.88031400 | -1.44340200 |
| N                               | -2.09050100 | -1.42230100 | -0.14246700 | C                               | 3.62642000  | -4.96137500 | -0.23793200 |
| N                               | 3.77667900  | 2.70834000  | 1.11565300  | H                               | 4.38787800  | -5.44687600 | 0.37931600  |
| N                               | -0.91998400 | -0.82751300 | 2.26207300  | H                               | 2.76131300  | -4.74627500 | 0.39196500  |
| N                               | 2.54264700  | -3.47782000 | -1.65616600 | H                               | 3.32160000  | -5.67006500 | -1.01352100 |
| C                               | -2.65670300 | -1.89598900 | 0.98666600  | C                               | 3.23592500  | -3.41285600 | -3.10806700 |
| C                               | -1.96900200 | -1.81138500 | 4.65422800  | H                               | 2.22281500  | -3.34733000 | -3.50522100 |
| H                               | -2.38481200 | -2.19341700 | 5.58239000  | H                               | 3.52853100  | -4.46720300 | -3.13251400 |
| C                               | -4.40666800 | -2.96341400 | -0.28494400 | C                               | 4.18991300  | -2.57219300 | -3.94048900 |
| H                               | -5.30934600 | -3.56605400 | -0.33411000 | H                               | 4.20864900  | -2.93047000 | -4.97372500 |
| C                               | -2.03658400 | -1.59045000 | 2.25138200  | H                               | 3.86866900  | -1.52884300 | -3.94808700 |
| C                               | -2.06032700 | 2.32337000  | -1.28239100 | H                               | 5.21141700  | -2.61699800 | -3.55118700 |
| C                               | -0.82755000 | -1.05132100 | 4.64852000  | S                               | -1.24312700 | -2.11948900 | 1.66561300  |
| H                               | -0.30101800 | -0.80736800 | 5.56416300  | S                               | -2.63311600 | -1.24086600 | -0.80020900 |
| C                               | -3.68116700 | 4.12404900  | -0.90746900 | N                               | -3.66641700 | -2.96956200 | 0.94725000  |
| H                               | -4.07824600 | 3.47017200  | -0.13040000 | C                               | -2.62769600 | -2.18236100 | 0.63122700  |
| H                               | -4.52425300 | 4.44333900  | -1.52849800 | C                               | -3.69608600 | -3.77988500 | 2.16025200  |
| C                               | 1.63368800  | -2.59824400 | -1.21120300 | H                               | -4.74043500 | -3.83662500 | 2.48336500  |
| C                               | -2.73715200 | 3.75103900  | -3.16034900 | H                               | -3.14250400 | -3.25532100 | 2.93927200  |
| H                               | -1.73296200 | 3.55573300  | -3.53718800 | C                               | -3.12238900 | -5.17109100 | 1.94657700  |
| H                               | -2.88976600 | 4.83461400  | -3.18347500 | H                               | -3.19583500 | -5.75771000 | 2.86697400  |
| C                               | -3.82850800 | -2.68475100 | 0.96609900  | H                               | -3.65871000 | -5.71129000 | 1.16093600  |
| C                               | -2.60867000 | -2.10446700 | 3.43718500  | H                               | -2.06977200 | -5.10813100 | 1.66431700  |
| C                               | -2.65402400 | -1.70449000 | -1.30327700 | C                               | -4.84005800 | -3.07580600 | 0.08576700  |
| H                               | -2.16194900 | -1.30132200 | -2.18117700 | H                               | -5.22627300 | -4.09442500 | 0.19186200  |
| C                               | 2.71330100  | 1.96574900  | 0.77473500  | H                               | -4.51910600 | -2.95447200 | -0.94919100 |
| C                               | -3.81994100 | -2.47231000 | -1.42334000 | C                               | -5.91052400 | -2.05471700 | 0.43395600  |
| H                               | -4.23424600 | -2.66662700 | -2.40604100 | H                               | -6.78381700 | -2.18504600 | -0.21165200 |
| C                               | 3.30042000  | -4.33637400 | -0.75108000 | H                               | -6.24210900 | -2.15657000 | 1.47162200  |
| H                               | 3.49958500  | -5.27063300 | -1.28564300 | H                               | -5.52828400 | -1.04214000 | 0.29116800  |
| H                               | 2.67004900  | -4.57902100 | 0.10465400  | S                               | -1.51014300 | 2.24479200  | 0.58201800  |
| C                               | -0.33999600 | -0.57791900 | 3.42348200  | S                               | -0.99946500 | 1.52437700  | -2.25600300 |
| H                               | 0.55630200  | 0.03371400  | 3.38425600  | N                               | -2.79794500 | 3.33182400  | -1.48289100 |
| C                               | 4.59664000  | -3.69012200 | -0.29033600 | C                               | -1.85795700 | 2.45690300  | -1.09450900 |
| H                               | 5.14657700  | -4.36912500 | 0.36782200  | C                               | -3.55862800 | 4.13028000  | -0.52705000 |
| H                               | 4.38549400  | -2.77185700 | 0.26102500  | H                               | -3.79257300 | 5.08109900  | -1.01646200 |
| H                               | 5.24530000  | -3.44263400 | -1.13565500 | H                               | -2.91728100 | 4.35297900  | 0.32604100  |
| C                               | 2.86053200  | -3.61669400 | -3.07421000 | C                               | -4.82864800 | 3.43185400  | -0.06918700 |
| H                               | 3.91866600  | -3.88796300 | -3.14058000 | H                               | -5.38233700 | 4.06841400  | 0.62715500  |
| H                               | 2.74301500  | -2.64295500 | -3.55011100 | H                               | -5.48761400 | 3.20277800  | -0.91172700 |
| C                               | -4.38352600 | -3.17348500 | 2.18752200  | H                               | -4.58362800 | 2.49742000  | 0.43929700  |
| H                               | -5.28605400 | -3.77604000 | 2.14305600  | C                               | -3.14758200 | 3.52294300  | -2.88693600 |
| C                               | -3.77442000 | 3.04521900  | -4.01807600 | H                               | -4.21370100 | 3.76773300  | -2.92166000 |
| H                               | -3.72583800 | 3.40839300  | -5.04865100 | H                               | -3.01380200 | 2.57400000  | -3.40682300 |
| H                               | -4.78935400 | 3.21933500  | -3.64836400 | C                               | -2.32439300 | 4.61536500  | -3.54930600 |
| H                               | -3.59023500 | 1.96919000  | -4.02779500 | H                               | -2.63984900 | 4.75154100  | -4.58774100 |
| C                               | 4.95521400  | 2.80416500  | 0.25984800  | H                               | -2.43922000 | 5.57423400  | -3.03502200 |
| H                               | 5.37207300  | 3.80681500  | 0.39721100  | H                               | -1.26602600 | 4.34760900  | -3.54737700 |
| H                               | 4.63359400  | 2.72456800  | -0.77898600 | N                               | 1.88855100  | 1.61708200  | -0.17736000 |

|                                                                                                     |             |             |             |                                                                                                     |             |             |             |
|-----------------------------------------------------------------------------------------------------|-------------|-------------|-------------|-----------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| C                                                                                                   | 5.99332100  | 1.74094700  | 0.57871700  | N                                                                                                   | 0.88804100  | 0.76451100  | 2.23078800  |
| H                                                                                                   | 6.87218000  | 1.86465200  | -0.06058700 | C                                                                                                   | 2.37675600  | 2.01854400  | -1.33690200 |
| H                                                                                                   | 5.58175600  | 0.74498700  | 0.40415600  | H                                                                                                   | 1.89699800  | 1.61352400  | -2.22038600 |
| H                                                                                                   | 6.32458700  | 1.80080300  | 1.61973500  | C                                                                                                   | 3.44792500  | 2.91493400  | -1.44991000 |
| C                                                                                                   | -3.79556800 | -2.89648600 | 3.37570600  | H                                                                                                   | 3.80330800  | 3.20363800  | -2.43252200 |
