

*Electronic Supplementary Information (ESI)*

**Binding Affinity of Pyridines with Am<sup>III</sup>/Cm<sup>III</sup> Elucidated by Density  
Functional Theory Calculations**

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**Table S1** The average  $M^n-O(H_2O)/M^n-O(ONO_2)$  distance( $\text{\AA}$ ) and the CN of  $M(H_2O)_{9-2x}(NO_3)_x^{3-x}$ , and the WBIs of  $M^n-O(H_2O)/M^n-O(ONO_2)$  of  $M(H_2O)_{9-2x}(NO_3)_x^{3-x}$ .

|                       | $M(H_2O)_9^{3+}$ | $M(H_2O)_7(NO_3)_2^{2+}$ | $M(H_2O)_5(NO_3)_2^{2+}$ | $M(H_2O)_3(NO_3)_3^{3-}$ |
|-----------------------|------------------|--------------------------|--------------------------|--------------------------|
| Bond ( $Am^n-OH_2$ )  | 2.539            | 2.542                    | 2.590                    | 2.546                    |
| Bond ( $Cm^n-OH_2$ )  | 2.526            | 2.528                    | 2.621                    | 2.547                    |
| Bond ( $Am^n-ONO_2$ ) | -                | 2.504                    | 2.538                    | 2.542                    |
| Bond ( $Cm^n-ONO_2$ ) | -                | 2.528                    | 2.543                    | 2.546                    |
| CN ( $Am^n$ )         | 7.849            | 7.861                    | 7.763                    | 7.842                    |
| CN ( $Cm^n$ )         | 7.877            | 7.871                    | 7.776                    | 7.836                    |
| WBI ( $Am^n-OH_2$ )   | -                | 0.265                    | 0.235                    | 0.268                    |
| WBI ( $Cm^n-OH_2$ )   | -                | 0.267                    | 0.229                    | 0.245                    |
| WBI ( $Am^n-ONO_2$ )  | 0.263            | 0.276                    | 0.264                    | 0.270                    |
| WBI ( $Cm^n-ONO_2$ )  | 0.261            | 0.258                    | 0.248                    | 0.259                    |

**Table S2.** Electron density  $\rho(r)$ , Laplacian  $\nabla^2\rho(r)$ , total electronic energy  $E_b$ , kinetic energy density  $G_b$ , potential energy density  $V_b$ , and  $G_b/\rho(r)$  of M-N bond critical point of  $[M(H_2O)_{8-2x}(NO_3)_x(L_n)]^{3-x}$  ( $x=0-3$ ).

| $[M(H_2O)_8(L_n)]^{3+}$       |      | $L_1$     | $L_2$    | $L_3$     | $L_4$     | $L_5$     | $L_6$    | $L_7$    |
|-------------------------------|------|-----------|----------|-----------|-----------|-----------|----------|----------|
| $\rho(r)$                     | Am-N | 0.041     | 0.022    | 0.037     | 0.048     | 0.036     | 0.030    | 0.020    |
|                               | Cm-N | 0.041     | 0.027    | 0.035     | 0.044     | 0.032     | 0.029    | 0.021    |
| $\nabla^2\rho(r)$             | Am-N | 0.120     | 0.065    | 0.106     | 0.143     | 0.108     | 0.088    | 0.059    |
|                               | Cm-N | 0.123     | 0.080    | 0.102     | 0.131     | 0.096     | 0.087    | 0.062    |
| $E_b$                         | Am-N | -2.33     | 4.74     | -1.59     | -4.16     | -1.32     | -4.66    | 5.24     |
|                               |      | E-03      | E-04     | E-03      | E-03      | E-03      | E-04     | E-04     |
|                               | Cm-N | -2.44     | 1.56     | -1.39     | -2.93     | -5.59     | -4.66    | 5.15     |
| $G_b$                         |      | E-03      | E-04     | E-03      | E-03      | E-04      | E-04     | E-04     |
|                               | Am-N | 0.032     | 0.016    | 0.028     | 0.040     | 0.028     | 0.023    | 0.014    |
|                               | Cm-N | 0.033     | 0.020    | 0.027     | 0.036     | 0.025     | 0.023    | 0.015    |
| $-V_b$                        | Am-N | 0.035     | 0.015    | 0.030     | 0.044     | 0.030     | 0.023    | 0.014    |
|                               | Cm-N | 0.036     | 0.020    | 0.028     | 0.039     | 0.025     | 0.023    | 0.015    |
| $G_b/\rho(r)$                 | Am-N | 0.791     | 0.719    | 0.756     | 0.831     | 0.790     | 0.750    | 0.710    |
|                               | Cm-N | 0.810     | 0.733    | 0.805     | 0.876     | 0.785     | 0.792    | 0.692    |
| $[M(H_2O)_6(NO_3)(L_n)]^{2+}$ |      | $L_1$     | $L_2$    | $L_3$     | $L_4$     | $L_5$     | $L_6$    | $L_7$    |
| $\rho(r)$                     | Am-N | 0.035     | 0.022    | 0.036     | 0.042     | 0.029     | 0.022    | 0.022    |
|                               | Cm-N | 0.035     | 0.022    | 0.037     | 0.038     | 0.029     | 0.024    | 0.022    |
| $\nabla^2\rho(r)$             | Am-N | 0.102     | 0.065    | 0.106     | 0.123     | 0.088     | 0.063    | 0.065    |
|                               | Cm-N | 0.106     | 0.065    | 0.111     | 0.115     | 0.089     | 0.069    | 0.065    |
| $E_b$                         | Am-N | -1.14E-03 | 5.33E-04 | -1.56E-03 | -2.39E-03 | -2.23E-04 | 4.18E-04 | 4.45E-04 |
|                               |      |           |          |           |           |           |          |          |
|                               | Cm-N | -1.15E-03 | 6.22E-04 | -1.69E-03 | -1.73E-03 | -1.90E-04 | 2.84E-04 | 5.70E-04 |
| $G_b$                         |      |           |          |           |           |           |          |          |
|                               | Am-N | 0.027     | 0.016    | 0.028     | 0.033     | 0.022     | 0.015    | 0.016    |
|                               | Cm-N | 0.028     | 0.016    | 0.029     | 0.03      | 0.023     | 0.017    | 0.016    |
| $-V_b$                        | Am-N | 0.028     | 0.015    | 0.03      | 0.036     | 0.023     | 0.015    | 0.015    |
|                               | Cm-N | 0.029     | 0.015    | 0.031     | 0.032     | 0.023     | 0.017    | 0.015    |
| $G_b/\rho(r)$                 | Am-N | 0.763     | 0.719    | 0.777     | 0.790     | 0.768     | 0.700    | 0.721    |

|                              | Cm-N           | 0.789          | 0.708          | 0.796          | 0.800          | 0.776          | 0.709          | 0.708    |
|------------------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------|
| $[M(H_2O)_4(NO_3)_2(L_n)]^+$ | L <sub>1</sub> | L <sub>2</sub> | L <sub>3</sub> | L <sub>4</sub> | L <sub>5</sub> | L <sub>6</sub> | L <sub>7</sub> |          |
| $\rho(r)$                    | Am-N           | 0.034          | 0.024          | 0.023          | 0.038          | 0.031          | 0.023          | 0.020    |
|                              | Cm-N           | 0.033          | 0.022          | 0.020          | 0.034          | 0.030          | 0.022          | 0.020    |
| $\nabla^2\rho(r)$            | Am-N           | 0.104          | 0.074          | 0.066          | 0.114          | 0.096          | 0.067          | 0.062    |
|                              | Cm-N           | 0.099          | 0.068          | 0.058          | 0.103          | 0.09           | 0.065          | 0.059    |
| $E_b$                        | Am-N           | -8.86E-04      | 5.34E-04       | -2.95E-04      | -1.55E-03      | -1.74E-04      | 4.54E-04       | 7.16E-04 |
|                              | Cm-N           | -6.54E-04      | 7.09E-04       | -5.83E-04      | -9.18E-04      | -1.74E-04      | 5.73E-04       | 8.03E-04 |
| $G_b$                        | Am-N           | 0.027          | 0.018          | 0.016          | 0.030          | 0.023          | 0.016          | 0.015    |
|                              | Cm-N           | 0.025          | 0.016          | 0.014          | 0.027          | 0.023          | 0.016          | 0.014    |
| $-V_b$                       | Am-N           | 0.028          | 0.017          | 0.016          | 0.032          | 0.023          | 0.016          | 0.014    |
|                              | Cm-N           | 0.026          | 0.016          | 0.013          | 0.028          | 0.023          | 0.015          | 0.013    |
| $G_b/\rho(r)$                | Am-N           | 0.787          | 0.745          | 0.704          | 0.792          | 0.734          | 0.709          | 0.737    |
|                              | Cm-N           | 0.768          | 0.740          | 0.690          | 0.786          | 0.759          | 0.708          | 0.700    |
| $M(H_2O)_2(NO_3)_3(L_n)$     | L <sub>1</sub> | L <sub>2</sub> | L <sub>3</sub> | L <sub>4</sub> | L <sub>5</sub> | L <sub>6</sub> | L <sub>7</sub> |          |
| $\rho(r)$                    | Am-N           | 0.041          | 0.024          | 0.032          | 0.040          | 0.039          | 0.022          | 0.020    |
|                              | Cm-N           | 0.036          | 0.025          | 0.029          | 0.041          | 0.041          | 0.025          | 0.019    |
| $\nabla^2\rho(r)$            | Am-N           | 0.128          | 0.075          | 0.098          | 0.127          | 0.126          | 0.066          | 0.060    |
|                              | Cm-N           | 0.111          | 0.076          | 0.087          | 0.127          | 0.132          | 0.072          | 0.059    |
| $E_b$                        | Am-N           | -2.02E-03      | 5.12E-04       | -7.03E-04      | -1.99E-03      | -1.99E-03      | 4.51E-04       | 6.64E-04 |
|                              | Cm-N           | -1.19E-03      | 5.36E-04       | -2.69E-04      | -2.04E-03      | -2.21E-03      | 2.93E-04       | 7.91E-04 |
| $G_b$                        | Am-N           | 0.034          | 0.018          | 0.025          | 0.034          | 0.034          | 0.016          | 0.014    |
|                              | Cm-N           | 0.029          | 0.019          | 0.022          | 0.034          | 0.035          | 0.019          | 0.014    |
| $-V_b$                       | Am-N           | 0.036          | 0.018          | 0.026          | 0.036          | 0.036          | 0.016          | 0.014    |
|                              | Cm-N           | 0.030          | 0.018          | 0.022          | 0.036          | 0.037          | 0.018          | 0.013    |
| $G_b/\rho(r)$                | Am-N           | 0.827          | 0.756          | 0.786          | 0.840          | 0.860          | 0.726          | 0.716    |
|                              | Cm-N           | 0.805          | 0.743          | 0.763          | 0.822          | 0.857          | 0.740          | 0.729    |

**Table S3.** Electron density  $\rho(r)$  of M-O bond critical point of  $[M(H_2O)_{8-2x}(NO_3)_x(L_n)]^{3-x}$  ( $x=0-3$ ).

|                                       |                |                |                |                |                |                |                |       |
|---------------------------------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|-------|
| $\rho(r)-[M(H_2O)_8(L_n)]^{3+}$       | L <sub>1</sub> | L <sub>2</sub> | L <sub>3</sub> | L <sub>4</sub> | L <sub>5</sub> | L <sub>6</sub> | L <sub>7</sub> |       |
| $M^0-OH_2$                            | Am-O           | 0.041          | 0.041          | 0.041          | 0.041          | 0.041          | 0.041          | 0.040 |
|                                       | Cm-O           | 0.040          | 0.040          | 0.041          | 0.041          | 0.041          | 0.040          | 0.039 |
| $\rho(r)-[M(H_2O)_6(NO_3)(L_n)]^{2+}$ | L <sub>1</sub> | L <sub>2</sub> | L <sub>3</sub> | L <sub>4</sub> | L <sub>5</sub> | L <sub>6</sub> | L <sub>7</sub> |       |
| $M^1-OH_2$                            | Am-O           | 0.040          | 0.039          | 0.041          | 0.041          | 0.042          | 0.041          | 0.038 |
|                                       | Cm-O           | 0.040          | 0.040          | 0.042          | 0.041          | 0.043          | 0.041          | 0.041 |
| $M^1-ONO_2$                           | Am-O           | 0.047          | 0.046          | 0.047          | 0.046          | 0.047          | 0.048          | 0.048 |
|                                       | Cm-O           | 0.043          | 0.045          | 0.044          | 0.044          | 0.044          | 0.044          | 0.044 |
| $\rho(r)-[M(H_2O)_4(NO_3)_2(L_n)]^+$  | L <sub>1</sub> | L <sub>2</sub> | L <sub>3</sub> | L <sub>4</sub> | L <sub>5</sub> | L <sub>6</sub> | L <sub>7</sub> |       |
| $M^2-OH_2$                            | Am-O           | 0.037          | 0.037          | 0.035          | 0.037          | 0.036          | 0.036          | 0.037 |
|                                       | Cm-O           | 0.036          | 0.036          | 0.036          | 0.036          | 0.035          | 0.036          | 0.037 |

|                                                                                                 |      |                |                |                |                |                |                |                |
|-------------------------------------------------------------------------------------------------|------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| M <sup>2</sup> -ONO <sub>2</sub>                                                                | Am-O | 0.044          | 0.045          | 0.044          | 0.044          | 0.044          | 0.045          | 0.045          |
|                                                                                                 | Cm-O | 0.043          | 0.044          | 0.042          | 0.043          | 0.043          | 0.044          | 0.044          |
| $\rho(r)$ -[M(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>n</sub> )] |      | L <sub>1</sub> | L <sub>2</sub> | L <sub>3</sub> | L <sub>4</sub> | L <sub>5</sub> | L <sub>6</sub> | L <sub>7</sub> |
| M <sup>3</sup> -OH <sub>2</sub>                                                                 | Am-O | 0.042          | 0.041          | 0.043          | 0.042          | 0.041          | 0.042          | 0.044          |
|                                                                                                 | Cm-O | 0.043          | 0.041          | 0.043          | 0.043          | 0.040          | 0.042          | 0.044          |
| M <sup>3</sup> -ONO <sub>2</sub>                                                                | Am-O | 0.044          | 0.045          | 0.044          | 0.044          | 0.044          | 0.044          | 0.045          |
|                                                                                                 | Cm-O | 0.042          | 0.043          | 0.043          | 0.042          | 0.042          | 0.043          | 0.044          |

**Table S4** The Gibbs free energy changes for the incorporation of nitrate ions on hydrated americium and curium structures. (in kJ/mol).

| reaction                                                                     | Am    | Cm    |
|------------------------------------------------------------------------------|-------|-------|
| $M(H_2O)_9^{3+} + NO_3^- \rightarrow M(H_2O)_7(NO_3)_2^{2+} + 2H_2O$         | -71.9 | -70.5 |
| $M(H_2O)_7(NO_3)_2^{2+} + NO_3^- \rightarrow M(H_2O)_5(NO_3)_2^{2+} + 2H_2O$ | -51.6 | -42.4 |
| $M(H_2O)_5(NO_3)_2^{2+} + NO_3^- \rightarrow M(H_2O)_3(NO_3)_3 + 2H_2O$      | -64.1 | -65.2 |