| H                                                                                                   | -4.21579200 | -3.27334100 | 4.30354300  | C                                                                                                   | 4.01763600  | 3.40949200  | -0.30455400 |
| C                                                                                                   | 3.29690100  | 4.89448300  | 2.17915800  | H                                                                                                   | 4.84675900  | 4.11031100  | -0.34755500 |
| H                                                                                                   | 3.38380200  | 5.45040200  | 3.11724700  | C                                                                                                   | 3.51899500  | 3.00421300  | 0.94613000  |
| H                                                                                                   | 2.24421500  | 4.87230400  | 1.89105400  | C                                                                                                   | 4.06319200  | 3.48743300  | 2.17461000  |
| H                                                                                                   | 3.85331500  | 5.44150700  | 1.41244100  | H                                                                                                   | 4.89100800  | 4.18941000  | 2.13478900  |
| C                                                                                                   | -2.98431100 | 5.32360600  | -0.28656600 | C                                                                                                   | 3.55708800  | 3.08285500  | 3.36377800  |
| H                                                                                                   | -3.68951500 | 5.90055300  | 0.31874100  | H                                                                                                   | 3.96926300  | 3.45432600  | 4.29735900  |
| H                                                                                                   | -2.57406600 | 5.99063800  | -1.05045100 | C                                                                                                   | 2.46985000  | 2.15842300  | 3.41854300  |
| H                                                                                                   | -2.16793300 | 4.99504700  | 0.35922100  | C                                                                                                   | 1.91075300  | 1.64933100  | 2.22452100  |
| C                                                                                                   | 3.82673900  | 3.48049700  | 2.35257800  | C                                                                                                   | 2.44211500  | 2.08985300  | 0.95897000  |
| H                                                                                                   | 4.87103400  | 3.49486300  | 2.68050800  | C                                                                                                   | 1.91950000  | 1.72548500  | 4.63751600  |
| H                                                                                                   | 3.25392900  | 2.95005000  | 3.11366100  | H                                                                                                   | 2.32848400  | 2.10044500  | 5.57155900  |
| C                                                                                                   | 1.99499100  | -4.65706400 | -3.76558400 | C                                                                                                   | 0.87299100  | 0.83913400  | 4.62735200  |
| H                                                                                                   | 2.28783400  | -4.75791300 | -4.81460700 | H                                                                                                   | 0.41786100  | 0.48426000  | 5.54495700  |
| H                                                                                                   | 0.94475600  | -4.36075900 | -3.73236800 | C                                                                                                   | 0.38983100  | 0.38300100  | 3.39435500  |
| H                                                                                                   | 2.09177200  | -5.63956300 | -3.29398700 | H                                                                                                   | -0.43448800 | -0.32262500 | 3.34985100  |
| Cf(S <sub>2</sub> CNEt <sub>2</sub> ) <sub>3</sub> (N <sub>2</sub> C <sub>12</sub> H <sub>8</sub> ) |             |             |             | Eu(S <sub>2</sub> CNEt <sub>2</sub> ) <sub>3</sub> (N <sub>2</sub> C <sub>12</sub> H <sub>8</sub> ) |             |             |             |
| Cf                                                                                                  | 0.08607700  | 0.11349900  | -0.06096800 | Eu                                                                                                  | 0.07026800  | 0.10435000  | -0.05986700 |
| S                                                                                                   | -0.99155900 | 1.45976500  | -2.26637900 | S                                                                                                   | -1.09607500 | 1.38861000  | -2.32016200 |
| S                                                                                                   | -2.29493000 | 1.65985900  | 0.39233700  | S                                                                                                   | 1.27139600  | 1.99734200  | 1.74891500  |
| N                                                                                                   | -2.99854500 | 3.12829000  | -1.71764800 | S                                                                                                   | -2.20085400 | 1.81355600  | 0.40222300  |
| C                                                                                                   | -2.18251700 | 2.17605800  | -1.24123900 | S                                                                                                   | 0.88971400  | -1.54979000 | -2.27322200 |
| C                                                                                                   | -4.01719100 | 3.76036300  | -0.88544700 | S                                                                                                   | 1.50344000  | -2.29167900 | 0.53724900  |
| H                                                                                                   | -4.37874300 | 3.02536900  | -0.16564200 | S                                                                                                   | 2.59316300  | 1.24542000  | -0.78305200 |
| H                                                                                                   | -4.85545900 | 4.01571400  | -1.54153200 | N                                                                                                   | -3.00351800 | 3.16178100  | -1.75014500 |
| C                                                                                                   | -3.49806500 | 4.99557100  | -0.16791800 | N                                                                                                   | -1.98150600 | -1.51666500 | -0.17043200 |
| H                                                                                                   | -4.29651700 | 5.45549300  | 0.42158800  | N                                                                                                   | 3.69590500  | 2.85205200  | 1.03682500  |
| H                                                                                                   | -2.68424700 | 4.72705700  | 0.50819100  | N                                                                                                   | -0.89947500 | -0.80635300 | 2.24369200  |
| H                                                                                                   | -3.12794100 | 5.74510300  | -0.87356800 | N                                                                                                   | 2.72779200  | -3.35005300 | -1.58039500 |
| C                                                                                                   | -2.91000400 | 3.61567800  | -3.09055300 | C                                                                                                   | -2.54663100 | -1.99552900 | 0.95703700  |
| H                                                                                                   | -1.86997100 | 3.55530100  | -3.41190200 | C                                                                                                   | -1.94228600 | -1.79799400 | 4.63524000  |
| H                                                                                                   | -3.18535200 | 4.67485000  | -3.07352000 | H                                                                                                   | -2.35587500 | -2.18343400 | 5.56298400  |
| C                                                                                                   | -3.80744400 | 2.84359800  | -4.04359200 | C                                                                                                   | -4.21271800 | -3.17844600 | -0.32500500 |