**Table S5.** The Gibbs free energy changes for the ligand exchange reaction with L<sub>5</sub>/L<sub>8</sub> (in kJ/mol)

| L <sub>8</sub> | $\Delta G_{mx}^{M0}$ | $\Delta G_{mx}^{M1}$ | $\Delta G_{mx}^{M2}$ | $\Delta G_{mx}^{M3}$ |
|----------------|----------------------|----------------------|----------------------|----------------------|
| Am             | 22.2                 | 16.8                 | 11.8                 | 2.6                  |
| Cm             | 21.7                 | 14.8                 | 11.0                 | 0.0                  |
| L <sub>5</sub> | $\Delta G_{mx}^{M0}$ | $\Delta G_{mx}^{M1}$ | $\Delta G_{mx}^{M2}$ | $\Delta G_{mx}^{M3}$ |
| Am             | 26.8                 | 19.7                 | 16.5                 | 4.3                  |
| Cm             | 24.4                 | 16.9                 | 14.9                 | 3.0                  |

**Table S6.** The Gibbs free energy changes for the ligand exchange reaction of [Am(NO<sub>3</sub>)<sub>x</sub>(H<sub>2</sub>O)<sub>8-2x</sub>(L<sub>n</sub>)]<sup>3-x</sup> (x=1-3) with L<sub>4</sub> in the presence or absence of Na<sup>+</sup> (in kJ/mol, Na<sup>+</sup>:NO<sub>3</sub><sup>-</sup>=1:1)

| L <sub>4</sub>          | $\Delta G_{mx}^{Am1}$ | $\Delta G_{mx}^{Am2}$ | $\Delta G_{mx}^{Am3}$ |
|-------------------------|-----------------------|-----------------------|-----------------------|
| without Na <sup>+</sup> | 12.4                  | 12.3                  | 1.2                   |
| with Na <sup>+</sup>    | 7.7                   | 3.2                   | 0.8                   |

**Table S7.** The Gibbs free energy changes for the ligand exchange reaction with or without TEDGA (in kJ/mol).

|                  |                             |                |                |                |                |                |                |
|------------------|-----------------------------|----------------|----------------|----------------|----------------|----------------|----------------|
| With<br>TEDGA    |                             | L <sub>1</sub> | L <sub>2</sub> | L <sub>3</sub> | L <sub>4</sub> | L <sub>5</sub> | L <sub>6</sub> |
|                  | $\Delta G_{mx}^{Am2}$       | -69.8          | -48.5          | -45.3          | -64.8          | -62.4          | -44.8          |
|                  | $\Delta G_{mx}^{Cm2}$       | -74.4          | -57.6          | -53.1          | -76.3          | -73.6          | -59.3          |
|                  | $\Delta \Delta G_{mx}^{M2}$ | -4.6           | -9.1           | -7.8           | -11.5          | -11.2          | -14.5          |
| Without<br>TEDGA |                             | L <sub>1</sub> | L <sub>2</sub> | L <sub>3</sub> | L <sub>4</sub> | L <sub>5</sub> | L <sub>6</sub> |
|                  | $\Delta G_{mx}^{Am2}$       | 17.7           | 31.7           | 44.9           | 12.3           | 16.5           | 36.2           |

|                                           |      |      |      |      |      |      |
|-------------------------------------------|------|------|------|------|------|------|
| $\Delta G_{\text{rx}}^{\text{Cm2}}$       | 13.9 | 27.4 | 36.0 | 9.4  | 14.9 | 28.1 |
| $\Delta \Delta G_{\text{rx}}^{\text{M2}}$ | -3.8 | -4.3 | -8.9 | -2.9 | -1.6 | -8.1 |

**Table S8** Gibbs free Energies in Solvate of related  $\text{M}(\text{H}_2\text{O})_{9-2\text{X}}(\text{NO}_3)_{\text{X}}^{3-\text{X}}$ ,  $\text{L}_n$ ,  $\text{H}_2\text{O}$  and  $\text{NO}_3^-$  compounds (in Hartree).

|                                                     | Gibbs free energy |                                                     | Gibbs free energy |
|-----------------------------------------------------|-------------------|-----------------------------------------------------|-------------------|
| $\text{Am}(\text{H}_2\text{O})_9^{3+}$              | -1283.296332      | $\text{Cm}(\text{H}_2\text{O})_9^{3+}$              | -1326.938738      |
| $\text{Am}(\text{H}_2\text{O})_7(\text{NO}_3)^{2+}$ | -1410.958051      | $\text{Cm}(\text{H}_2\text{O})_7(\text{NO}_3)^{2+}$ | -1454.599916      |
| $\text{Am}(\text{H}_2\text{O})_5(\text{NO}_3)_2^+$  | -1538.612022      | $\text{Cm}(\text{H}_2\text{O})_5(\text{NO}_3)_2^+$  | -1582.250413      |
| $\text{Am}(\text{H}_2\text{O})_3(\text{NO}_3)_3$    | -1666.270773      | $\text{Cm}(\text{H}_2\text{O})_3(\text{NO}_3)_3$    | -1709.909576      |
| $\text{L}_1$                                        | -248.290843       | $\text{L}_2$                                        | -707.927938       |
| $\text{L}_3$                                        | -366.191812       | $\text{L}_4$                                        | -366.190078       |
| $\text{L}_5$                                        | -362.824826       | $\text{L}_6$                                        | -685.809776       |
| $\text{L}_7$                                        | -585.431527       | $\text{H}_2\text{O}$                                | -76.451022        |
| $\text{NO}_3^-$                                     | -280.536391       |                                                     |                   |

**Table S9** Gibbs free Energies in Solvate of related  $\text{M}(\text{H}_2\text{O})_8(\text{L}_n)^{3+}$  compounds (in Hartree).

|                                                    | Gibbs free energy |                                                    | Gibbs free energy |
|----------------------------------------------------|-------------------|----------------------------------------------------|-------------------|
| $\text{Am}(\text{H}_2\text{O})_8(\text{L}_1)^{3+}$ | -1455.121813      | $\text{Cm}(\text{H}_2\text{O})_8(\text{L}_1)^{3+}$ | -1498.76892       |
| $\text{Am}(\text{H}_2\text{O})_8(\text{L}_2)^{3+}$ | -1914.752698      | $\text{Cm}(\text{H}_2\text{O})_8(\text{L}_2)^{3+}$ | -1958.394822      |
| $\text{Am}(\text{H}_2\text{O})_8(\text{L}_3)^{3+}$ | -1573.015666      | $\text{Cm}(\text{H}_2\text{O})_8(\text{L}_3)^{3+}$ | -1616.657294      |
| $\text{Am}(\text{H}_2\text{O})_8(\text{L}_4)^{3+}$ | -1573.027236      | $\text{Cm}(\text{H}_2\text{O})_8(\text{L}_4)^{3+}$ | -1616.669974      |
| $\text{Am}(\text{H}_2\text{O})_8(\text{L}_5)^{3+}$ | -1569.659928      | $\text{Cm}(\text{H}_2\text{O})_8(\text{L}_5)^{3+}$ | -1613.303266      |
| $\text{Am}(\text{H}_2\text{O})_8(\text{L}_6)^{3+}$ | -1892.634696      | $\text{Cm}(\text{H}_2\text{O})_8(\text{L}_6)^{3+}$ | -1936.279044      |
| $\text{Am}(\text{H}_2\text{O})_8(\text{L}_7)^{3+}$ | -1792.252521      | $\text{Cm}(\text{H}_2\text{O})_8(\text{L}_7)^{3+}$ | -1835.894757      |

**Table S10** Gibbs free Energies in Solvate of related  $\text{M}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_n)^{2+}$  compounds (in Hartree).

|                                                                 | Gibbs free energy |                                                                 | Gibbs free energy |
|-----------------------------------------------------------------|-------------------|-----------------------------------------------------------------|-------------------|
| $\text{Am}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_1)^{2+}$ | -1582.788989      | $\text{Cm}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_1)^{2+}$ | -1626.432194      |
| $\text{Am}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_2)^{2+}$ | -2042.418054      | $\text{Cm}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_2)^{2+}$ | -2086.060172      |
| $\text{Am}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_3)^{2+}$ | -1700.681659      | $\text{Cm}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_3)^{2+}$ | -1744.323895      |
| $\text{Am}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_4)^{2+}$ | -1700.692390      | $\text{Cm}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_4)^{2+}$ | -1744.332838      |
| $\text{Am}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_5)^{2+}$ | -1697.324375      | $\text{Cm}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_5)^{2+}$ | -1740.967269      |
| $\text{Am}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_6)^{2+}$ | -2020.301984      | $\text{Cm}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_6)^{2+}$ | -2063.944305      |
| $\text{Am}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_7)^{2+}$ | -1919.921537      | $\text{Cm}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_7)^{2+}$ | -1963.562939      |

**Table S11** Gibbs free Energies in Solvate of related  $\text{M}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_n)^+$  compounds (in Hartree).

|                                                                | Gibbs free energy |                                                                | Gibbs free energy |
|----------------------------------------------------------------|-------------------|----------------------------------------------------------------|-------------------|
| $\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_1)^+$ | -1710.445113      | $\text{Cm}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_1)^+$ | -1754.084954      |
| $\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_2)^+$ | -2170.076865      | $\text{Cm}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_2)^+$ | -2213.716886      |
| $\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_3)^+$ | -1828.335720      | $\text{Cm}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_3)^+$ | -1871.977502      |

|                                                                |              |                                                                |              |
|----------------------------------------------------------------|--------------|----------------------------------------------------------------|--------------|
| $\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_4)^+$ | -1828.346408 | $\text{Cm}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_4)^+$ | -1871.985904 |
| $\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_5)^+$ | -1824.979537 | $\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_5)^+$ | -1868.618540 |
| $\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_6)^+$ | -2147.957000 | $\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_6)^+$ | -2191.598460 |
| $\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_7)^+$ | -2047.577365 | $\text{Cm}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_7)^+$ | -2091.219001 |

**Table S12** Gibbs free Energies in Solvate of related  $\text{M}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_n)$  compounds (in Hartree).

|                                                              | Gibbs free energy |                                                              | Gibbs free energy |
|--------------------------------------------------------------|-------------------|--------------------------------------------------------------|-------------------|
| $\text{Am}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_1)$ | -1838.10931       | $\text{Cm}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_1)$ | -1881.747029      |
| $\text{Am}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_2)$ | -2297.736663      | $\text{Cm}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_2)$ | -2341.375734      |
| $\text{Am}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_3)$ | -1956.003670      | $\text{Cm}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_3)$ | -1999.639919      |
| $\text{Am}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_4)$ | -1956.009386      | $\text{Cm}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_4)$ | -1999.649414      |
| $\text{Am}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_5)$ | -1952.642944      | $\text{Cm}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_5)$ | -1996.282233      |
| $\text{Am}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_6)$ | -2275.619346      | $\text{Cm}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_6)$ | -2319.259441      |
| $\text{Am}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_7)$ | -2175.236931      | $\text{Cm}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_7)$ | -2218.875316      |

**Table S13** Gibbs free Energies in Solvate of related  $[\text{M}(\text{H}_2\text{O})_{8-2x}(\text{NO}_3)_x(\text{L}_8)]^{3-x}$  compounds (in Hartree).

|                                                                   | Gibbs free energy |                                                                   | Gibbs free energy |
|-------------------------------------------------------------------|-------------------|-------------------------------------------------------------------|-------------------|
| $[\text{Am}(\text{H}_2\text{O})_8(\text{L}_8)]^{3+}$              | -1684.191745      | $[\text{Cm}(\text{H}_2\text{O})_8(\text{L}_8)]^{3+}$              | -1727.834352      |
| $[\text{Am}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_8)]^{2+}$ | -1811.855527      | $[\text{Cm}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_8)]^{2+}$ | -1855.498165      |
| $[\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_8)]^+$  | -1939.511378      | $[\text{Cm}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_8)]^+$  | -1983.150085      |
| $[\text{Am}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_8)]$    | -2067.173636      | $[\text{Cm}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_8)]$    | -2110.813427      |
| $\text{L}_8$                                                      | -477.354886       |                                                                   |                   |

**Table S14** Gibbs free Energies in Solvate of related  $[\text{M}(\text{H}_2\text{O})_5(\text{NO}_3)_2(\text{TEDGA})(\text{L}_n)]^+$  compounds (in Hartree).

| Am             | Gibbs free energy | Cm           | Gibbs free energy |
|----------------|-------------------|--------------|-------------------|
| $\text{L}_1$   | -2287.970278      | $\text{L}_1$ | -2331.610417      |
| $\text{L}_2$   | -2747.599274      | $\text{L}_2$ | -2791.241133      |
| $\text{L}_3$   | -2405.86193       | $\text{L}_3$ | -2449.503295      |
| $\text{L}_4$   | -2405.867619      | $\text{L}_4$ | -2449.510366      |
| $\text{L}_5$   | -2402.501456      | $\text{L}_5$ | -2446.144109      |
| $\text{L}_6$   | -2725.479703      | $\text{L}_6$ | -2769.123609      |
| $\text{TEDGA}$ | -806.844934       |              |                   |

**Table S15** Gibbs free Energies in Solvate of related  $[\text{Am}(\text{H}_2\text{O})_{8-2x}(\text{NO}_3)_x(\text{Na})_x]$  and  $[\text{Am}(\text{H}_2\text{O})_{8-2x}(\text{NO}_3)_x(\text{L}_4)(\text{Na})_x]$  compounds (in Hartree).

|                                                                 | Gibbs free energy |                                                                             | Gibbs free energy |
|-----------------------------------------------------------------|-------------------|-----------------------------------------------------------------------------|-------------------|
| $[\text{Am}(\text{H}_2\text{O})_7(\text{NO}_3)(\text{Na})]$     | -1573.207446      | $[\text{Am}(\text{H}_2\text{O})_6(\text{NO}_3)(\text{L}_4)(\text{Na})]$     | -1862.943587      |
| $[\text{Am}(\text{H}_2\text{O})_5(\text{NO}_3)_2(\text{Na})_2]$ | -1863.121338      | $[\text{Am}(\text{H}_2\text{O})_4(\text{NO}_3)_2(\text{L}_4)(\text{Na})_2]$ | -2152.859159      |
| $[\text{Am}(\text{H}_2\text{O})_3(\text{NO}_3)_3(\text{Na})_3]$ | -2153.040512      | $[\text{Am}(\text{H}_2\text{O})_2(\text{NO}_3)_3(\text{L}_4)(\text{Na})_3]$ | -2442.779272      |

**Table S16** The kinetic datas of Gibbs free energy for the ligand exchange reactions of  $\text{M}(\text{H}_2\text{O})_9^{3+}$

and pyridine ligand L<sub>1</sub>. (in Hartree).