| H                                                                                                   | -3.74203000 | 3.26405200  | -5.05119300 | H                                                                                                   | -5.08161400 | -3.82849400 | -0.37885800 |
| H                                                                                                   | -3.49968700 | 1.79723900  | -4.09128200 | C                                                                                                   | -1.97117800 | -1.63065200 | 2.22736500  |
| H                                                                                                   | -4.85527900 | 2.88236600  | -3.73113600 | C                                                                                                   | -2.18657500 | 2.21163700  | -1.26981200 |
| S                                                                                                   | 1.14566700  | 2.14463700  | 1.62693400  | C                                                                                                   | -0.84503900 | -0.97542800 | 4.63588200  |
| S                                                                                                   | 2.66767700  | 1.10273800  | -0.68112500 | H                                                                                                   | -0.35234100 | -0.68360500 | 5.55632800  |
| N                                                                                                   | 3.61254300  | 2.94847700  | 0.99884100  | C                                                                                                   | -3.94069500 | 3.88248200  | -0.89472600 |
| C                                                                                                   | 2.59131300  | 2.14048300  | 0.68027000  | H                                                                                                   | -4.27643700 | 3.20834300  | -0.10603000 |
| C                                                                                                   | 3.57229600  | 3.84366700  | 2.15018400  | H                                                                                                   | -4.81331900 | 4.12692200  | -1.50885900 |
| H                                                                                                   | 4.59539000  | 3.92437700  | 2.53119500  | C                                                                                                   | 1.79440100  | -2.48713400 | -1.15118600 |
| H                                                                                                   | 2.97037300  | 3.37585700  | 2.92961200  | C                                                                                                   | -2.99358400 | 3.55967000  | -3.15422400 |
| C                                                                                                   | 3.01669300  | 5.21521900  | 1.80322900  | H                                                                                                   | -1.98101400 | 3.43896200  | -3.53997300 |
| H                                                                                                   | 3.03549200  | 5.86615400  | 2.68219200  | H                                                                                                   | -3.22989900 | 4.62786100  | -3.18686800 |
| H                                                                                                   | 3.60123300  | 5.69886500  | 1.01514800  | C                                                                                                   | -3.67477300 | -2.84557900 | 0.93071100  |
| H                                                                                                   | 1.98305300  | 5.13026000  | 1.46259100  | C                                                                                                   | -2.53889900 | -2.15125600 | 3.41234000  |
| C                                                                                                   | 4.83328600  | 2.99519900  | 0.20002000  | C                                                                                                   | -2.50668700 | -1.85079900 | -1.33514900 |
| H                                                                                                   | 5.21518300  | 4.01951700  | 0.25427200  | H                                                                                                   | -2.01682300 | -1.44316000 | -2.21192900 |
| H                                                                                                   | 4.57091400  | 2.79944000  | -0.84012200 | C                                                                                                   | 2.63745600  | 2.10149500  | 0.69892900  |
| C                                                                                                   | 5.88015000  | 2.00373800  | 0.68033500  | C                                                                                                   | -3.62979100 | -2.67922400 | -1.46173300 |
| H                                                                                                   | 6.78928000  | 2.08984800  | 0.07825700  | H                                                                                                   | -4.01368900 | -2.91394300 | -2.44798500 |

|                                                                                                     |             |             |             |                                                                           |             |             |             |
|-----------------------------------------------------------------------------------------------------|-------------|-------------|-------------|---------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                                   | 6.15193000  | 2.17961700  | 1.72547300  | C                                                                         | 3.52663900  | -4.15237900 | -0.65968600 |
| H                                                                                                   | 5.50505800  | 0.98266400  | 0.58808100  | H                                                                         | 3.74935500  | -5.09689500 | -1.16629400 |
| S                                                                                                   | 1.39242100  | -2.31185200 | 0.57439500  | H                                                                         | 2.91715200  | -4.38727100 | 0.21317600  |
| S                                                                                                   | 0.98235400  | -1.50629100 | -2.24745500 | C                                                                         | -0.35899100 | -0.50097400 | 3.41063800  |
| N                                                                                                   | 2.64625000  | -3.44686700 | -1.48740600 | H                                                                         | 0.50394800  | 0.15721300  | 3.37640800  |
| C                                                                                                   | 1.75844800  | -2.51929800 | -1.09835500 | C                                                                         | 4.80758400  | -3.44999800 | -0.23988800 |
| C                                                                                                   | 3.33502500  | -4.31077500 | -0.53428600 | H                                                                         | 5.39014600  | -4.09001900 | 0.42921100  |
| H                                                                                                   | 3.51463500  | -5.26630900 | -1.03734100 | H                                                                         | 4.57444800  | -2.52295600 | 0.28737500  |
| H                                                                                                   | 2.66459500  | -4.50569600 | 0.30324000  | H                                                                         | 5.43449100  | -3.20712100 | -1.10280300 |
| C                                                                                                   | 4.63969700  | -3.70668500 | -0.04104300 | C                                                                         | 3.03039100  | -3.52525200 | -2.99745500 |
| H                                                                                                   | 5.13787900  | -4.39177400 | 0.65117900  | H                                                                         | 4.09677400  | -3.76012500 | -3.07129000 |
| H                                                                                                   | 5.32734300  | -3.50524900 | -0.86756500 | H                                                                         | 2.87049000  | -2.57295000 | -3.50351700 |
| H                                                                                                   | 4.44761500  | -2.76818800 | 0.48243300  | C                                                                         | -4.22749600 | -3.33947900 | 2.15110300  |
| C                                                                                                   | 3.00734500  | -3.63292100 | -2.88894100 | H                                                                         | -5.09543300 | -3.99053600 | 2.10172300  |
| H                                                                                                   | 4.05619900  | -3.94472300 | -2.91207500 | C                                                                         | -3.98156000 | 2.76619600  | -3.99340000 |
| H                                                                                                   | 2.94282700  | -2.66728200 | -3.39125100 | H                                                                         | -3.97085000 | 3.11995500  | -5.02831800 |
| C                                                                                                   | 2.12751500  | -4.65695400 | -3.58683200 | H                                                                         | -5.00334900 | 2.86614500  | -3.61520200 |
| H                                                                                                   | 2.45134900  | -4.79287900 | -4.62272600 | H                                                                         | -3.71541200 | 1.70741700  | -3.99332100 |
| H                                                                                                   | 2.17179500  | -5.63111300 | -3.09064200 | C                                                                         | 4.85371000  | 2.98691300  | 0.15855600  |
| H                                                                                                   | 1.08861300  | -4.32155300 | -3.59618800 | H                                                                         | 5.25965900  | 3.99162900  | 0.31261400  |
| N                                                                                                   | -1.89332600 | -1.57134500 | -0.20733200 | H                                                                         | 4.51015700  | 2.92959500  | -0.87484600 |
| N                                                                                                   | -0.89371800 | -0.76080700 | 2.20194000  | C                                                                         | 5.91302100  | 1.93058700  | 0.42686500  |
| C                                                                                                   | -2.38614500 | -1.94118200 | -1.37516300 | H                                                                         | 6.77531300  | 2.08257900  | -0.22868300 |
| H                                                                                                   | -1.89263400 | -1.53329600 | -2.25013100 | H                                                                         | 5.51096100  | 0.93361300  | 0.23651900  |
| C                                                                                                   | -3.47759000 | -2.81072700 | -1.50508300 | H                                                                         | 6.26707900  | 1.96899300  | 1.46136500  |
| H                                                                                                   | -3.83696600 | -3.07490300 | -2.49315700 | C                                                                         | -3.67948300 | -3.00812600 | 3.34444200  |
| C                                                                                                   | -4.06188200 | -3.31260800 | -0.36979500 | H                                                                         | -4.09763000 | -3.38899000 | 4.27157600  |
| H                                                                                                   | -4.90565700 | -3.99458800 | -0.42772000 | C                                                                         | 3.20878500  | 4.99951500  | 2.17354600  |
| C                                                                                                   | -3.55980000 | -2.93777600 | 0.88903900  | H                                                                         | 3.30816100  | 5.52915500  | 3.12550800  |
| C                                                                                                   | -4.11622000 | -3.42444700 | 2.11086300  | H                                                                         | 2.15055700  | 4.97048100  | 1.90716500  |
| H                                                                                                   | -4.95750900 | -4.10961400 | 2.06161100  | H                                                                         | 3.74063100  | 5.57680600  | 1.41162000  |
| C                                                                                                   | -3.60578400 | -3.04270600 | 3.30615100  | C                                                                         | -3.33409100 | 5.14053800  | -0.29511000 |
| H                                                                                                   | -4.02821900 | -3.41676600 | 4.23410000  | H                                                                         | -4.07589600 | 5.66679000  | 0.31263400  |
| C                                                                                                   | -2.50217600 | -2.13844000 | 3.37529900  | H                                                                         | -2.98688400 | 5.82907400  | -1.07104200 |
| C                                                                                                   | -1.93045600 | -1.62912700 | 2.18810900  | H                                                                         | -2.48672600 | 4.88550000  | 0.34390400  |
| C                                                                                                   | -2.46431700 | -2.04737000 | 0.91778100  | C                                                                         | 3.76239900  | 3.58909400  | 2.29392300  |
| C                                                                                                   | -1.94794000 | -1.72413600 | 4.59889200  | H                                                                         | 4.81329900  | 3.60942200  | 2.59970600  |
| H                                                                                                   | -2.36483900 | -2.09925700 | 5.52936400  | H                                                                         | 3.21437800  | 3.02826200  | 3.05163400  |
| C                                                                                                   | -0.88774700 | -0.85368100 | 4.59751300  | C                                                                         | 2.19418800  | -4.61899600 | -3.64105700 |
| H                                                                                                   | -0.43026800 | -0.51246400 | 5.51912200  | H                                                                         | 2.47526400  | -4.74377900 | -4.69075600 |
| C                                                                                                   | -0.39342400 | -0.39485800 | 3.36991100  | H                                                                         | 1.13434200  | -4.36025700 | -3.60079500 |
| H                                                                                                   | 0.43812300  | 0.30236500  | 3.33176200  | H                                                                         | 2.33416400  | -5.58119500 | -3.13937500 |
| Gd(S <sub>2</sub> CNEt <sub>2</sub> ) <sub>3</sub> (N <sub>2</sub> C <sub>12</sub> H <sub>8</sub> ) |             |             |             | Am(S <sub>2</sub> CNEt <sub>2</sub> ) <sub>3</sub> ((MeCN) <sub>2</sub> ) |             |             |             |
| Gd                                                                                                  | 0.07410300  | 0.13151800  | -0.07233400 | Am                                                                        | -0.08450800 | -0.26338500 | 0.40005200  |
| S                                                                                                   | -1.14262100 | 1.37731000  | -2.27602900 | S                                                                         | -1.89039200 | -1.26935800 | -1.59296600 |
| S                                                                                                   | -2.33745200 | 1.60616900  | 0.43492300  | S                                                                         | 0.08866500  | 2.49067400  | 1.23845300  |
| N                                                                                                   | -3.17384500 | 2.99588800  | -1.67834300 | S                                                                         | -2.90071800 | 0.02661600  | 0.87837600  |
| C                                                                                                   | -2.30860000 | 2.08089800  | -1.21517500 | S                                                                         | 1.46606300  | -2.07632300 | -1.21363600 |
| C                                                                                                   | -4.17489300 | 3.61895100  | -0.81818700 | S                                                                         | 2.63665300  | -0.74450300 | 1.16766800  |