|                                                                        | Gibbs free energy |                                                                        | Gibbs free energy |
|------------------------------------------------------------------------|-------------------|------------------------------------------------------------------------|-------------------|
| [Am(H <sub>2</sub> O) <sub>9</sub> ] <sup>3+</sup> -ts                 | -1283.288449      | [Cm(H <sub>2</sub> O) <sub>9</sub> ] <sup>3+</sup> -ts                 | -1326.935008      |
| [Am(H <sub>2</sub> O) <sub>8</sub> ] <sup>3+</sup>                     | -1206.844152      | [Cm(H <sub>2</sub> O) <sub>8</sub> ] <sup>3+</sup>                     | -1250.488972      |
| [Am(H <sub>2</sub> O) <sub>8</sub> .L <sub>1</sub> ] <sup>3+</sup> -ts | -1455.119060      | [Cm(H <sub>2</sub> O) <sub>8</sub> .L <sub>1</sub> ] <sup>3+</sup> -ts | -1498.761253      |

# Cartesian Coordinates and thermal energies of all species in this study:

|                |             |             |             |                |             |             |             |
|----------------|-------------|-------------|-------------|----------------|-------------|-------------|-------------|
| L <sub>1</sub> |             |             |             | H              | 3.34559800  | -0.13096800 | 1.27813400  |
| C              | -1.14319100 | 0.72062900  | -0.00000700 | H              | 2.19975800  | 1.21281400  | 1.32509800  |
| C              | -1.19695700 | -0.67165300 | 0.00002200  | C              | 2.28220900  | 0.12577200  | -1.27007900 |
| C              | 0.00003400  | -1.38283300 | -0.00000400 | H              | 3.34582800  | -0.12834800 | -1.27800800 |
| C              | 1.19698300  | -0.67161100 | -0.00002500 | H              | 1.82733600  | -0.29132900 | -2.17246600 |
| C              | 1.14315100  | 0.72068500  | 0.00000600  | H              | 2.19995900  | 1.21547500  | -1.32255200 |
| H              | -2.06044100 | 1.30278400  | 0.00004900  |                |             |             |             |
| H              | -2.15349600 | -1.18004400 | 0.00005400  | L <sub>4</sub> |             |             |             |
| H              | 0.00004500  | -2.46674200 | -0.00000500 | C              | 2.13990300  | -1.00651400 | 0.00017000  |
| H              | 2.15355500  | -1.17994200 | -0.00005200 | C              | 0.77052400  | -1.26114200 | 0.00022100  |
| H              | 2.06038800  | 1.30286200  | -0.00003300 | C              | -0.13237200 | -0.19505900 | 0.00004000  |
| N              | -0.00002500 | 1.41854000  | 0.00000500  | C              | 0.41897900  | 1.09175900  | -0.00020400 |
|                |             |             |             | C              | 1.80113900  | 1.24569500  | -0.00026300 |
| L <sub>2</sub> |             |             |             | H              | 2.84562700  | -1.83290100 | 0.00029400  |
| C              | -0.19855700 | 1.21335400  | -0.00006000 | H              | 0.41364400  | -2.28523600 | 0.00040800  |
| C              | 0.46098300  | -0.01277100 | -0.00024000 | H              | -0.21232600 | 1.97268300  | -0.00035000 |
| C              | -1.46302300 | -1.21054100 | 0.00005200  | H              | 2.23548600  | 2.24169700  | -0.00043600 |
| C              | -2.23727800 | -0.05680100 | 0.00003300  | N              | 2.66764400  | 0.22311800  | -0.00007500 |
| C              | -1.58835200 | 1.17719600  | 0.00002300  | C              | -1.63282900 | -0.43201100 | 0.00011200  |
| H              | 0.34974900  | 2.14515200  | 0.00000900  | H              | -1.78313300 | -1.51661300 | 0.00035300  |
| H              | -3.31748500 | -0.12399700 | 0.00007400  | C              | -2.29588900 | 0.13093500  | 1.27053900  |
| H              | -2.15377200 | 2.10124700  | 0.00008100  | H              | -3.36342200 | -0.10537400 | 1.27541400  |
| N              | -0.12007800 | -1.19266400 | -0.00008200 | H              | -1.84931900 | -0.29510900 | 2.17258000  |
| Cl             | 2.23788700  | -0.01436900 | 0.00008900  | H              | -2.19419500 | 1.21868100  | 1.32391700  |
| H              | -1.92465500 | -2.19210300 | 0.00005800  | C              | -2.29592300 | 0.13037800  | -1.27054200 |
|                |             |             |             | H              | -1.84936300 | -0.29604300 | -2.17240900 |
| L <sub>3</sub> |             |             |             | H              | -3.36345200 | -0.10595400 | -1.27529700 |
| C              | 0.11095600  | -0.18459600 | -0.00022200 | H              | -2.19425100 | 1.21810300  | -1.32438900 |
| C              | -0.42706400 | 1.10943100  | 0.00057600  |                |             |             |             |
| C              | -1.80654600 | 1.27572000  | 0.00075000  | L <sub>5</sub> |             |             |             |
| C              | -2.62062400 | 0.14494300  | 0.00012900  | C              | -0.42042700 | -0.28136200 | -0.00065100 |
| C              | -2.00396100 | -1.10115500 | -0.00063800 | C              | -0.01686400 | 1.06226100  | -0.00065300 |
| H              | 0.22650400  | 1.97359700  | 0.00105900  | C              | 1.34681700  | 1.33030900  | -0.00007300 |
| H              | -2.23964800 | 2.26960000  | 0.00135700  | C              | 2.25729100  | 0.27575600  | 0.00054200  |
| H              | -3.70082900 | 0.22382600  | 0.00023000  | C              | 1.74525900  | -1.01740300 | 0.00042300  |
| H              | -2.60197600 | -2.00851900 | -0.00112800 | H              | -0.73313700 | 1.87119700  | -0.00129000 |
| N              | -0.67519200 | -1.27347000 | -0.00081800 | H              | 1.69147700  | 2.35805600  | -0.00014100 |
| C              | 1.61143900  | -0.42838300 | -0.00041400 | H              | 3.32592400  | 0.44711700  | 0.00086500  |
| H              | 1.72650100  | -1.51585700 | -0.00149300 | H              | 2.41400700  | -1.87355300 | 0.00073700  |
| C              | 2.28199100  | 0.12321300  | 1.27048900  | N              | 0.43840200  | -1.30067500 | -0.00027000 |
| H              | 1.82691100  | -0.29566300 | 2.17195000  | O              | -1.71581100 | -0.68158800 | -0.00070100 |

|                              |             |             |             |                                                 |             |             |             |
|------------------------------|-------------|-------------|-------------|-------------------------------------------------|-------------|-------------|-------------|
| C                            | -2.74253300 | 0.31459000  | 0.00095000  | O                                               | -1.97678200 | 0.12751100  | 1.09804800  |
| H                            | -3.68223800 | -0.23336100 | 0.00231800  | O                                               | -1.97118200 | 0.20112900  | -1.07839800 |
| H                            | -2.68673200 | 0.94145400  | 0.89534500  | N                                               | -2.60179400 | 0.19889200  | 0.00934600  |
| H                            | -2.68888600 | 0.94162000  | -0.89355900 | O                                               | -3.85764800 | 0.26866300  | 0.00861900  |
| L <sub>6</sub>               |             |             |             |                                                 |             |             |             |
| C                            | -0.00784500 | -0.35044500 | -0.05016800 |                                                 |             |             |             |
| C                            | 1.00277900  | -1.31837800 | -0.05413200 | Am(H <sub>2</sub> O) <sub>9</sub> <sup>3+</sup> |             |             |             |
| C                            | 2.32305600  | -0.88262600 | -0.01594800 | Am                                              | 0.09235400  | 0.02987600  | -0.04624200 |
| C                            | 2.59399100  | 0.48293400  | 0.02505200  | O                                               | 0.44144300  | 2.14612900  | 1.39100400  |
| C                            | 1.51460400  | 1.36156900  | 0.02666500  | O                                               | -0.92886900 | 2.12828900  | -1.10174700 |
| H                            | 0.77614500  | -2.37455800 | -0.08561800 | H                                               | -0.05629400 | 2.96389900  | 1.27342100  |
| H                            | 3.12991200  | -1.60646600 | -0.01826500 | H                                               | -0.56946000 | 2.82358700  | -1.66492700 |
| H                            | 3.60865500  | 0.85872500  | 0.05509500  | H                                               | -1.85857600 | 2.33374100  | -0.94445300 |
| H                            | 1.67617800  | 2.43500800  | 0.05855100  | O                                               | 0.25633300  | -0.14294400 | -2.53133800 |
| N                            | 0.23913700  | 0.96329700  | -0.01004700 | O                                               | -0.42826800 | -1.67163300 | 1.76094800  |
| S                            | -1.75630000 | -0.70880100 | -0.09647000 | O                                               | -1.71965400 | -1.66350100 | -0.85694700 |
| C                            | -1.83225000 | -2.52973300 | -0.15885400 | O                                               | -2.15024600 | 0.65056800  | 0.98694400  |
| H                            | -2.89433900 | -2.77149900 | -0.19188300 | O                                               | 1.99671800  | 1.47689500  | -0.84830700 |
| H                            | -1.35240900 | -2.91538400 | -1.05790000 | O                                               | 0.97055800  | -2.25718800 | -0.60805400 |
| H                            | -1.39437000 | -2.97600800 | 0.73342700  | O                                               | 2.15705300  | -0.28981700 | 1.29439700  |
| L <sub>7</sub>               |             |             |             |                                                 |             |             |             |
| C                            | 0.08151800  | 0.02891900  | -0.00000200 | H                                               | 0.81883700  | 2.16193800  | 2.27872500  |
| C                            | 0.78324800  | 1.22836900  | -0.00008400 | H                                               | -0.21147400 | 0.43581500  | -3.14542800 |
| C                            | 2.17572400  | 1.16429900  | -0.00006800 | H                                               | 0.59106500  | -0.89357500 | -3.03606700 |
| C                            | 2.78972600  | -0.08209800 | 0.00001800  | H                                               | -0.97280800 | -1.57746100 | 2.55119300  |
| C                            | 1.98652600  | -1.22326200 | 0.00009200  | H                                               | -0.05467500 | -2.56103300 | 1.76643600  |
| H                            | 0.26297800  | 2.17595900  | -0.00015100 | H                                               | -2.20186400 | -1.60460900 | -1.69049300 |
| H                            | 2.76476700  | 2.07322400  | -0.00012500 | H                                               | -2.25789300 | 1.17372100  | 1.79064600  |
| H                            | 3.86826100  | -0.17692400 | 0.00003000  | H                                               | 2.13190400  | 2.34506700  | -0.44798700 |
| H                            | 2.43401200  | -2.21200600 | 0.00016800  | H                                               | 0.40507300  | -2.87850600 | -1.08322500 |
| N                            | 0.65272800  | -1.17827600 | 0.00008300  | H                                               | 2.33165700  | -0.94873000 | 1.97645000  |
| C                            | -1.43076400 | 0.00177200  | 0.00000200  | H                                               | -2.21499600 | -2.26185500 | -0.28477100 |
| F                            | -1.91949800 | -0.63939300 | 1.08415500  | H                                               | -2.95265800 | 0.12498700  | 0.88489900  |
| F                            | -1.96268100 | 1.24341000  | -0.00013100 | H                                               | 2.25339500  | 1.53461200  | -1.77666000 |
| F                            | -1.91948600 | -0.63960600 | -1.08405200 | H                                               | 1.88472500  | -2.55067200 | -0.70134300 |
|                              |             |             |             |                                                 |             |             |             |
|                              |             |             |             | Cm(H <sub>2</sub> O) <sub>9</sub> <sup>3+</sup> |             |             |             |
| H <sub>2</sub> O             |             |             |             | Cm                                              | -0.00069900 | -0.02141500 | 0.02310100  |
| O                            | 0.00000000  | 0.00000000  | 0.11945800  | O                                               | 1.68947500  | 1.83940600  | 0.14819900  |
| H                            | 0.00000000  | 0.75530700  | -0.47783200 | O                                               | 1.97994800  | -0.99145200 | 1.26864400  |
| H                            | 0.00000000  | -0.75530700 | -0.47783200 | H                                               | 2.56450800  | 1.78163200  | -0.25570500 |
|                              |             |             |             |                                                 |             |             |             |
| NO <sub>3</sub> <sup>-</sup> |             |             |             | H                                               | 2.65080900  | -0.52870600 | 1.78535500  |
|                              |             |             |             | H                                               | 1.78354100  | 2.31851500  | 0.98134400  |