| H                                                                                                   | -4.48487800 | 2.89185100  | -0.06705200 | S                                                                         | 0.65285600  | 1.67224000  | -1.55003400 |
| H                                                                                                   | -5.04677000 | 3.83449900  | -1.44404400 | N                                                                         | -4.43837300 | -0.58329800 | -1.21208100 |
| C                                                                                                   | -3.66291300 | 4.88552200  | -0.15206200 | N                                                                         | -0.61609400 | -2.63743100 | 1.44580800  |
| H                                                                                                   | -4.44971500 | 5.33729800  | 0.45900600  | N                                                                         | 0.87388000  | 4.17954600  | -0.67198400 |
| H                                                                                                   | -2.81481400 | 4.65689700  | 0.49595000  | N                                                                         | -0.16565900 | -0.06039600 | 3.04248300  |
| H                                                                                                   | -3.34382600 | 5.62743300  | -0.88994700 | N                                                                         | 4.08665900  | -1.79332500 | -0.80873700 |
| C                                                                                                   | -3.15877100 | 3.45287100  | -3.06447800 | C                                                                         | -3.19935900 | -0.61199900 | -0.69398300 |
| H                                                                                                   | -2.13210900 | 3.41607100  | -3.42938500 | C                                                                         | -5.57448300 | -0.03520000 | -0.47941300 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -3.46522800 | 4.50357200  | -3.05922600 | H | -5.42210600 | -0.22236700 | 0.58401100  |
| C | -4.07254700 | 2.63261000  | -3.96002200 | H | -6.45959500 | -0.60126400 | -0.78756000 |
| H | -4.06260900 | 3.03036800  | -4.97884400 | C | 2.85202900  | -1.56968200 | -0.33186000 |
| H | -3.73633200 | 1.59461600  | -3.99706600 | C | -4.72774600 | -1.07235700 | -2.55584600 |
| H | -5.10681400 | 2.64875500  | -3.60351900 | H | -3.85038000 | -0.90204300 | -3.18038800 |
| S | 1.13241100  | 2.14618900  | 1.63673300  | H | -5.53878000 | -0.45536500 | -2.95538700 |
| S | 2.59927300  | 1.24628700  | -0.76798300 | C | 0.57076500  | 2.91008300  | -0.35969600 |
| N | 3.54322700  | 3.05730000  | 0.94766500  | C | 5.28504600  | -1.36724500 | -0.09358700 |
| C | 2.53811000  | 2.22688400  | 0.63351800  | H | 6.07143000  | -2.09393000 | -0.32200100 |
| C | 3.51957800  | 3.90262600  | 2.13643500  | H | 5.08831800  | -1.42625000 | 0.97716000  |
| H | 4.55390500  | 4.00274700  | 2.48072500  | C | 5.72104600  | 0.03777300  | -0.47597300 |
| H | 2.96557500  | 3.38290200  | 2.91849000  | H | 6.63491800  | 0.31119100  | 0.05963800  |
| C | 2.90645600  | 5.26767000  | 1.86982600  | H | 4.94246000  | 0.75784000  | -0.21728900 |
| H | 2.93986200  | 5.88232200  | 2.77412800  | H | 5.92318100  | 0.11829900  | -1.54805900 |
| H | 3.44301100  | 5.80261900  | 1.08074600  | C | 4.31532500  | -2.44654800 | -2.09345700 |
| H | 1.86317500  | 5.16226400  | 1.56630900  | H | 5.22544400  | -2.01144100 | -2.51802600 |
| C | 4.73004100  | 3.17800500  | 0.10668500  | H | 3.49064300  | -2.19249100 | -2.75975200 |
| H | 5.08026900  | 4.21168800  | 0.18970000  | C | -5.11437900 | -2.54215200 | -2.57210800 |
| H | 4.43428300  | 3.01612600  | -0.93033900 | H | -5.36027500 | -2.85955100 | -3.58961000 |
| C | 5.82649600  | 2.20415500  | 0.50567400  | H | -5.98623000 | -2.73649800 | -1.94003800 |
| H | 6.70800600  | 2.34500100  | -0.12643500 | H | -4.28453500 | -3.15551400 | -2.21564600 |
| H | 6.13331800  | 2.34730700  | 1.54609800  | C | 1.27477200  | 4.57076500  | -2.01940100 |
| H | 5.48124000  | 1.17544600  | 0.38584200  | H | 0.91219900  | 5.59108600  | -2.17987400 |
| S | 1.53938400  | -2.18743100 | 0.59840200  | H | 0.76021200  | 3.92678700  | -2.73303800 |
| S | 1.04015400  | -1.47835100 | -2.23976400 | C | 2.77901800  | 4.49562200  | -2.22388900 |
| N | 2.83890200  | -3.28126400 | -1.45596500 | H | 3.04218600  | 4.82463200  | -3.23336400 |
| C | 1.89577000  | -2.40623400 | -1.07474900 | H | 3.12732700  | 3.46873900  | -2.09770700 |
| C | 3.59584300  | -4.07586200 | -0.49421800 | H | 3.31441900  | 5.13209800  | -1.51303000 |
| H | 3.83230500  | -5.02844200 | -0.97904500 | C | -0.53606400 | 5.93252900  | 0.36562000  |
| H | 2.95088500  | -4.29612800 | 0.35684300  | H | -0.52462100 | 6.75186200  | 1.09049500  |
| C | 4.86372700  | -3.37568100 | -0.03309000 | H | -1.30403600 | 5.21812800  | 0.66824900  |
| H | 5.41488500  | -4.01010400 | 0.66721900  | H | -0.81645400 | 6.34904100  | -0.60634700 |
| H | 5.52602600  | -3.14870000 | -0.87357600 | C | -5.77043500 | 1.45066700  | -0.73279300 |
| H | 4.61660500  | -2.43985700 | 0.47177600  | H | -6.64859200 | 1.81590700  | -0.19219400 |
| C | 3.19482200  | -3.47555900 | -2.85777700 | H | -5.91929100 | 1.66136800  | -1.79589100 |
| H | 4.26168500  | -3.71786100 | -2.88770400 | H | -4.89889900 | 2.01086600  | -0.38921500 |
| H | 3.06108800  | -2.52818900 | -3.38070400 | C | 0.82339600  | 5.25468500  | 0.31224900  |
| C | 2.37704700  | -4.57167300 | -3.52081200 | H | 1.60468400  | 5.97336700  | 0.04489300  |
| H | 2.69684800  | -4.70959300 | -4.55769500 | H | 1.08207900  | 4.84100000  | 1.28737200  |
| H | 2.49233500  | -5.52902500 | -3.00379600 | C | 4.45172300  | -3.95477400 | -1.96506900 |
| H | 1.31796400  | -4.30674000 | -3.52362200 | H | 4.65952700  | -4.40214500 | -2.94139300 |
| N | -1.82878100 | -1.61691200 | -0.23271700 | H | 3.52562400  | -4.38810900 | -1.58229600 |
| N | -0.86472200 | -0.78186600 | 2.19113900  | H | 5.26731600  | -4.22954500 | -1.28938400 |
| C | -2.30486300 | -2.00291400 | -1.40221700 | C | -0.83547400 | -3.76026400 | 1.54048600  |
| H | -1.82719600 | -1.57309800 | -2.27496200 | C | -0.16445400 | 0.20619700  | 4.15950300  |
| C | -3.36190300 | -2.91279900 | -1.53758300 | C | -0.15706300 | 0.56129700  | 5.56140400  |
| H | -3.70830000 | -3.18754500 | -2.52739000 | H | 0.52670400  | -0.08833900 | 6.11096300  |
| C | -3.92884900 | -3.43940600 | -0.40503200 | H | 0.16910000  | 1.59677400  | 5.67656700  |
| H | -4.74604000 | -4.15276700 | -0.46610200 | H | -1.15987500 | 0.45809900  | 5.98012500  |
| C | -3.44351200 | -3.04971600 | 0.85573700  | C | -1.10603000 | -5.17814100 | 1.62083900  |
| C | -3.98508200 | -3.56362600 | 2.07296800  | H | -2.16530100 | -5.34896900 | 1.82163400  |
| H | -4.79992300 | -4.27952600 | 2.01678400  | H | -0.84490600 | -5.65113500 | 0.67190900  |
| C | -3.49272000 | -3.17028600 | 3.27178900  | H | -0.51436200 | -5.63330700 | 2.41722700  |
| H | -3.90311900 | -3.56524800 | 4.19646900  |   |             |             |             |
| C | -2.42368900 | -2.22629900 | 3.34868700  |   |             |             |             |
| C | -1.86816700 | -1.68764400 | 2.16635900  |   |             |             |             |
| C | -2.38238000 | -2.11803600 | 0.89107200  |   |             |             |             |
| C | -1.88849200 | -1.80124000 | 4.57711800  |   |             |             |             |

|                                                                           |             |             |             |                                                                           |                                     |
|---------------------------------------------------------------------------|-------------|-------------|-------------|---------------------------------------------------------------------------|-------------------------------------|
| H                                                                         | -2.29430800 | -2.19863500 | 5.50322500  |                                                                           |                                     |
| C                                                                         | -0.86063400 | -0.89316300 | 4.58579700  |                                                                           |                                     |
| H                                                                         | -0.41780900 | -0.54308300 | 5.51124300  |                                                                           |                                     |
| C                                                                         | -0.38073500 | -0.40749400 | 3.36275200  |                                                                           |                                     |
| H                                                                         | 0.42722300  | 0.31744300  | 3.33220400  |                                                                           |                                     |
| Cm(S <sub>2</sub> CNEt <sub>2</sub> ) <sub>3</sub> ((MeCN) <sub>2</sub> ) |             |             |             | Cf(S <sub>2</sub> CNEt <sub>2</sub> ) <sub>3</sub> ((MeCN) <sub>2</sub> ) |                                     |
| Cm                                                                        | -0.00142900 | -0.27252800 | 0.35324400  | Cf                                                                        | -0.00064000 -0.25674100 0.31161000  |
| S                                                                         | -1.71298200 | -1.65066300 | -1.50516000 | S                                                                         | -1.68937400 -1.65291400 -1.49784600 |
| S                                                                         | -2.79254300 | -0.41551700 | 0.97334900  | S                                                                         | -2.75436000 -0.36667000 0.95434300  |
| N                                                                         | -4.31074000 | -1.27504400 | -1.04212800 | N                                                                         | -4.28755700 -1.28440000 -1.02566800 |
| C                                                                         | -3.06063600 | -1.13357900 | -0.57222300 | C                                                                         | -3.03543900 -1.12223100 -0.56856400 |
| C                                                                         | -5.48078400 | -0.85133500 | -0.28035500 | C                                                                         | -5.45388000 -0.84704200 -0.26604400 |
| H                                                                         | -5.27046000 | -0.98835400 | 0.78068500  | H                                                                         | -5.23402700 -0.95458200 0.79649800  |
| H                                                                         | -6.29826100 | -1.53107800 | -0.54191900 | H                                                                         | -6.26971600 -1.53782200 -0.50262000 |
| C                                                                         | -5.86884700 | 0.59108600  | -0.56175600 | C                                                                         | -5.85189300 0.58537000 -0.58251500  |
| H                                                                         | -6.76607700 | 0.86028600  | 0.00331300  | H                                                                         | -6.74569400 0.86517500 -0.01717200  |
| H                                                                         | -5.06223300 | 1.26425300  | -0.26572000 | H                                                                         | -5.04625600 1.27010700 -0.31139900  |
| H                                                                         | -6.08007000 | 0.75129300  | -1.62308500 | H                                                                         | -6.07284200 0.71609300 -1.64590800  |
| C                                                                         | -4.58427200 | -1.83338600 | -2.36211500 | C                                                                         | -4.56680900 -1.87899800 -2.32832400 |
| H                                                                         | -3.75713200 | -1.57395200 | -3.02334000 | H                                                                         | -3.74523100 -1.63329400 -3.00169500 |
| H                                                                         | -5.47889000 | -1.33194800 | -2.74457800 | H                                                                         | -5.46629600 -1.39236100 -2.71846800 |
| C                                                                         | -4.78684700 | -3.33930400 | -2.32917100 | C                                                                         | -4.76151300 -3.38451400 -2.25407600 |
| H                                                                         | -5.02673200 | -3.71258300 | -3.32898500 | H                                                                         | -5.00591100 -3.78552200 -3.24199400 |
| H                                                                         | -3.87603500 | -3.83642300 | -1.98980500 | H                                                                         | -3.84600700 -3.86791000 -1.90753200 |
| H                                                                         | -5.60560500 | -3.62136300 | -1.66029100 | H                                                                         | -5.57449900 -3.65267200 -1.57256200 |
| S                                                                         | -0.08909100 | 2.45616200  | 1.29377400  | S                                                                         | -0.08932300 2.41313400 1.30786800   |
| S                                                                         | 0.02839500  | 1.79725800  | -1.59522200 | S                                                                         | 0.01598000 1.79475400 -1.58338200   |
| N                                                                         | -0.07889300 | 4.28545600  | -0.64710100 | N                                                                         | -0.08466400 4.27332100 -0.60558700  |
| C                                                                         | -0.04938900 | 2.97795300  | -0.34542100 | C                                                                         | -0.05563800 2.96280400 -0.32014600  |
| C                                                                         | -0.13033100 | 5.31827200  | 0.38141600  | C                                                                         | -0.13270000 5.29189200 0.43723200   |
| H                                                                         | 0.41699400  | 6.18457400  | -0.00376700 | H                                                                         | 0.41385400 6.16328600 0.06265800    |
| H                                                                         | 0.40744800  | 4.95739600  | 1.25859500  | H                                                                         | 0.40762600 4.91846200 1.30766300    |
| C                                                                         | -1.55399700 | 5.70206300  | 0.75069800  | C                                                                         | -1.55520200 5.67065900 0.81598900   |
| H                                                                         | -1.55115700 | 6.49869000  | 1.50057100  | H                                                                         | -1.54993300 6.45609900 1.57752600   |
| H                                                                         | -2.11197000 | 6.06234000  | -0.11863400 | H                                                                         | -2.11532800 6.04396500 -0.04642400  |
| H                                                                         | -2.08233300 | 4.84183700  | 1.16619400  | H                                                                         | -2.08286500 4.80466100 1.22021200   |
| C                                                                         | -0.06220400 | 4.76409400  | -2.02562200 | C                                                                         | -0.07093800 4.76901500 -1.97804000  |
| H                                                                         | -0.64580100 | 5.68990100  | -2.05185000 | H                                                                         | -0.65446300 5.69510700 -1.99163400  |
| H                                                                         | -0.57971000 | 4.03528700  | -2.64990700 | H                                                                         | -0.59028700 4.04827000 -2.61019200  |
| C                                                                         | 1.34698800  | 5.00137600  | -2.54318900 | C                                                                         | 1.33716300 5.01232600 -2.49581100   |
| H                                                                         | 1.31577100  | 5.38979700  | -3.56530800 | H                                                                         | 1.30372100 5.41314000 -3.51304900   |
| H                                                                         | 1.88650900  | 5.72533600  | -1.92520400 | H                                                                         | 1.87810600 5.72865500 -1.87026600   |
| H                                                                         | 1.91005200  | 4.06625700  | -2.55045600 | H                                                                         | 1.90029500 4.07741800 -2.51568000   |
| S                                                                         | 2.75632000  | -0.31122600 | 1.11671000  | S                                                                         | 2.71868500 -0.25375200 1.09227800   |
| S                                                                         | 1.85453100  | -1.57863900 | -1.41607100 | S                                                                         | 1.83351500 -1.57431800 -1.41283300  |
| N                                                                         | 4.40796900  | -1.09744800 | -0.82207800 | N                                                                         | 4.38690900 -1.10062800 -0.80831100  |
| C                                                                         | 3.13109800  | -1.01044100 | -0.41512400 | C                                                                         | 3.10754000 -0.99189500 -0.41524500  |