|                                                                                 |             |             |             |                                                                                 |             |             |             |
|---------------------------------------------------------------------------------|-------------|-------------|-------------|---------------------------------------------------------------------------------|-------------|-------------|-------------|
| O                                                                               | -1.73997100 | 1.79260300  | 0.24737100  | N                                                                               | -2.64447900 | 0.20196200  | 0.01065900  |
| O                                                                               | 0.03380500  | 1.10975300  | 2.26762700  | O                                                                               | -3.84933400 | 0.26775000  | 0.00825000  |
| O                                                                               | 1.96763600  | -0.56586700 | -1.47809700 | Am                                                                              | 0.29797800  | 0.01507000  | 0.00098900  |
| O                                                                               | -1.95162200 | -0.76779300 | -1.44331500 | O                                                                               | 2.58167500  | 1.21886900  | -0.26613400 |
| O                                                                               | 0.01821300  | -2.51984100 | -0.20491400 | H                                                                               | 3.41047400  | 0.97368000  | -0.69294400 |
| O                                                                               | -0.10371900 | 1.55217700  | -1.96589300 | H                                                                               | 2.78487900  | 1.89834000  | 0.38853200  |
| O                                                                               | -1.95160100 | -0.92575600 | 1.32045100  |                                                                                 |             |             |             |
| H                                                                               | -2.62632000 | 1.63669900  | 0.59707800  | Cm(H <sub>2</sub> O) <sub>7</sub> (NO <sub>3</sub> ) <sub>2</sub> <sup>2+</sup> |             |             |             |
| H                                                                               | 0.32800100  | 0.74463800  | 3.11110800  | O                                                                               | -2.09459700 | 1.74947700  | -0.03764800 |
| H                                                                               | 2.03682800  | -0.56012500 | -2.43978600 | H                                                                               | -3.02718000 | 1.73625100  | 0.20517700  |
| H                                                                               | -2.60228900 | -0.22657500 | -1.90702600 | O                                                                               | -0.19193400 | -2.28122400 | -0.99452000 |
| H                                                                               | -0.55606300 | -3.13011800 | 0.27321200  | O                                                                               | 2.00765500  | 0.17796300  | 0.97614200  |
| H                                                                               | 1.94493100  | -1.89770600 | 1.59944800  | O                                                                               | -0.41349300 | -1.79295600 | 1.85048800  |
| H                                                                               | 0.57195700  | 2.23966100  | -2.02519900 | O                                                                               | -0.22307100 | 1.12517600  | 2.28880500  |
| H                                                                               | -0.34313700 | 1.31226400  | -2.86953400 | O                                                                               | -0.44577300 | 0.70460500  | -2.39413800 |
| H                                                                               | -2.08246000 | -1.05232900 | 2.26743700  | O                                                                               | 1.86684400  | -0.40665600 | -1.10202500 |
| H                                                                               | -2.71611000 | -1.29412600 | 0.86079500  | O                                                                               | 0.52806400  | 2.36020700  | -0.37847800 |
| H                                                                               | -1.82595100 | 2.40021900  | -0.49874600 | H                                                                               | -1.80254200 | 2.66851800  | -0.08242400 |
| H                                                                               | -0.64945900 | 1.76418300  | 2.46056000  | H                                                                               | -0.95375900 | -2.78413800 | -1.30689100 |
| H                                                                               | 2.71864800  | -1.06234600 | -1.13054400 | H                                                                               | 0.56313300  | -2.51894100 | -1.54668600 |
| H                                                                               | -1.88777200 | -1.60197900 | -1.92494200 | H                                                                               | -0.03571400 | -2.66325200 | 1.67143700  |
| H                                                                               | 0.57404000  | -3.04590800 | -0.79238100 | H                                                                               | 0.59983900  | 1.28691200  | 2.76564200  |
|                                                                                 |             |             |             | H                                                                               | 0.15969200  | 0.32925100  | -3.04573100 |
| Am(H <sub>2</sub> O) <sub>7</sub> (NO <sub>3</sub> ) <sub>2</sub> <sup>2+</sup> |             |             |             | H                                                                               | 1.19949500  | 2.79063100  | 0.16454400  |
| O                                                                               | 2.08681500  | -1.74043900 | 0.08075900  | H                                                                               | -0.23026000 | -1.58526100 | 2.77488200  |
| H                                                                               | 3.00699300  | -1.70308900 | 0.36569400  | H                                                                               | -0.89972300 | 1.69302600  | 2.67585100  |
| O                                                                               | 0.14711200  | 2.01676800  | -1.49639900 | H                                                                               | -1.27234700 | 0.89060100  | -2.85631400 |
| O                                                                               | -1.95964800 | 0.12674600  | 1.08828000  | H                                                                               | 0.73394800  | 2.56046800  | -1.30047500 |
| O                                                                               | 0.44155300  | 2.09800500  | 1.41048700  | N                                                                               | 2.62121800  | -0.15211700 | -0.09612900 |
| O                                                                               | 0.29315000  | -0.69294700 | 2.43407000  | O                                                                               | 3.82617900  | -0.21688700 | -0.16037300 |
| O                                                                               | 0.22012000  | -1.14865800 | -2.26194800 | O                                                                               | -2.60179400 | -1.17789400 | 0.28069800  |
| O                                                                               | -1.95394500 | 0.19973700  | -1.06957400 | H                                                                               | -3.41647100 | -1.17368500 | -0.23459300 |
| O                                                                               | -0.56438600 | -2.42166300 | 0.05347700  | H                                                                               | -2.70585000 | -1.81052600 | 1.00128900  |
| H                                                                               | 1.76585800  | -2.63951500 | 0.22799400  | Cm                                                                              | -0.34278400 | -0.00747400 | 0.05156700  |
| H                                                                               | 0.93553500  | 2.42414700  | -1.87489500 |                                                                                 |             |             |             |
| H                                                                               | -0.59873900 | 2.20679500  | -2.07749500 | Am(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> <sup>+</sup>  |             |             |             |
| H                                                                               | 0.04767800  | 2.92126600  | 1.09564700  | O                                                                               | 0.49195600  | -0.00825200 | -2.74279400 |
| H                                                                               | -0.53308400 | -0.82937900 | 2.91383000  | H                                                                               | -0.28583400 | -0.16454800 | -3.29173600 |
| H                                                                               | 1.02662900  | -1.40516300 | -2.72710700 | O                                                                               | 0.21627300  | -0.13420100 | 2.49558600  |
| H                                                                               | -1.18511900 | -2.80688400 | 0.68325700  | O                                                                               | 0.77803000  | 1.68046300  | 1.46531300  |
| H                                                                               | 0.27713200  | 2.04855500  | 2.36051800  | O                                                                               | 1.65261200  | 1.75060500  | -1.12144800 |
| H                                                                               | 0.96729800  | -1.22528000 | 2.87307700  | O                                                                               | 1.27248600  | -2.39851300 | 1.24476700  |
| H                                                                               | -0.40591400 | -0.85674800 | -2.93664500 | O                                                                               | 3.06771100  | -0.17671600 | 0.65646200  |
| H                                                                               | -0.80302100 | -2.75252700 | -0.82222000 | O                                                                               | 2.69672600  | -1.11472400 | -1.25613800 |

|                                                                                |             |             |             |                                                                   |             |             |             |
|--------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                              | 1.23068800  | -0.42480300 | -3.20496100 | O                                                                 | 2.44126900  | -0.16419100 | 1.05027100  |
| H                                                                              | 1.60629900  | 2.59180100  | -0.65172000 | O                                                                 | -2.20893100 | -0.37937500 | -0.95461600 |
| H                                                                              | 0.77976600  | -3.17963600 | 0.96228700  | O                                                                 | -0.49345900 | 2.09364800  | -0.93438400 |
| H                                                                              | 1.29431400  | 1.88344300  | -2.00948000 | O                                                                 | 0.19005300  | -0.51653700 | -2.45560700 |
| H                                                                              | 1.19611200  | -2.33826700 | 2.20529000  | O                                                                 | 2.33219100  | 0.60662300  | -0.96751400 |
| N                                                                              | 3.55517800  | -0.73034700 | -0.38166600 | O                                                                 | -1.81729500 | -1.61375000 | 0.77936100  |
| O                                                                              | 4.74506900  | -0.88560900 | -0.54122700 | O                                                                 | -1.36227800 | 1.69777200  | 1.01098600  |
| N                                                                              | 0.46246600  | 1.11482100  | 2.57092100  | O                                                                 | 0.06135900  | -0.55856400 | 2.55849300  |
| O                                                                              | 0.40601100  | 1.72926700  | 3.61302300  | H                                                                 | -0.64021300 | -0.37645600 | -2.92826700 |
| O                                                                              | 0.19026600  | -2.58452200 | -1.21372200 | H                                                                 | 0.65509400  | -0.12991200 | 3.18593900  |
| H                                                                              | -0.64689300 | -2.61990900 | -1.69367500 | H                                                                 | 0.88304500  | -0.07500800 | -2.96280900 |
| H                                                                              | 0.86141900  | -2.97353800 | -1.78820700 | H                                                                 | -0.78728600 | -0.67859100 | 3.00110800  |
| Am                                                                             | 0.64900200  | -0.32470800 | -0.06331200 | N                                                                 | -1.24726100 | 2.49341600  | 0.01753400  |
| O                                                                              | -1.81976900 | -0.68693500 | -0.81095800 | O                                                                 | -1.81970900 | 3.56335100  | -0.02092500 |
| H                                                                              | -2.30444700 | 0.04441500  | -1.21506700 | N                                                                 | -2.65510000 | -1.22607000 | -0.10903300 |
| H                                                                              | -2.41930800 | -1.05710100 | -0.14936900 | O                                                                 | -3.79525600 | -1.63280200 | -0.13984200 |
| Cm(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> <sup>+</sup> |             |             |             | N                                                                 | 3.06467500  | 0.29741200  | 0.03136800  |
| O                                                                              | 0.66204100  | -0.07096300 | -2.76593100 | O                                                                 | 4.26845900  | 0.42832200  | 0.01944500  |
| H                                                                              | -0.06428000 | -0.24626400 | -3.37594900 | O                                                                 | 1.08810200  | -2.41203900 | -0.67700800 |
| O                                                                              | 0.37583800  | -0.09521000 | 2.47133800  | H                                                                 | 1.00470300  | -3.23876800 | -0.18736500 |
| O                                                                              | 0.73627400  | 1.77426600  | 1.44942500  | H                                                                 | 0.84130300  | -2.59653300 | -1.59270900 |
| O                                                                              | 1.66878100  | 1.79258200  | -1.10908500 | Am                                                                | 0.12558000  | -0.15481900 | 0.06786700  |
| O                                                                              | 1.26237800  | -2.37019800 | 1.14077200  | Cm(H <sub>2</sub> O) <sub>3</sub> (NO <sub>3</sub> ) <sub>3</sub> |             |             |             |
| O                                                                              | 3.03118700  | -0.07516400 | 0.71402000  | O                                                                 | 2.47207300  | -0.12242300 | 1.08228800  |
| O                                                                              | 2.71782900  | -1.06853200 | -1.17947600 | O                                                                 | -2.23446000 | -0.36904200 | -0.96275100 |
| H                                                                              | 1.44654000  | -0.48301000 | -3.14986500 | O                                                                 | -0.49013500 | 2.06794500  | -0.93671100 |
| H                                                                              | 1.61997500  | 2.62346400  | -0.62129700 | O                                                                 | 0.19211200  | -0.50382300 | -2.45599700 |
| H                                                                              | 0.81167100  | -3.12543100 | 0.73923200  | O                                                                 | 2.35193900  | 0.52295400  | -0.97993700 |
| H                                                                              | 1.37596200  | 1.95649300  | -2.01499000 | O                                                                 | -1.82500000 | -1.57682100 | 0.78779200  |
| H                                                                              | 1.12427000  | -2.40818100 | 2.09475900  | O                                                                 | -1.38248000 | 1.69348200  | 1.00167700  |
| N                                                                              | 3.54976100  | -0.65812000 | -0.29027900 | O                                                                 | 0.06203400  | -0.54180700 | 2.57178800  |
| O                                                                              | 4.74398500  | -0.81977800 | -0.41058600 | H                                                                 | -0.63913300 | -0.35899400 | -2.92516000 |
| N                                                                              | 0.56490800  | 1.16443600  | 2.55883800  | H                                                                 | 0.67561400  | -0.17809900 | 3.22018900  |
| O                                                                              | 0.58508400  | 1.74388300  | 3.62423000  | H                                                                 | 0.88426000  | -0.05985300 | -2.96187000 |
| O                                                                              | 0.07971500  | -2.59449400 | -1.23453500 | H                                                                 | -0.77258800 | -0.71261300 | 3.02359900  |
| H                                                                              | -0.85747500 | -2.53572300 | -1.47118600 | N                                                                 | -1.27113100 | 2.47146400  | -0.00488300 |
| H                                                                              | 0.54616000  | -2.95080200 | -1.99946900 | O                                                                 | -1.86826500 | 3.52392500  | -0.07888100 |
| O                                                                              | -1.95718900 | -0.91176000 | -0.73149300 | N                                                                 | -2.66685600 | -1.20791000 | -0.10741400 |
| H                                                                              | -2.45366900 | -0.29946000 | -1.28920600 | O                                                                 | -3.80335200 | -1.63151100 | -0.12879000 |
| H                                                                              | -2.52625700 | -1.08754300 | 0.02912500  | N                                                                 | 3.08853000  | 0.27490000  | 0.03515600  |
| Cm                                                                             | 0.63264600  | -0.26200300 | -0.10022000 | O                                                                 | 4.29322200  | 0.40513000  | 0.00611900  |
| Am(H <sub>2</sub> O) <sub>3</sub> (NO <sub>3</sub> ) <sub>3</sub>              |             |             |             | O                                                                 | 1.07898700  | -2.37944500 | -0.67270900 |
|                                                                                |             |             |             | H                                                                 | 0.98770200  | -3.21849400 | -0.20618000 |

|                                                                   |             |             |             |                                                                   |             |             |             |
|-------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                 | 0.85914200  | -2.53860800 | -1.60023200 | O                                                                 | 0.24694600  | -0.72984300 | -2.16129200 |
| Cm                                                                | 0.13682800  | -0.13323000 | 0.08519900  | O                                                                 | -2.89513900 | 1.16048400  | -0.83952900 |
|                                                                   |             |             |             | O                                                                 | -0.58626600 | 2.08942200  | -1.76284000 |
| Am(H <sub>2</sub> O) <sub>8</sub> (L <sub>1</sub> ) <sup>3+</sup> |             |             |             | O                                                                 | -1.27813100 | 2.26909700  | 1.28301200  |
| Am                                                                | -0.68878600 | -0.04261700 | -0.02813500 | O                                                                 | -0.21829400 | -2.17460200 | 0.72011000  |
| O                                                                 | 0.10256100  | -0.60871900 | 2.27461600  | O                                                                 | -2.19731700 | -1.48651300 | -1.17524600 |
| H                                                                 | 0.99376200  | -0.60834800 | 2.64357500  | O                                                                 | -2.49583000 | -0.27756300 | 1.69554100  |
| O                                                                 | 0.06899000  | -1.01738000 | -2.24016000 | H                                                                 | -0.42338700 | -0.07100900 | 3.10483000  |
| O                                                                 | -2.56290100 | 1.49846100  | -0.64309400 | H                                                                 | 1.10790500  | -0.63916500 | -2.58587800 |
| O                                                                 | -0.04521200 | 1.67784100  | -1.77148600 | H                                                                 | -0.27640100 | -1.36222100 | -2.66978700 |
| O                                                                 | -0.34949000 | 2.11811600  | 1.22831700  | H                                                                 | -2.82200600 | 1.87387600  | -1.48698800 |
| O                                                                 | -0.17971700 | -2.51545700 | 0.24247000  | H                                                                 | -3.76358100 | 1.21396000  | -0.42317500 |
| O                                                                 | -2.56132600 | -1.39177300 | -1.13312700 | H                                                                 | -0.21091000 | 1.86533200  | -2.62459400 |
| O                                                                 | -2.51214400 | 0.10168500  | 1.81072800  | H                                                                 | -1.89365800 | 2.95197000  | 0.98992400  |
| H                                                                 | -0.52765200 | -0.57022200 | 3.00532600  | H                                                                 | 0.10606100  | -2.23445400 | 1.62883800  |
| H                                                                 | 0.93691000  | -1.33855600 | -2.51395300 | H                                                                 | -2.99430700 | -1.07859700 | -1.54003100 |
| H                                                                 | -0.59195200 | -1.52641200 | -2.72809100 | H                                                                 | -2.92695400 | 0.44665700  | 2.16611900  |
| H                                                                 | -2.54808600 | 2.05378200  | -1.43205500 | H                                                                 | -0.20534900 | 2.94228600  | -1.51550500 |
| H                                                                 | -3.41933000 | 1.60685200  | -0.21358800 | H                                                                 | -0.69165800 | 2.68078200  | 1.92996400  |
| H                                                                 | 0.27828400  | 1.34437500  | -2.61760000 | H                                                                 | -0.27638300 | -3.06851400 | 0.36255700  |
| H                                                                 | -0.84511600 | 2.93261700  | 1.07742300  | H                                                                 | -2.44226900 | -2.37087100 | -0.87773200 |
| H                                                                 | -0.11209300 | -2.90262800 | 1.12435700  | H                                                                 | -3.05357800 | -1.05812800 | 1.79746300  |
| H                                                                 | -3.36232800 | -0.95565100 | -1.44939300 | N                                                                 | 2.24249900  | -0.06140600 | 0.04373700  |
| H                                                                 | -2.70406200 | 0.88615900  | 2.33899100  | C                                                                 | 3.10919700  | 0.93852000  | 0.17255200  |
| H                                                                 | 0.14403600  | 2.62292600  | -1.73726000 | C                                                                 | 2.75660900  | -1.29267600 | -0.15876500 |
| H                                                                 | 0.09155000  | 2.21079500  | 2.08166700  | C                                                                 | 4.49121000  | 0.79958000  | 0.10242600  |
| H                                                                 | -0.14153500 | -3.23830000 | -0.39528300 | C                                                                 | 4.11689100  | -1.54279300 | -0.24289400 |
| H                                                                 | -2.81660700 | -2.28217600 | -0.86215100 | H                                                                 | 2.03563500  | -2.09264200 | -0.25025600 |
| H                                                                 | -3.26146700 | -0.49767700 | 1.91515200  | C                                                                 | 5.00050800  | -0.47446900 | -0.11225700 |
| N                                                                 | 1.96703300  | -0.04075100 | 0.05063200  | H                                                                 | 5.13505300  | 1.66018900  | 0.21438900  |
| C                                                                 | 2.61073000  | 1.14281200  | 0.06096500  | H                                                                 | 4.47002200  | -2.55197800 | -0.40664000 |
| C                                                                 | 2.71547500  | -1.16128100 | 0.05627500  | H                                                                 | 6.07094100  | -0.62658700 | -0.17349000 |
| C                                                                 | 3.99460200  | 1.24903800  | 0.07091100  | Cl                                                                | 2.45943700  | 2.54935000  | 0.46425600  |
| H                                                                 | 1.99002300  | 2.02884400  | 0.06860500  |                                                                   |             |             |             |
| C                                                                 | 4.10371800  | -1.14203200 | 0.06396300  | Am(H <sub>2</sub> O) <sub>8</sub> (L <sub>3</sub> ) <sup>3+</sup> |             |             |             |
| H                                                                 | 2.17446600  | -2.09807000 | 0.05981600  | Am                                                                | 0.92000600  | 0.01348600  | -0.01441100 |
| C                                                                 | 4.75828500  | 0.08555600  | 0.06956500  | O                                                                 | 0.03551800  | 0.24529900  | 2.32435600  |
| H                                                                 | 4.45685300  | 2.22738900  | 0.07960600  | H                                                                 | -0.86554600 | 0.38170400  | 2.63966600  |
| H                                                                 | 4.65203400  | -2.07497400 | 0.06668300  | O                                                                 | 0.48420700  | 1.41692700  | -2.03960900 |
| H                                                                 | 5.84036900  | 0.13478000  | 0.07526100  | O                                                                 | 2.78081700  | -1.61794500 | -0.91543500 |
| Am(H <sub>2</sub> O) <sub>8</sub> (L <sub>2</sub> ) <sup>3+</sup> |             |             |             | O                                                                 | 0.09353000  | -1.43938800 | -1.89102600 |
| Am                                                                | -0.69140600 | 0.17798300  | -0.03049300 | O                                                                 | 0.79090600  | -2.26691700 | 1.00595600  |
| O                                                                 | 0.21058800  | -0.12291700 | 2.37811800  | O                                                                 | 1.24283100  | 2.33685100  | 0.90714500  |
| H                                                                 | 1.06301300  | 0.17288400  | 2.72053200  | O                                                                 | 2.99120900  | 1.14146900  | -1.05120700 |