| C                                                                         | 5.51958100  | -0.62901400 | -0.00122400 | C                                                                         | 5.49404400 -0.61896900 0.01081700   |
| H                                                                         | 6.37706300  | -1.27231400 | -0.22391200 | H                                                                         | 6.34872100 -1.27442000 -0.18571500  |
| H                                                                         | 5.26266800  | -0.78058400 | 1.04750900  | H                                                                         | 5.22523900 -0.74039100 1.06053300   |
| C                                                                         | 5.85984300  | 0.82999600  | -0.25785900 | C                                                                         | 5.84807500 0.83009200 -0.28116500   |
| H                                                                         | 6.71620000  | 1.13324000  | 0.35163400  | H                                                                         | 6.70056700 1.14324200 0.32872700    |
| H                                                                         | 6.11596000  | 1.00491600  | -1.30692300 | H                                                                         | 6.11597000 0.97503200 -1.33186300   |
| H                                                                         | 5.01215800  | 1.46714400  | 0.00080200  | H                                                                         | 5.00271600 1.48008400 -0.04811200   |
| C                                                                         | 4.77050300  | -1.63796900 | -2.12797600 | C                                                                         | 4.75645000 -1.67851100 -2.09593300  |
| H                                                                         | 5.66159900  | -1.09817400 | -2.46357000 | H                                                                         | 5.65403500 -1.15412700 -2.43866000  |
| H                                                                         | 3.96761300  | -1.41007100 | -2.82949600 | H                                                                         | 3.96103300 -1.46407700 -2.81018200  |

|                                                                           |             |             |             |                                                                           |             |             |             |
|---------------------------------------------------------------------------|-------------|-------------|-------------|---------------------------------------------------------------------------|-------------|-------------|-------------|
| C                                                                         | 5.03362700  | -3.13435100 | -2.08853700 | C                                                                         | 5.00853600  | -3.17510700 | -2.01427400 |
| H                                                                         | 5.33840800  | -3.49290900 | -3.07598700 | H                                                                         | 5.31886600  | -3.56223300 | -2.98913300 |
| H                                                                         | 5.82901700  | -3.38526800 | -1.38020700 | H                                                                         | 5.79621800  | -3.41240700 | -1.29277000 |
| H                                                                         | 4.12847300  | -3.67027600 | -1.79636300 | H                                                                         | 4.09713700  | -3.69661000 | -1.71544700 |
| N                                                                         | 0.02367200  | -2.75407800 | 1.26157300  | N                                                                         | 0.02834400  | -2.68408200 | 1.25994500  |
| N                                                                         | -0.07031900 | -0.19756700 | 2.98399000  | N                                                                         | -0.06694600 | -0.21620900 | 2.89666900  |
| C                                                                         | -0.10285700 | 0.02763000  | 4.10946500  | C                                                                         | -0.09879700 | -0.03956900 | 4.03078200  |
| C                                                                         | -0.14384900 | 0.32981500  | 5.52308400  | C                                                                         | -0.13899000 | 0.20195700  | 5.45626300  |
| H                                                                         | 0.74430800  | -0.06716500 | 6.01823300  | H                                                                         | 0.74985200  | -0.21469100 | 5.93381100  |
| H                                                                         | -0.17496800 | 1.41157800  | 5.66665100  | H                                                                         | -0.17109300 | 1.27643800  | 5.64676100  |
| H                                                                         | -1.03263800 | -0.11282700 | 5.97663400  | H                                                                         | -1.02694000 | -0.26034800 | 5.89158400  |
| C                                                                         | 0.04352300  | -3.89988800 | 1.32621200  | C                                                                         | 0.04951800  | -3.82727000 | 1.36004100  |
| C                                                                         | 0.06933100  | -5.34472400 | 1.36872100  | C                                                                         | 0.07699100  | -5.27025800 | 1.44554500  |
| H                                                                         | 0.96318600  | -5.69184200 | 1.89029200  | H                                                                         | 0.97056000  | -5.60071500 | 1.97835700  |
| H                                                                         | -0.81452100 | -5.72405500 | 1.88487600  | H                                                                         | -0.80689200 | -5.63521200 | 1.97195900  |
| H                                                                         | 0.07957800  | -5.73727900 | 0.34984000  | H                                                                         | 0.08885100  | -5.69346000 | 0.43901200  |
| Eu(S <sub>2</sub> CNEt <sub>2</sub> ) <sub>3</sub> ((MeCN) <sub>2</sub> ) |             |             |             | Gd(S <sub>2</sub> CNEt <sub>2</sub> ) <sub>3</sub> ((MeCN) <sub>2</sub> ) |             |             |             |
| Eu                                                                        | -0.12755700 | -0.28440100 | 0.43353800  | Gd                                                                        | -0.00128700 | -0.30752100 | 0.38136800  |
| S                                                                         | -1.96359600 | -1.19742600 | -1.56540900 | S                                                                         | -1.67929700 | -1.67324200 | -1.46456600 |
| S                                                                         | 0.14654600  | 2.45642200  | 1.25560900  | S                                                                         | -2.76043600 | -0.38504300 | 0.97963600  |
| S                                                                         | -2.91844200 | 0.14451700  | 0.89942100  | N                                                                         | -4.27802900 | -1.27659000 | -1.02300600 |
| S                                                                         | 1.37923100  | -2.12977300 | -1.17916000 | C                                                                         | -3.02895400 | -1.13261000 | -0.55086000 |
| S                                                                         | 2.57769000  | -0.79671200 | 1.18643200  | C                                                                         | -5.44856100 | -0.83131100 | -0.27471300 |
| S                                                                         | 0.69230100  | 1.60530000  | -1.52123900 | H                                                                         | -5.24306400 | -0.94799200 | 0.78976400  |
| N                                                                         | -4.48861500 | -0.43695500 | -1.17480900 | H                                                                         | -6.26877600 | -1.51190300 | -0.52536200 |
| N                                                                         | -0.72908400 | -2.63039800 | 1.43143400  | C                                                                         | -5.82814300 | 0.60714300  | -0.58650100 |
| N                                                                         | 1.10365200  | 4.08371200  | -0.63006500 | H                                                                         | -6.72657700 | 0.89197000  | -0.03106200 |
| N                                                                         | -0.22600000 | -0.10210800 | 3.04922700  | H                                                                         | -5.01955700 | 1.28217700  | -0.30033600 |