|                                                                   |             |             |             |                                                                   |             |             |             |
|-------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------|-------------|-------------|-------------|
| O                                                                 | 2.73605700  | -0.23216400 | 1.73675900  | O                                                                 | 1.34362800  | -2.16679100 | 1.16845800  |
| H                                                                 | 0.59936500  | 0.09479200  | 3.09360200  | O                                                                 | 0.88386500  | 2.41975200  | 0.64169100  |
| H                                                                 | -0.29862600 | 1.77062000  | -2.47843200 | O                                                                 | 3.09698600  | 1.45023200  | -1.16928100 |
| H                                                                 | 1.26449600  | 1.82533400  | -2.43786500 | O                                                                 | 3.12822500  | 0.36486600  | 1.71675700  |
| H                                                                 | 2.66009100  | -2.15277600 | -1.70979100 | H                                                                 | 0.98351900  | 0.40160900  | 3.08996900  |
| H                                                                 | 3.56752000  | -1.95199000 | -0.46691500 | H                                                                 | -0.32623900 | 1.32833300  | -2.51891300 |
| H                                                                 | -0.16842500 | -1.03486900 | -2.72771700 | H                                                                 | 1.19727600  | 1.66534400  | -2.59676400 |
| H                                                                 | 1.25467800  | -3.04758000 | 0.67942400  | H                                                                 | 3.37205300  | -1.94124100 | -1.46745000 |
| H                                                                 | 0.98424300  | 2.52530400  | 1.81814700  | H                                                                 | 4.21375900  | -1.47285400 | -0.24941800 |
| H                                                                 | 3.58747300  | 0.46414800  | -1.39887700 | H                                                                 | 0.35560000  | -1.51728000 | -2.58000800 |
| H                                                                 | 2.94714700  | -1.06458000 | 2.17721100  | H                                                                 | 1.95395400  | -2.89966200 | 1.02156500  |
| H                                                                 | -0.11623000 | -2.37938100 | -1.95134400 | H                                                                 | 0.68572800  | 2.69086900  | 1.54634300  |
| H                                                                 | 0.27916200  | -2.53355600 | 1.77948700  | H                                                                 | 3.86091000  | 0.92905300  | -1.44963600 |
| H                                                                 | 1.52225300  | 3.17133200  | 0.51100000  | H                                                                 | 3.52085100  | -0.31325100 | 2.28068300  |
| H                                                                 | 3.54671500  | 1.84773200  | -0.69933000 | H                                                                 | 0.67539500  | -2.71222400 | -1.64466700 |
| H                                                                 | 3.45231800  | 0.38293700  | 1.93596100  | H                                                                 | 0.97586400  | -2.26469500 | 2.05563300  |
| N                                                                 | -1.70187700 | 0.68553600  | -0.02552800 | H                                                                 | 0.87055400  | 3.21677100  | 0.09766100  |
| C                                                                 | -2.82505700 | -0.07255200 | -0.02126800 | H                                                                 | 3.41444200  | 2.34231600  | -0.98318000 |
| C                                                                 | -1.84070600 | 2.03137200  | -0.01575100 | H                                                                 | 3.75443400  | 1.09911800  | 1.69495200  |
| C                                                                 | -4.08998900 | 0.52770600  | -0.00877200 | N                                                                 | -1.29292800 | -0.10195500 | -0.00130600 |
| C                                                                 | -3.06110100 | 2.68192300  | -0.00689500 | C                                                                 | -1.92676100 | -1.28955500 | 0.00644700  |
| C                                                                 | -4.21717700 | 1.90736300  | -0.00315300 | C                                                                 | -2.05859200 | 1.00862900  | 0.00010100  |
| H                                                                 | -4.97324200 | -0.09697400 | -0.00179800 | C                                                                 | -3.30800800 | -1.40651000 | 0.00885800  |
| H                                                                 | -3.09597500 | 3.76322900  | -0.00025100 | C                                                                 | -3.44247900 | 0.97100500  | -0.00103200 |
| H                                                                 | -5.19691200 | 2.36962400  | 0.00632200  | C                                                                 | -4.10836900 | -0.26094200 | 0.00112400  |
| C                                                                 | -2.72391000 | -1.58852000 | -0.01304000 | H                                                                 | -3.75424500 | -2.39336800 | 0.01608900  |
| H                                                                 | -1.67220500 | -1.85924800 | -0.08691400 | H                                                                 | -3.98868400 | 1.90571600  | -0.00198500 |
| C                                                                 | -3.43654200 | -2.21051600 | -1.22925800 | H                                                                 | -1.30093200 | -2.17272100 | 0.01531200  |
| H                                                                 | -3.27388700 | -3.29114200 | -1.23839400 | C                                                                 | -5.62133700 | -0.35610500 | 0.00187500  |
| H                                                                 | -4.51524800 | -2.03755800 | -1.19713300 | H                                                                 | -5.87492300 | -1.42037800 | -0.01824900 |
| H                                                                 | -3.05565000 | -1.80029800 | -2.16739200 | C                                                                 | -6.21752500 | 0.24449500  | 1.28903800  |
| C                                                                 | -3.26184200 | -2.17738600 | 1.30612500  | H                                                                 | -7.30194900 | 0.10905700  | 1.29469400  |
| H                                                                 | -3.13237100 | -3.26255100 | 1.30633700  | H                                                                 | -5.80953100 | -0.24040300 | 2.17919100  |
| H                                                                 | -2.73044100 | -1.77405400 | 2.17141800  | H                                                                 | -6.01269600 | 1.31629200  | 1.36056700  |
| H                                                                 | -4.32683600 | -1.96676000 | 1.43387300  | C                                                                 | -6.22734800 | 0.29575900  | -1.25485400 |
| H                                                                 | -0.92501400 | 2.60605700  | -0.00585000 | H                                                                 | -5.82343600 | -0.14976500 | -2.16718700 |
| Am(H <sub>2</sub> O) <sub>8</sub> (L <sub>4</sub> ) <sup>3+</sup> |             |             |             | H                                                                 | -7.31130100 | 0.15666200  | -1.25937800 |
| Am                                                                | 1.29414300  | 0.02479000  | -0.01529400 | H                                                                 | -6.02767200 | 1.37050900  | -1.28303800 |
| O                                                                 | 0.40571900  | 0.17973700  | 2.34883900  | H                                                                 | -1.53222100 | 1.95459600  | 0.01029800  |
| H                                                                 | -0.50535200 | 0.23958400  | 2.65993900  | Am(H <sub>2</sub> O) <sub>8</sub> (L <sub>5</sub> ) <sup>3+</sup> |             |             |             |
| O                                                                 | 0.52562900  | 1.19371300  | -2.08741200 | O                                                                 | 0.31595000  | -0.22422500 | 2.30357300  |
| O                                                                 | 3.40375200  | -1.30241800 | -0.74482300 | H                                                                 | 1.21293100  | -0.03384000 | 2.60324000  |
| O                                                                 | 0.75625900  | -1.75501200 | -1.73454500 | O                                                                 | 0.13670500  | -1.12481700 | -2.08066500 |

|                                                                   |             |             |             |                                                                   |             |             |             |
|-------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------|-------------|-------------|-------------|
| O                                                                 | -2.72466300 | 1.36566700  | -0.86744400 | O                                                                 | -1.36501600 | 1.96950500  | 1.62434400  |
| O                                                                 | -0.04795800 | 1.98652300  | -1.52857400 | O                                                                 | -0.35877300 | -2.38092200 | 0.58156200  |
| O                                                                 | -1.19474600 | 2.10233100  | 1.39957200  | O                                                                 | -2.43939600 | -1.37399500 | -1.24070800 |
| O                                                                 | -0.35740300 | -2.33702700 | 0.67308900  | O                                                                 | -2.57301100 | -0.48904700 | 1.69089300  |
| O                                                                 | -2.40527800 | -1.40193300 | -1.23423100 | H                                                                 | -0.40393500 | -0.46188000 | 3.15613800  |
| O                                                                 | -2.46740400 | -0.32710500 | 1.68298100  | H                                                                 | 1.00048100  | -1.15080700 | -2.41157300 |
| H                                                                 | -0.25509900 | -0.22791100 | 3.08234600  | H                                                                 | -0.50445200 | -1.57498600 | -2.51331300 |
| H                                                                 | 0.91909200  | -1.05023100 | -2.63926700 | H                                                                 | -2.45761900 | 2.09454500  | -1.44991500 |
| H                                                                 | -0.54124300 | -1.60996500 | -2.56904300 | H                                                                 | -3.59759400 | 1.57193700  | -0.51233400 |
| H                                                                 | -2.62414500 | 2.09218800  | -1.49519300 | H                                                                 | 0.10226600  | 1.56362700  | -2.60744300 |
| H                                                                 | -3.60974500 | 1.43830800  | -0.48975200 | H                                                                 | -1.76836300 | 2.77079400  | 1.26730400  |
| H                                                                 | 0.06958900  | 1.85623300  | -2.47819600 | H                                                                 | -0.14164800 | -2.63753800 | 1.48655500  |
| H                                                                 | -1.64989500 | 2.84658300  | 0.98670600  | H                                                                 | -3.18640200 | -0.88605400 | -1.61058000 |
| H                                                                 | -0.05049400 | -2.51899800 | 1.57028100  | H                                                                 | -2.95880200 | 0.25184700  | 2.17586300  |
| H                                                                 | -3.12365900 | -0.87082600 | -1.60246700 | H                                                                 | 0.47162900  | 2.50247500  | -1.42348100 |
| H                                                                 | -2.81857900 | 0.43609100  | 2.15893800  | H                                                                 | -0.76964800 | 2.24685400  | 2.33244100  |
| H                                                                 | 0.77987400  | 2.37638300  | -1.18986900 | H                                                                 | -0.28037300 | -3.16720200 | 0.02787000  |
| H                                                                 | -0.57436500 | 2.47449100  | 2.03894900  | H                                                                 | -2.76178000 | -2.25599700 | -1.01782300 |
| H                                                                 | -0.37638100 | -3.17369400 | 0.19345900  | H                                                                 | -3.23623000 | -1.18821300 | 1.65353600  |
| H                                                                 | -2.80121300 | -2.22476300 | -0.92154700 | N                                                                 | 2.06170300  | 0.23396300  | 0.11697100  |
| H                                                                 | -3.08809900 | -1.05602700 | 1.79808100  | C                                                                 | 2.88095900  | 1.30778100  | 0.12032700  |
| N                                                                 | 2.07159900  | 0.05447600  | -0.09842300 | C                                                                 | 2.63005200  | -0.98531500 | 0.00824900  |
| C                                                                 | 2.86997700  | 1.13322500  | -0.05530700 | C                                                                 | 4.26610500  | 1.18844500  | -0.02528500 |
| C                                                                 | 2.65924600  | -1.15983500 | -0.15254400 | C                                                                 | 3.99156300  | -1.18996100 | -0.13838700 |
| C                                                                 | 4.26418400  | 1.04602400  | -0.06573400 | H                                                                 | 1.95094300  | -1.82725700 | 0.03888500  |
| C                                                                 | 4.03008200  | -1.34324300 | -0.16367400 | C                                                                 | 4.82312600  | -0.07428800 | -0.16593800 |
| H                                                                 | 1.98763100  | -2.00725700 | -0.18138600 | H                                                                 | 4.89976500  | 2.06252800  | -0.02071100 |
| C                                                                 | 4.84351900  | -0.21303600 | -0.11980600 | H                                                                 | 4.38132100  | -2.19468100 | -0.22926100 |
| H                                                                 | 4.87824200  | 1.93324800  | -0.03688700 | H                                                                 | 5.89463700  | -0.18240000 | -0.28225200 |
| H                                                                 | 4.44347900  | -2.34147700 | -0.20415900 | Am                                                                | -0.73773900 | 0.04974700  | 0.04519600  |
| H                                                                 | 5.92248500  | -0.30697500 | -0.12962200 | S                                                                 | 2.08291400  | 2.88480600  | 0.37997300  |
| O                                                                 | 2.19546600  | 2.30914800  | -0.00385900 | C                                                                 | 3.34727100  | 4.10835800  | -0.10224500 |
| C                                                                 | 2.93177200  | 3.53876200  | 0.18598100  | H                                                                 | 3.70706100  | 3.91872300  | -1.11197200 |
| H                                                                 | 3.57522400  | 3.73698700  | -0.67234900 | H                                                                 | 2.82802500  | 5.06576700  | -0.07699100 |
| H                                                                 | 2.17503700  | 4.31388500  | 0.26928400  | H                                                                 | 4.16649100  | 4.12846900  | 0.61388300  |
| H                                                                 | 3.51691100  | 3.48914800  | 1.10461600  |                                                                   |             |             |             |
| Am                                                                | -0.64400400 | 0.05415400  | -0.02420000 | Am(H <sub>2</sub> O) <sub>8</sub> (L <sub>7</sub> ) <sup>3+</sup> |             |             |             |
|                                                                   |             |             |             | Am                                                                | -0.77788800 | 0.08975800  | 0.09567300  |
| Am(H <sub>2</sub> O) <sub>8</sub> (L <sub>6</sub> ) <sup>3+</sup> |             |             |             | O                                                                 | 0.20134200  | -0.31909700 | -2.26074500 |
| O                                                                 | 0.16930200  | -0.35206100 | 2.38706900  | H                                                                 | 1.10321400  | -0.03065200 | -2.44896600 |
| H                                                                 | 1.05003600  | -0.12278100 | 2.70745900  | O                                                                 | 0.18668500  | 1.08899400  | 2.28340900  |
| O                                                                 | 0.13902600  | -1.08719500 | -1.98286500 | O                                                                 | -2.88875500 | -0.97600100 | 0.93792100  |
| O                                                                 | -2.69302600 | 1.41198100  | -0.80718700 | O                                                                 | -0.42612800 | -1.47052900 | 2.01697200  |
| O                                                                 | -0.19224800 | 1.86222400  | -1.73759500 | O                                                                 | -0.94199500 | -2.26874400 | -0.76320500 |

|                                                                   |             |             |             |                                                                   |             |             |             |
|-------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------|-------------|-------------|-------------|
| O                                                                 | -1.02120400 | 2.30273600  | -1.25689600 | H                                                                 | 0.92135100  | -1.36048500 | -2.54669700 |
| O                                                                 | -2.24102800 | 1.86864800  | 1.14345000  | H                                                                 | -0.60790900 | -1.53116000 | -2.76734100 |
| O                                                                 | -2.61106300 | 0.02135000  | -1.68027500 | H                                                                 | -2.55731000 | 2.06767400  | -1.43009400 |
| H                                                                 | -0.32215800 | -0.11063400 | -3.04489500 | H                                                                 | -3.39376100 | 1.64980300  | -0.18043500 |
| H                                                                 | 1.07857700  | 1.46100200  | 2.28503000  | H                                                                 | 0.27487400  | 1.29049100  | -2.60522200 |
| H                                                                 | -0.40557500 | 1.78809900  | 2.59421000  | H                                                                 | -0.79574000 | 2.92963900  | 1.04595400  |
| H                                                                 | -0.03344400 | -1.06121500 | 2.79948300  | H                                                                 | -0.16166000 | -2.97447900 | 1.08628300  |
| H                                                                 | -1.59386400 | -2.94049600 | -0.52864100 | H                                                                 | -3.33502900 | -0.88692200 | -1.38677600 |
| H                                                                 | -1.35634300 | 2.30735900  | -2.16196000 | H                                                                 | -2.69897600 | 0.87747800  | 2.35800400  |
| H                                                                 | -3.08289400 | 1.66799900  | 1.57125900  | H                                                                 | 0.18779700  | 2.57842700  | -1.73186900 |
| H                                                                 | -0.46425500 | -2.42397900 | 2.15498700  | H                                                                 | 0.06346100  | 2.12511300  | 2.06319700  |
| H                                                                 | -0.56142200 | -2.50192500 | -1.61981500 | H                                                                 | -0.14270000 | -3.19217300 | -0.45183700 |
| H                                                                 | -0.30790100 | 2.95424400  | -1.23526300 | H                                                                 | -2.86585100 | -2.26030200 | -0.83373600 |
| H                                                                 | -2.37619800 | 2.64332400  | 0.58059200  | H                                                                 | -3.28299700 | -0.48779600 | 1.91674500  |
| N                                                                 | 2.05295200  | -0.86548600 | 0.07071000  | N                                                                 | 1.96529200  | -0.01104800 | 0.03548200  |
| C                                                                 | 2.15636300  | -2.18409400 | 0.28367900  | C                                                                 | 2.61198600  | 1.17070200  | 0.04299100  |
| C                                                                 | 3.20120100  | -0.16882800 | -0.01083200 | C                                                                 | 2.71115000  | -1.13339900 | 0.06025500  |
| C                                                                 | 3.37430600  | -2.84197700 | 0.43633400  | C                                                                 | 3.99571000  | 1.27385600  | 0.07115500  |
| C                                                                 | 4.45992500  | -0.73361200 | 0.13433500  | H                                                                 | 1.99309000  | 2.05761000  | 0.03679300  |
| C                                                                 | 4.54633600  | -2.10420200 | 0.37007600  | C                                                                 | 4.09920000  | -1.11707200 | 0.08740500  |
| H                                                                 | 3.38763700  | -3.91093600 | 0.60291700  | H                                                                 | 2.16824300  | -2.06903600 | 0.06580800  |
| H                                                                 | 5.34674700  | -0.12134300 | 0.05925500  | C                                                                 | 4.75671300  | 0.10883500  | 0.09165000  |
| H                                                                 | 5.51232200  | -2.57833800 | 0.48876700  | H                                                                 | 4.45996200  | 2.25127000  | 0.07773600  |
| H                                                                 | 1.22866200  | -2.73740300 | 0.32186600  | H                                                                 | 4.64495500  | -2.05131000 | 0.10676900  |
| C                                                                 | 3.07364700  | 1.30689800  | -0.31973900 | H                                                                 | 5.83870000  | 0.15568400  | 0.11330300  |
| F                                                                 | 2.41071600  | 1.98698800  | 0.64987200  | Cm                                                                | -0.67798000 | -0.06209400 | -0.02175100 |
| F                                                                 | 4.26194600  | 1.90125400  | -0.47138300 |                                                                   |             |             |             |
| F                                                                 | 2.37222200  | 1.50870800  | -1.46459200 | Cm(H <sub>2</sub> O) <sub>8</sub> (L <sub>2</sub> ) <sup>3+</sup> |             |             |             |
| H                                                                 | -2.96195100 | -1.34046700 | 1.82835900  | O                                                                 | 0.22814600  | -0.26545400 | 2.40258200  |
| H                                                                 | -3.77654200 | -0.92050400 | 0.56532900  | H                                                                 | 1.08030000  | 0.00177600  | 2.76849700  |
| H                                                                 | -2.87588500 | -0.81596300 | -2.08213700 | O                                                                 | 0.16737500  | -0.84339100 | -2.15211800 |
| H                                                                 | -3.36788300 | 0.61484400  | -1.77048900 | O                                                                 | -2.74249900 | 1.36966000  | -0.79959400 |
|                                                                   |             |             |             | O                                                                 | -0.30622800 | 1.88011600  | -1.81803300 |
| Cm(H <sub>2</sub> O) <sub>8</sub> (L <sub>1</sub> ) <sup>3+</sup> |             |             |             | O                                                                 | -1.32720600 | 2.15661800  | 1.49414700  |
| O                                                                 | 0.13015200  | -0.48532900 | 2.30904500  | O                                                                 | -0.21669700 | -2.23629000 | 0.61003900  |
| H                                                                 | 1.00064400  | -0.71914000 | 2.65229900  | O                                                                 | -2.33083400 | -1.38755200 | -1.09848700 |
| O                                                                 | 0.05514900  | -1.05580700 | -2.24996900 | O                                                                 | -2.46729100 | -0.32151200 | 1.72692500  |
| O                                                                 | -2.59581000 | 1.45564400  | -0.68548200 | H                                                                 | -0.40490600 | -0.28295900 | 3.13193400  |
| O                                                                 | -0.04163800 | 1.64227900  | -1.76371100 | H                                                                 | 1.04490000  | -0.97356600 | -2.53114100 |
| O                                                                 | -0.31876900 | 2.10081800  | 1.17690200  | H                                                                 | -0.42978900 | -1.47258600 | -2.57768200 |
| O                                                                 | -0.14954900 | -2.51630700 | 0.23671100  | H                                                                 | -2.60322700 | 1.98997000  | -1.52702200 |
| O                                                                 | -2.55871400 | -1.38524700 | -1.10090300 | H                                                                 | -3.65217100 | 1.46315200  | -0.49237000 |
| O                                                                 | -2.52687800 | 0.10220000  | 1.80988900  | H                                                                 | 0.02168200  | 1.49470300  | -2.64111700 |
| H                                                                 | -0.51728200 | -0.62941600 | 3.01097600  | H                                                                 | -1.83068600 | 2.87216600  | 1.08558800  |

|                                                                   |             |             |             |                                                                   |             |             |             |
|-------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                 | 0.06930600  | -2.40480100 | 1.51765200  | H                                                                 | 3.61149400  | 1.88348400  | -0.54399600 |
| H                                                                 | -3.10280700 | -0.94983100 | -1.48002100 | H                                                                 | 3.62433100  | 0.19731500  | 1.86383500  |
| H                                                                 | -2.84601100 | 0.44418300  | 2.17858800  | N                                                                 | -1.58745200 | 0.89848800  | 0.05541200  |
| H                                                                 | 0.14772000  | 2.72453900  | -1.70016000 | C                                                                 | -2.72538700 | 0.16521400  | 0.09000900  |
| H                                                                 | -0.71328300 | 2.56982600  | 2.11463400  | C                                                                 | -1.69918400 | 2.24570600  | 0.02424300  |
| H                                                                 | -0.25404700 | -3.08164900 | 0.14715800  | C                                                                 | -3.97915800 | 0.78753000  | 0.08300000  |
| H                                                                 | -2.60505700 | -2.27799600 | -0.84810300 | C                                                                 | -2.90701700 | 2.91998800  | 0.01541400  |
| H                                                                 | -3.13685500 | -1.01571900 | 1.71553400  | C                                                                 | -4.07854700 | 2.16905600  | 0.04373300  |
| N                                                                 | 2.16952900  | 0.05945300  | 0.02013100  | H                                                                 | -4.87374500 | 0.17949300  | 0.11100200  |
| C                                                                 | 3.02386300  | 1.07127400  | 0.16209000  | H                                                                 | -2.92155200 | 4.00147700  | -0.01058200 |
| C                                                                 | 2.70628100  | -1.16355600 | -0.18884400 | H                                                                 | -5.04879800 | 2.65107200  | 0.03863200  |
| C                                                                 | 4.40743500  | 0.94979900  | 0.09264200  | C                                                                 | -2.64126600 | -1.34873100 | 0.14796500  |
| C                                                                 | 4.06920500  | -1.39376800 | -0.27090500 | H                                                                 | -1.58708400 | -1.62264100 | 0.13880600  |
| H                                                                 | 2.00106900  | -1.97689800 | -0.28156000 | C                                                                 | -3.29888400 | -1.99902000 | -1.08417000 |
| C                                                                 | 4.93688000  | -0.31403300 | -0.13130700 | H                                                                 | -3.14489600 | -3.08085900 | -1.05895500 |
| H                                                                 | 5.03837400  | 1.81844700  | 0.21448500  | H                                                                 | -4.37638200 | -1.81643500 | -1.10682900 |
| H                                                                 | 4.43557100  | -2.39750100 | -0.43851300 | H                                                                 | -2.87147900 | -1.61446700 | -2.01282500 |
| H                                                                 | 6.00950500  | -0.45012600 | -0.19030700 | C                                                                 | -3.24807100 | -1.89751900 | 1.45419100  |
| Cl                                                                | 2.35756300  | 2.66644700  | 0.47863000  | H                                                                 | -3.10177600 | -2.97951400 | 1.50343700  |
| Cm                                                                | -0.66541900 | 0.15248300  | 0.04299700  | H                                                                 | -2.77807400 | -1.45113500 | 2.33394600  |
| Cm(H <sub>2</sub> O) <sub>8</sub> (L <sub>3</sub> ) <sup>3+</sup> |             |             |             | H                                                                 | -4.32230100 | -1.70307300 | 1.50999500  |
| O                                                                 | 0.27826200  | 0.48199100  | 2.40048700  | H                                                                 | -0.77153400 | 2.80043900  | 0.01378600  |
| H                                                                 | -0.62339300 | 0.50524100  | 2.74304700  | Cm                                                                | 1.01277900  | 0.08353200  | 0.00684300  |
| O                                                                 | 0.62660000  | 1.48407200  | -2.04154700 | Cm(H <sub>2</sub> O) <sub>8</sub> (L <sub>4</sub> ) <sup>3+</sup> |             |             |             |
| O                                                                 | 2.65667900  | -1.70956300 | -0.85289000 | O                                                                 | 0.50408600  | 0.42892600  | 2.35233200  |
| O                                                                 | 0.06727300  | -1.24333400 | -1.88922400 | H                                                                 | -0.38174000 | 0.31554300  | 2.71733100  |
| O                                                                 | 0.64420700  | -2.21298000 | 0.93383200  | O                                                                 | 0.62225200  | 1.14392600  | -2.15098800 |
| O                                                                 | 1.42083600  | 2.41076100  | 0.86827800  | O                                                                 | 3.25692800  | -1.49161200 | -0.66076500 |
| O                                                                 | 3.11733800  | 1.16463200  | -0.95683600 | O                                                                 | 0.74817000  | -1.65298900 | -1.80035300 |
| O                                                                 | 2.83068100  | -0.33385900 | 1.72455900  | O                                                                 | 1.13215000  | -2.17402900 | 1.11795900  |
| H                                                                 | 0.85426300  | 0.18160400  | 3.11507800  | O                                                                 | 0.84660300  | 2.44868800  | 0.51645900  |
| H                                                                 | -0.15221500 | 1.90163000  | -2.42886400 | O                                                                 | 3.22883200  | 1.53600100  | -0.80457600 |
| H                                                                 | 1.40841100  | 1.91750700  | -2.40828800 | O                                                                 | 3.16671600  | 0.19857700  | 1.75689700  |
| H                                                                 | 2.61985800  | -2.06532500 | -1.74936500 | H                                                                 | 1.12085100  | 0.50014200  | 3.09161900  |
| H                                                                 | 3.54058800  | -1.89116100 | -0.51048200 | H                                                                 | -0.26458600 | 1.34397600  | -2.47498200 |
| H                                                                 | -0.06783000 | -0.81034300 | -2.74136100 | H                                                                 | 1.23825000  | 1.67624500  | -2.66997000 |
| H                                                                 | 1.17000800  | -2.94525400 | 0.58774800  | H                                                                 | 3.22280000  | -1.93424700 | -1.51795000 |
| H                                                                 | 1.16431200  | 2.57181900  | 1.78587700  | H                                                                 | 4.17439100  | -1.50360300 | -0.36304700 |
| H                                                                 | 3.76042900  | 0.62387900  | -1.43228700 | H                                                                 | 0.41397600  | -1.32495900 | -2.64420800 |
| H                                                                 | 2.98714200  | -1.18461100 | 2.15297000  | H                                                                 | 1.79539500  | -2.85557500 | 0.94841600  |
| H                                                                 | -0.16577500 | -2.17366400 | -1.99443300 | H                                                                 | 0.62368100  | 2.69849300  | 1.42201900  |
| H                                                                 | 0.17442800  | -2.52705400 | 1.71589100  | H                                                                 | 3.96824400  | 1.24554800  | -1.35252700 |
| H                                                                 | 1.65116900  | 3.26138500  | 0.47491300  | H                                                                 | 3.48811100  | -0.50609600 | 2.33344500  |