| N                                                                         | 4.00416400  | -1.94660600 | -0.75007700 | H                                                                         | -6.03372200 | 0.74717100  | -1.65177900 |
| C                                                                         | -3.24742000 | -0.49740100 | -0.66482100 | C                                                                         | -4.54833700 | -1.85834700 | -2.33335000 |
| C                                                                         | -5.60368100 | 0.14753800  | -0.43826400 | H                                                                         | -3.71658600 | -1.61588300 | -2.99535000 |
| H                                                                         | -5.44886700 | -0.03659200 | 0.62544400  | H                                                                         | -5.43822800 | -1.35944200 | -2.72993600 |
| H                                                                         | -6.50633800 | -0.39604200 | -0.73589100 | C                                                                         | -4.75951100 | -3.36227500 | -2.27305200 |
| C                                                                         | 2.77405300  | -1.66114400 | -0.29304600 | H                                                                         | -4.99632000 | -3.75317300 | -3.26685900 |
| C                                                                         | -4.79989500 | -0.92483400 | -2.51399000 | H                                                                         | -3.85329600 | -3.85791900 | -1.91951500 |
| H                                                                         | -3.92182200 | -0.78287500 | -3.14471700 | H                                                                         | -5.58331100 | -3.62705000 | -1.60327800 |
| H                                                                         | -5.59523900 | -0.28702200 | -2.91238400 | S                                                                         | -0.09234000 | 2.37788600  | 1.34983200  |
| C                                                                         | 0.69111300  | 2.84236400  | -0.32997400 | S                                                                         | 0.01909000  | 1.72975700  | -1.53692000 |
| C                                                                         | 5.21119300  | -1.55927500 | -0.02814000 | N                                                                         | -0.08984800 | 4.21591000  | -0.58315300 |
| H                                                                         | 5.96761700  | -2.32420800 | -0.23179400 | C                                                                         | -0.05748800 | 2.90749300  | -0.28480800 |
| H                                                                         | 4.99897100  | -1.58803200 | 1.04092000  | C                                                                         | -0.14113400 | 5.24513700  | 0.44873700  |
| C                                                                         | 5.71437300  | -0.18279600 | -0.43160000 | H                                                                         | 0.40335800  | 6.11405200  | 0.06537100  |
| H                                                                         | 6.63346200  | 0.05992000  | 0.10990300  | H                                                                         | 0.39975200  | 4.88259400  | 1.32341900  |
| H                                                                         | 4.96605900  | 0.57627900  | -0.19605800 | C                                                                         | -1.56475500 | 5.62455000  | 0.82286400  |
| H                                                                         | 5.93219500  | -0.13209800 | -1.50246200 | H                                                                         | -1.56189900 | 6.41807400  | 1.57604300  |
| C                                                                         | 4.21901600  | -2.63255900 | -2.01973600 | H                                                                         | -2.12529700 | 5.98731800  | -0.04379000 |
| H                                                                         | 5.15123200  | -2.24412500 | -2.44178900 | H                                                                         | -2.09051600 | 4.76153500  | 1.23583000  |
| H                                                                         | 3.41296700  | -2.35634100 | -2.70001100 | C                                                                         | -0.07716800 | 4.69813800  | -1.96029100 |
| C                                                                         | -5.22855100 | -2.38303400 | -2.51998500 | H                                                                         | -0.66253300 | 5.62293700  | -1.98300900 |
| H                                                                         | -5.48934800 | -2.69866300 | -3.53431800 | H                                                                         | -0.59510200 | 3.97033800  | -2.58548600 |
| H                                                                         | -6.10197700 | -2.54885800 | -1.88199300 | C                                                                         | 1.33026000  | 4.93951000  | -2.48090000 |
| H                                                                         | -4.41469000 | -3.01817100 | -2.16483300 | H                                                                         | 1.29573200  | 5.33096500  | -3.50177500 |
| C                                                                         | 1.56359600  | 4.44309800  | -1.96723100 | H                                                                         | 1.87002100  | 5.66255200  | -1.86205700 |
| H                                                                         | 1.29096300  | 5.49050200  | -2.13143100 | H                                                                         | 1.89512400  | 4.00551900  | -2.49240000 |
| H                                                                         | 1.01179700  | 3.84611200  | -2.69394600 | S                                                                         | 2.72338200  | -0.26891500 | 1.12210400  |
| C                                                                         | 3.06024900  | 4.24240100  | -2.14090700 | S                                                                         | 1.82748800  | -1.59401100 | -1.37682500 |
| H                                                                         | 3.37108200  | 4.54864400  | -3.14398300 | N                                                                         | 4.37963900  | -1.08033600 | -0.80289100 |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | 3.31867500  | 3.18986800  | -2.00958600 | C | 3.10296800  | -0.99632600 | -0.39426400 |
| H | 3.63206500  | 4.83145800  | -1.41763000 | C | 5.48893400  | -0.58555400 | 0.00525500  |
| C | -0.17558300 | 5.94365500  | 0.39031400  | H | 6.35152500  | -1.22593500 | -0.20594100 |
| H | -0.10997800 | 6.75676700  | 1.11931700  | H | 5.23573200  | -0.71779200 | 1.05756800  |
| H | -1.00595700 | 5.29462400  | 0.67488500  | C | 5.81644200  | 0.87074800  | -0.28177200 |
| H | -0.40194600 | 6.38519900  | -0.58468100 | H | 6.67228000  | 1.19312000  | 0.31858900  |
| C | -5.76073700 | 1.63652800  | -0.70038000 | H | 6.06771500  | 1.02657700  | -1.33500400 |
| H | -6.62504100 | 2.02907500  | -0.15660100 | H | 4.96450700  | 1.50618900  | -0.03316000 |
| H | -5.91095000 | 1.84421900  | -1.76386600 | C | 4.74260000  | -1.64244500 | -2.09934900 |
| H | -4.87213000 | 2.17524500  | -0.36643200 | H | 5.62746100  | -1.10113800 | -2.44877700 |
| C | 1.12372800  | 5.15544700  | 0.35855200  | H | 3.93520200  | -1.43522700 | -2.80222400 |
| H | 1.96694000  | 5.80785700  | 0.10996700  | C | 5.01972800  | -3.13535400 | -2.03244100 |
| H | 1.32895600  | 4.71791000  | 1.33613700  | H | 5.32394200  | -3.51005200 | -3.01406600 |
| C | 4.29015600  | -4.14263600 | -1.86298200 | H | 5.82017400  | -3.36530200 | -1.32268100 |
| H | 4.48884300  | -4.61635700 | -2.82874700 | H | 4.12073900  | -3.67386200 | -1.72630700 |
| H | 3.34253700  | -4.52909800 | -1.48274500 | N | 0.03282500  | -2.74948900 | 1.27035800  |
| H | 5.08640000  | -4.43910900 | -1.17348500 | N | -0.07019900 | -0.27660900 | 2.97802300  |
| C | -0.97994500 | -3.74173000 | 1.56946400  | C | -0.10394500 | -0.07569400 | 4.10795600  |
| C | -0.21429800 | 0.15090700  | 4.16914700  | C | -0.14666800 | 0.19700100  | 5.52761600  |
| C | -0.19201500 | 0.48865700  | 5.57516300  | H | 0.73959500  | -0.21210800 | 6.01627300  |
| H | 0.48451900  | -0.17890000 | 6.11205400  | H | -0.17540000 | 1.27560500  | 5.69373800  |
| H | 0.15256100  | 1.51695600  | 5.70058400  | H | -1.03735400 | -0.25248200 | 5.97062800  |
| H | -1.19353100 | 0.39740600  | 5.99969100  | C | 0.06116100  | -3.89123200 | 1.38178100  |
| C | -1.28971800 | -5.14725400 | 1.70706500  | C | 0.09845500  | -5.33292300 | 1.48444400  |
| H | -2.35613000 | -5.28124900 | 1.89784400  | H | 0.93244500  | -5.64655900 | 2.11503000  |
| H | -1.02704400 | -5.66953000 | 0.78481600  | H | -0.83302500 | -5.70522800 | 1.91491700  |
| H | -0.72307500 | -5.58189400 | 2.53260000  | H | 0.22538300  | -5.76531300 | 0.48984000  |