|                                                                   |             |             |             |                                                                   |             |             |             |
|-------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                 | 0.50742600  | -2.58524300 | -1.74020700 | H                                                                 | 0.00485600  | -2.51449600 | 1.48146300  |
| H                                                                 | 0.77253600  | -2.33438200 | 1.99912500  | H                                                                 | -3.15492000 | -1.01161100 | -1.52341300 |
| H                                                                 | 0.74239700  | 3.23107000  | -0.03859300 | H                                                                 | -2.77417700 | 0.53717600  | 2.18065100  |
| H                                                                 | 3.31098300  | 2.49159200  | -0.70034100 | H                                                                 | 0.74870700  | 2.36244500  | -1.21413900 |
| H                                                                 | 3.91649100  | 0.78194900  | 1.58415900  | H                                                                 | -0.52798100 | 2.50921300  | 2.00980000  |
| N                                                                 | -1.27224400 | -0.08900000 | 0.04790100  | H                                                                 | -0.29287500 | -3.16973400 | 0.09795400  |
| C                                                                 | -1.89376300 | -1.28330600 | 0.05339900  | H                                                                 | -2.69859300 | -2.31294700 | -0.81180600 |
| C                                                                 | -2.05354800 | 1.01029100  | 0.03204300  | H                                                                 | -3.15528500 | -0.93291100 | 1.82520100  |
| C                                                                 | -3.27353800 | -1.41770500 | 0.03539600  | N                                                                 | 2.06817100  | 0.03843000  | -0.09320600 |
| C                                                                 | -3.43701400 | 0.95667300  | 0.01038900  | C                                                                 | 2.86583800  | 1.11715800  | -0.04570900 |
| C                                                                 | -4.08832600 | -0.28266100 | 0.00813500  | C                                                                 | 2.65885600  | -1.17426900 | -0.14189100 |
| H                                                                 | -3.70764300 | -2.41006000 | 0.04137000  | C                                                                 | 4.26067600  | 1.03130900  | -0.03933600 |
| H                                                                 | -3.99362900 | 1.88519400  | -0.00378600 | C                                                                 | 4.02997600  | -1.35752900 | -0.13785500 |
| H                                                                 | -1.25742800 | -2.15837700 | 0.08154200  | H                                                                 | 1.98879200  | -2.02216300 | -0.17489500 |
| C                                                                 | -5.59995600 | -0.39634900 | -0.01314900 | C                                                                 | 4.84218400  | -0.22711100 | -0.08406600 |
| H                                                                 | -5.83991700 | -1.46319500 | -0.05504500 | H                                                                 | 4.87397700  | 1.91881600  | -0.00458600 |
| C                                                                 | -6.21887500 | 0.17355100  | 1.27744100  | H                                                                 | 4.44393300  | -2.35581000 | -0.17297000 |
| H                                                                 | -7.30166500 | 0.02550300  | 1.26770400  | H                                                                 | 5.92129100  | -0.32022400 | -0.07922800 |
| H                                                                 | -5.81567900 | -0.32245800 | 2.16365200  | Cm                                                                | -0.68955400 | 0.06413600  | -0.03020000 |
| H                                                                 | -6.02733800 | 1.24616700  | 1.37039300  | O                                                                 | 2.19099700  | 2.29327200  | -0.00761100 |
| C                                                                 | -6.20002100 | 0.27047000  | -1.26461100 | C                                                                 | 2.92677300  | 3.52320500  | 0.17584300  |
| H                                                                 | -5.77900100 | -0.15197600 | -2.18021200 | H                                                                 | 3.57876200  | 3.71180500  | -0.67835500 |
| H                                                                 | -7.28177900 | 0.11655500  | -1.28503300 | H                                                                 | 2.17095700  | 4.30072700  | 0.24390800  |
| H                                                                 | -6.01568900 | 1.34831700  | -1.27048600 | H                                                                 | 3.50388700  | 3.48362900  | 1.10023200  |
| H                                                                 | -1.54146600 | 1.96356700  | 0.04371700  |                                                                   |             |             |             |
| Cm                                                                | 1.34358300  | 0.04253600  | -0.00434500 | Cm(H <sub>2</sub> O) <sub>8</sub> (L <sub>6</sub> ) <sup>3+</sup> |             |             |             |
|                                                                   |             |             |             | O                                                                 | 0.16354200  | -0.37093800 | 2.39400700  |
| Cm(H <sub>2</sub> O) <sub>8</sub> (L <sub>5</sub> ) <sup>3+</sup> |             |             |             | H                                                                 | 1.04268700  | -0.12915600 | 2.70982700  |
| O                                                                 | 0.27176300  | -0.26678100 | 2.29922000  | O                                                                 | 0.16765400  | -1.07918500 | -2.01355600 |
| H                                                                 | 1.16983500  | -0.06784500 | 2.59039200  | O                                                                 | -2.69459100 | 1.38158300  | -0.81757600 |
| O                                                                 | 0.09705400  | -0.91654400 | -2.20499100 | O                                                                 | -0.18468500 | 1.83792300  | -1.70629700 |
| O                                                                 | -2.76377100 | 1.32947700  | -0.84107900 | O                                                                 | -1.38128200 | 2.01152800  | 1.60666800  |
| O                                                                 | -0.07830300 | 1.97077500  | -1.55176700 | O                                                                 | -0.34793900 | -2.37784400 | 0.57168500  |
| O                                                                 | -1.17090700 | 2.14817100  | 1.38632600  | O                                                                 | -2.41729800 | -1.39016900 | -1.19476800 |
| O                                                                 | -0.28623800 | -2.33323900 | 0.57841200  | O                                                                 | -2.56209900 | -0.45033700 | 1.70086600  |
| O                                                                 | -2.39241100 | -1.45486900 | -1.12945300 | H                                                                 | -0.41139000 | -0.45965200 | 3.16448300  |
| O                                                                 | -2.48227100 | -0.25231100 | 1.70660300  | H                                                                 | 1.02238200  | -1.12216400 | -2.45767600 |
| H                                                                 | -0.29392100 | -0.25849900 | 3.08184700  | H                                                                 | -0.47401200 | -1.55465600 | -2.55651400 |
| H                                                                 | 0.95755700  | -0.92816200 | -2.63966200 | H                                                                 | -2.47363900 | 2.06045400  | -1.46881400 |
| H                                                                 | -0.47862500 | -1.53947500 | -2.66615000 | H                                                                 | -3.60008200 | 1.53116000  | -0.52000900 |
| H                                                                 | -2.70135900 | 2.04137400  | -1.49010000 | H                                                                 | 0.12980000  | 1.52310400  | -2.56333200 |
| H                                                                 | -3.63915900 | 1.38301500  | -0.43911700 | H                                                                 | -1.78450900 | 2.80046000  | 1.22305600  |
| H                                                                 | 0.06346000  | 1.78008600  | -2.48783100 | H                                                                 | -0.13243900 | -2.64776900 | 1.47340400  |
| H                                                                 | -1.61333100 | 2.90298200  | 0.97846200  | H                                                                 | -3.17017100 | -0.91894100 | -1.57437300 |

|                                                                   |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                 | -2.91305900 | 0.31292300  | 2.17848400  | N                                                                                   | 2.04496000  | -0.91380100 | 0.05026600  |
| H                                                                 | 0.46341800  | 2.49442400  | -1.39329200 | C                                                                                   | 2.14734800  | -2.23547900 | 0.24479300  |
| H                                                                 | -0.78459400 | 2.31957700  | 2.30103400  | C                                                                                   | 3.19338700  | -0.21428100 | -0.01095200 |
| H                                                                 | -0.27364400 | -3.15622500 | 0.00605000  | C                                                                                   | 3.36382200  | -2.89474800 | 0.40032100  |
| H                                                                 | -2.72158900 | -2.27825300 | -0.97087000 | C                                                                                   | 4.45034400  | -0.78142100 | 0.14161400  |
| H                                                                 | -3.25261300 | -1.12304900 | 1.67201500  | C                                                                                   | 4.53564700  | -2.15497100 | 0.35888800  |
| N                                                                 | 2.05517100  | 0.22244200  | 0.12735100  | H                                                                                   | 3.37601100  | -3.96630400 | 0.54908000  |
| C                                                                 | 2.87206700  | 1.29795200  | 0.13087300  | H                                                                                   | 5.33770500  | -0.16826800 | 0.08315900  |
| C                                                                 | 2.62335000  | -0.99358700 | -0.01386600 | H                                                                                   | 5.50085900  | -2.62987600 | 0.48065100  |
| C                                                                 | 4.25418400  | 1.18435300  | -0.04557500 | H                                                                                   | 1.22020400  | -2.79095900 | 0.26232700  |
| C                                                                 | 3.98177400  | -1.19257400 | -0.19253000 | C                                                                                   | 3.07538900  | 1.26390200  | -0.31804300 |
| H                                                                 | 1.94660100  | -1.83701300 | 0.01437200  | F                                                                                   | 2.40318700  | 1.95083300  | 0.63658000  |
| C                                                                 | 4.81036200  | -0.07470000 | -0.21885000 | F                                                                                   | 4.27038800  | 1.85037700  | -0.45377500 |
| H                                                                 | 4.88632200  | 2.05948800  | -0.04110000 | F                                                                                   | 2.39564900  | 1.46548600  | -1.47711900 |
| H                                                                 | 4.37119900  | -2.19471700 | -0.30965800 | H                                                                                   | -2.77502500 | -1.44540200 | 1.88649100  |
| H                                                                 | 5.87923400  | -0.17849200 | -0.36070700 | H                                                                                   | -3.71275600 | -1.05554500 | 0.70509600  |
| S                                                                 | 2.07213600  | 2.86670100  | 0.42564200  | H                                                                                   | -2.88538900 | -0.72547300 | -2.08086300 |
| C                                                                 | 3.33336300  | 4.10122700  | -0.03545000 | H                                                                                   | -3.37038800 | 0.67247400  | -1.64060300 |
| H                                                                 | 3.68293800  | 3.93875900  | -1.05349900 | Cm                                                                                  | -0.73868200 | 0.05646200  | 0.06617700  |
| H                                                                 | 2.81619500  | 5.05838000  | 0.02105000  |                                                                                     |             |             |             |
| H                                                                 | 4.15984500  | 4.10038700  | 0.67256300  | Am(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>1</sub> ) <sup>2+</sup> |             |             |             |
| Cm                                                                | -0.73596600 | 0.03838900  | 0.06154600  | O                                                                                   | -0.69863500 | 2.09631400  | 1.17994700  |
|                                                                   |             |             |             | H                                                                                   | -1.54594200 | 2.15739600  | 1.63571800  |
| Cm(H <sub>2</sub> O) <sub>8</sub> (L <sub>7</sub> ) <sup>3+</sup> |             |             |             | O                                                                                   | -0.15539500 | -1.24408000 | -2.04433300 |
| O                                                                 | 0.16585500  | -0.27236100 | -2.29345800 | O                                                                                   | 2.60219500  | -0.98208600 | 0.57998200  |
| H                                                                 | 1.06962300  | 0.01016600  | -2.48422600 | O                                                                                   | -0.12012300 | -2.32199200 | 0.55030100  |
| O                                                                 | 0.05310700  | 1.16238800  | 2.29994100  | O                                                                                   | 0.71150300  | -0.36268900 | 2.54146700  |
| O                                                                 | -2.78951400 | -1.15007800 | 0.96778500  | O                                                                                   | 0.68392200  | 2.10550400  | -1.48527100 |
| O                                                                 | -0.31044400 | -1.45903500 | 2.04638000  | O                                                                                   | 2.40393400  | -0.14193200 | -1.40193900 |
| O                                                                 | -0.92328100 | -2.26585100 | -0.77362200 | O                                                                                   | 1.99610700  | 1.90401700  | 0.98231500  |
| O                                                                 | -1.00767700 | 2.45878900  | -1.20118800 | H                                                                                   | -0.06046300 | 2.63719800  | 1.66378500  |
| O                                                                 | -2.30560300 | 1.80312900  | 1.02291100  | H                                                                                   | -0.99555300 | -1.20196800 | -2.51712000 |
| O                                                                 | -2.60543200 | 0.08272100  | -1.63194700 | H                                                                                   | 0.54013900  | -1.30873000 | -2.71138200 |
| H                                                                 | -0.37112100 | -0.00458800 | -3.05014500 | H                                                                                   | -0.15023400 | -2.92406300 | -0.20420100 |
| H                                                                 | 0.92363000  | 1.57780100  | 2.35359000  | H                                                                                   | 1.52684100  | -0.71302700 | 2.92004700  |
| H                                                                 | -0.59457100 | 1.84064900  | 2.53695400  | H                                                                                   | 0.06593200  | 2.84389000  | -1.54827500 |
| H                                                                 | 0.01941400  | -0.99239500 | 2.82586200  | H                                                                                   | 2.72585900  | 1.72287600  | 1.58688200  |
| H                                                                 | -1.62027500 | -2.87704800 | -0.50384200 | H                                                                                   | 0.25189900  | -2.80578800 | 1.29710900  |
| H                                                                 | -1.37553700 | 2.48746400  | -2.09317700 | H                                                                                   | 0.18160500  | -0.02345100 | 3.27226900  |
| H                                                                 | -3.17262000 | 1.68656100  | 1.42949200  | H                                                                                   | 1.14895800  | 2.05095900  | -2.32906900 |
| H                                                                 | -0.24369700 | -2.40687900 | 2.20868400  | H                                                                                   | 2.33092500  | 2.50908200  | 0.30809300  |
| H                                                                 | -0.59677700 | -2.53451200 | -1.64180200 | N                                                                                   | -2.34097200 | -0.14055900 | -0.12300400 |
| H                                                                 | -0.25348800 | 3.06204100  | -1.21193500 | C                                                                                   | -3.01852200 | -1.04721500 | 0.60298400  |
| H                                                                 | -2.33383000 | 2.59381200  | 0.46430600  | C                                                                                   | -3.04767600 | 0.70830300  | -0.89169700 |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| C                                                                                   | -4.40531500 | -1.13487400 | 0.59062600  | O                                                                                   | 4.47799500  | 0.03301600  | -1.42875300 |
| H                                                                                   | -2.41938000 | -1.72646600 | 1.19557400  | Cl                                                                                  | -2.64794700 | 2.18040800  | -0.64651300 |
| C                                                                                   | -4.43414400 | 0.68634900  | -0.96488200 | Am                                                                                  | 0.61692200  | -0.02397800 | 0.10432500  |
| H                                                                                   | -2.47928100 | 1.42938800  | -1.46822400 |                                                                                     |             |             |             |
| C                                                                                   | -5.12800300 | -0.25253100 | -0.20695200 | Am(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>3</sub> ) <sup>2+</sup> |             |             |             |
| H                                                                                   | -4.90186700 | -1.88334400 | 1.19439200  | O                                                                                   | -0.56856900 | 1.62481400  | -1.84420300 |
| H                                                                                   | -4.95082300 | 1.39239800  | -1.60193700 | H                                                                                   | 0.15349900  | 1.78600300  | -2.46339400 |
| H                                                                                   | -6.20998200 | -0.29596900 | -0.23903400 | O                                                                                   | 0.37498300  | 0.25172100  | 2.40357600  |
| N                                                                                   | 3.14967200  | -0.74982700 | -0.55161100 | O                                                                                   | -2.67101600 | -1.34038700 | -0.59374900 |
| O                                                                                   | 4.28451600  | -1.07374000 | -0.80456100 | O                                                                                   | -0.65393400 | -2.18646700 | 1.22883900  |
| Am                                                                                  | 0.38301900  | 0.09150100  | 0.06519600  | O                                                                                   | -0.10520000 | -1.48537800 | -1.81460300 |
|                                                                                     |             |             |             | O                                                                                   | -0.94508200 | 2.42852700  | 0.90049500  |
| Am(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>2</sub> ) <sup>2+</sup> |             |             |             | O                                                                                   | -2.32069000 | 0.08724800  | 2.13217100  |
| O                                                                                   | -0.50169600 | 0.37843100  | 2.35586400  | O                                                                                   | -2.94387600 | 0.80207700  | -0.72062900 |
| H                                                                                   | -1.41119900 | 0.61239000  | 2.57428100  | H                                                                                   | -1.39428400 | 1.77421600  | -2.32274000 |
| O                                                                                   | 0.02545000  | 0.09672700  | -2.37069500 | H                                                                                   | 1.25694800  | 0.52869700  | 2.67661400  |
| O                                                                                   | 2.95608100  | -0.90788100 | -0.18138500 | H                                                                                   | -0.21165700 | 0.31796400  | 3.16800200  |
| O                                                                                   | 0.29416100  | -2.30002900 | -0.88923200 | H                                                                                   | -0.12207300 | -2.39074500 | 2.00734600  |
| O                                                                                   | 1.12356500  | -1.89776800 | 1.75417100  | H                                                                                   | -0.83283000 | -2.03402300 | -2.13651500 |
| O                                                                                   | 0.82172900  | 2.53772600  | 0.25524800  | H                                                                                   | -1.27393900 | 3.15219900  | 0.35347300  |
| O                                                                                   | 2.47861900  | 0.89526300  | -1.27142400 | H                                                                                   | -2.76237400 | -0.73002300 | 2.39558000  |
| O                                                                                   | 2.13408400  | 0.91210400  | 1.97587000  | H                                                                                   | -1.07801100 | -3.00341800 | 0.93957600  |
| H                                                                                   | 0.07854500  | 0.81510400  | 2.99351800  | H                                                                                   | 0.41006600  | -1.23303200 | -2.59054400 |
| H                                                                                   | -0.85217800 | 0.27081600  | -2.73159100 | H                                                                                   | -0.74014100 | 2.79372300  | 1.76949200  |
| H                                                                                   | 0.66235600  | 0.53999700  | -2.94562900 | H                                                                                   | -2.97800300 | 0.79028900  | 2.20705000  |
| H                                                                                   | 0.28314500  | -2.41882100 | -1.84717600 | N                                                                                   | 1.93962700  | 0.63815900  | -0.21045700 |
| H                                                                                   | 1.99439100  | -2.28696800 | 1.90052700  | C                                                                                   | 3.01298300  | -0.18353300 | -0.28339400 |
| H                                                                                   | 0.07032300  | 3.10719800  | 0.46381800  | C                                                                                   | 2.15081100  | 1.97314100  | -0.22525300 |
| H                                                                                   | 2.95236100  | 0.49905800  | 2.27705700  | C                                                                                   | 4.30769300  | 0.34031000  | -0.37371100 |
| H                                                                                   | 0.66311900  | -3.09783500 | -0.49178900 | C                                                                                   | 3.40447800  | 2.55218300  | -0.31589000 |
| H                                                                                   | 0.67509100  | -1.87621000 | 2.60865100  | C                                                                                   | 4.51124800  | 1.71150400  | -0.39153200 |
| H                                                                                   | 1.31200200  | 2.97429300  | -0.45357800 | H                                                                                   | 5.15210100  | -0.33394700 | -0.42787200 |
| H                                                                                   | 2.31454700  | 1.85397000  | 1.85549300  | H                                                                                   | 3.50355500  | 3.62957900  | -0.32339300 |
| N                                                                                   | -2.29100700 | -0.41412100 | -0.23407600 | H                                                                                   | 5.51334300  | 2.11747600  | -0.46107900 |
| C                                                                                   | -2.72905300 | -1.67680000 | -0.05132800 | C                                                                                   | 2.80553500  | -1.68805300 | -0.24344600 |
| C                                                                                   | -3.21305900 | 0.53138200  | -0.37425700 | H                                                                                   | 1.73463200  | -1.88060700 | -0.30000700 |
| C                                                                                   | -4.07394100 | -2.00892000 | 0.00422900  | C                                                                                   | 3.32343700  | -2.28151400 | 1.08138400  |
| H                                                                                   | -1.95890700 | -2.43141500 | 0.03646100  | H                                                                                   | 3.10705100  | -3.35220400 | 1.11871000  |
| C                                                                                   | -4.58492900 | 0.31039800  | -0.33409500 | H                                                                                   | 4.40494000  | -2.15321000 | 1.17949900  |
| C                                                                                   | -5.01810700 | -0.99487500 | -0.13611600 | H                                                                                   | 2.84662800  | -1.80911300 | 1.94345100  |
| H                                                                                   | -4.36965900 | -3.03876800 | 0.15286000  | C                                                                                   | 3.44592500  | -2.39228800 | -1.45430900 |
| H                                                                                   | -5.27832200 | 1.13039600  | -0.45501900 | H                                                                                   | 3.19532000  | -3.45581200 | -1.43535000 |
| H                                                                                   | -6.07824100 | -1.21277300 | -0.09680700 | H                                                                                   | 3.08439600  | -1.97603800 | -2.39780800 |
| N                                                                                   | 3.35958000  | 0.00344000  | -0.98047700 | H                                                                                   | 4.53575300  | -2.30856600 | -1.44401700 |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                   | 1.26935800  | 2.59691500  | -0.15099700 | H                                                                                   | -1.49031100 | 1.92029200  | -0.03080200 |
| N                                                                                   | -3.44811800 | -0.36501600 | -0.89109300 | O                                                                                   | 3.61889900  | -0.87645000 | -0.70829100 |
| O                                                                                   | -4.57226600 | -0.53211800 | -1.29394100 | O                                                                                   | 2.91765300  | 1.10082100  | -1.23244900 |
| Am                                                                                  | -0.70081800 | 0.04588700  | 0.12240900  | N                                                                                   | 3.88117200  | 0.25205400  | -1.24909700 |
|                                                                                     |             |             |             | O                                                                                   | 4.95584000  | 0.50686700  | -1.73561800 |
| Am(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>4</sub> ) <sup>2+</sup> |             |             |             |                                                                                     |             |             |             |
| Am                                                                                  | 1.24457000  | -0.33409700 | -0.04381100 | Am(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>5</sub> ) <sup>2+</sup> |             |             |             |
| O                                                                                   | 0.32264000  | -0.39433800 | 2.30344100  | O                                                                                   | -0.68183900 | 1.85466700  | 1.43489300  |
| H                                                                                   | -0.57075200 | -0.36337600 | 2.66317600  | H                                                                                   | -1.60025900 | 2.14591200  | 1.45392900  |
| O                                                                                   | 0.43781100  | 0.45094000  | -2.29504500 | O                                                                                   | -0.13734400 | -1.59288200 | -1.74769500 |
| O                                                                                   | 0.75568800  | -2.34119800 | -1.46042000 | O                                                                                   | 2.76916100  | -0.83246200 | 0.65854700  |
| O                                                                                   | 2.05079000  | -2.49906800 | 1.04408300  | O                                                                                   | 0.03820500  | -2.44547200 | 0.90788000  |
| O                                                                                   | 0.90219900  | 2.09665500  | 0.55921500  | O                                                                                   | 0.85048600  | -0.20592400 | 2.67672100  |
| O                                                                                   | 2.88256000  | 0.35133200  | 1.87069400  | O                                                                                   | 0.28884800  | 1.64731600  | -1.61511300 |
| H                                                                                   | 0.94035500  | -0.13976800 | 3.00107800  | O                                                                                   | 2.32863600  | -0.35931400 | -1.40265200 |
| H                                                                                   | -0.46863800 | 0.58723100  | -2.59317500 | O                                                                                   | 1.90740900  | 1.99929000  | 0.65442900  |
| H                                                                                   | 1.01351800  | 0.99328700  | -2.84821000 | H                                                                                   | -0.12026000 | 2.63722800  | 1.51195800  |
| H                                                                                   | 0.62681900  | -2.32187800 | -2.41619800 | H                                                                                   | -0.97097900 | -1.59795200 | -2.23325000 |
| H                                                                                   | 2.94912200  | -2.84163700 | 0.95956100  | H                                                                                   | 0.56898700  | -1.72868900 | -2.39264600 |
| H                                                                                   | 0.54228300  | 2.46695700  | 1.37426900  | H                                                                                   | 0.05834700  | -3.15429600 | 0.25295100  |
| H                                                                                   | 3.70212200  | -0.13620200 | 2.01915300  | H                                                                                   | 1.69228300  | -0.43728000 | 3.08793000  |
| H                                                                                   | 1.07557000  | -3.21913400 | -1.21986800 | H                                                                                   | -0.64698500 | 1.87612800  | -1.77897100 |
| H                                                                                   | 1.72841500  | -2.76705300 | 1.91321700  | H                                                                                   | 2.74165400  | 1.98353700  | 1.13919600  |
| H                                                                                   | 1.33978100  | 2.81720500  | 0.08872700  | H                                                                                   | 0.23718500  | -2.82955000 | 1.77013600  |
| H                                                                                   | 3.10416900  | 1.28594700  | 1.96716200  | H                                                                                   | 0.43545900  | 0.46682000  | 3.23097800  |
| N                                                                                   | -1.39188400 | -0.14303000 | -0.10799600 | H                                                                                   | 0.70984700  | 1.48786500  | -2.46870000 |
| C                                                                                   | -2.10736400 | -1.28491300 | -0.14296100 | H                                                                                   | 2.03978200  | 2.56427600  | -0.11782500 |
| C                                                                                   | -2.07956900 | 1.01226400  | -0.05154900 | N                                                                                   | -2.32274300 | -0.03078900 | -0.34090900 |
| C                                                                                   | -3.49152400 | -1.31382800 | -0.11221400 | C                                                                                   | -2.94630600 | -1.10269000 | 0.19408200  |
| C                                                                                   | -3.46578500 | 1.06440700  | -0.01984400 | C                                                                                   | -3.08556700 | 0.89366300  | -0.94276200 |
| C                                                                                   | -4.21301700 | -0.11633200 | -0.04497300 | C                                                                                   | -4.31525600 | -1.29726500 | 0.14143600  |
| H                                                                                   | -3.99388300 | -2.27249800 | -0.14217500 | H                                                                                   | -2.30588200 | -1.83119400 | 0.67672900  |
| H                                                                                   | -3.95777100 | 2.02844100  | 0.02661300  | C                                                                                   | -4.47411500 | 0.77930300  | -1.05436900 |
| H                                                                                   | -1.54227900 | -2.20677900 | -0.20971800 | C                                                                                   | -5.08889100 | -0.33429500 | -0.50154300 |
| C                                                                                   | -5.72877800 | -0.09538700 | -0.00270700 | H                                                                                   | -4.75608300 | -2.17713800 | 0.58948800  |
| H                                                                                   | -6.03306700 | 0.95444700  | 0.04972600  | H                                                                                   | -5.05807800 | 1.53591000  | -1.55569000 |
| C                                                                                   | -6.33461000 | -0.69794600 | -1.28411300 | H                                                                                   | -6.16393100 | -0.44484800 | -0.57397800 |
| H                                                                                   | -7.42424400 | -0.61845500 | -1.25443200 | N                                                                                   | 3.19596100  | -0.76041200 | -0.54521000 |
| H                                                                                   | -5.97933400 | -0.17474100 | -2.17521100 | O                                                                                   | 4.32761200  | -1.04209200 | -0.85338400 |
| H                                                                                   | -6.07875700 | -1.75625500 | -1.38629400 | Am                                                                                  | 0.42444600  | -0.06466300 | 0.19360700  |
| C                                                                                   | -6.26298100 | -0.80421700 | 1.25612700  | O                                                                                   | -2.39047200 | 1.95678700  | -1.42078200 |
| H                                                                                   | -5.85375400 | -0.35903500 | 2.16629200  | C                                                                                   | -3.10885400 | 3.06917500  | -1.99984600 |
| H                                                                                   | -7.35202500 | -0.72182100 | 1.29676300  | H                                                                                   | -3.80655900 | 3.48738400  | -1.27354300 |
| H                                                                                   | -6.00761000 | -1.86757600 | 1.25301800  | H                                                                                   | -2.34826500 | 3.80496000  | -2.24643200 |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                   | -3.63240000 | 2.75802700  | -2.90471700 | O                                                                                   | 0.15347500  | -0.25474400 | -2.29999100 |
| Am(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>6</sub> ) <sup>2+</sup> |             |             |             | H                                                                                   | 0.99169600  | 0.13277400  | -2.58250100 |
|                                                                                     |             |             |             | O                                                                                   | 0.25886800  | 0.94230300  | 2.43494400  |
| Am                                                                                  | 0.83783800  | -0.13734000 | 0.24874600  | O                                                                                   | -2.95562100 | -0.84969000 | 0.48353900  |
| O                                                                                   | -0.05681000 | -0.01465900 | 2.60995500  | O                                                                                   | -0.56269500 | -1.55504300 | 2.01468700  |
| H                                                                                   | -0.85374800 | -0.41914800 | 2.97259200  | O                                                                                   | -0.69442800 | -2.27217800 | -0.74167100 |
| O                                                                                   | -0.29212500 | 1.02988300  | -1.70470800 | O                                                                                   | -1.15326100 | 2.34401300  | -1.16090000 |
| O                                                                                   | 3.02554100  | -0.78758900 | -0.80502200 | O                                                                                   | -2.12411000 | 1.86183500  | 1.31632800  |
| O                                                                                   | 0.27311400  | -1.76443100 | -1.59136700 | O                                                                                   | -2.60262100 | -0.00745300 | -1.47194500 |
| O                                                                                   | 1.80903300  | -2.30193000 | 1.10564100  | H                                                                                   | -0.47541900 | -0.09669600 | -3.01585000 |
| O                                                                                   | 0.83708800  | 2.27142300  | 1.16196900  | H                                                                                   | 1.16744300  | 1.26371900  | 2.50001400  |
| O                                                                                   | 2.50423900  | 1.30526900  | -0.92645500 | H                                                                                   | -0.31511100 | 1.67081800  | 2.71218900  |
| O                                                                                   | 2.61744000  | 0.34452200  | 2.02956700  | H                                                                                   | -0.31702500 | -1.09072200 | 2.82797100  |
| H                                                                                   | 0.62182900  | -0.02829400 | 3.29737400  | H                                                                                   | -1.20772900 | -3.05099100 | -0.49821000 |
| H                                                                                   | -1.11899100 | 1.49612000  | -1.48091400 | H                                                                                   | -1.81456900 | 2.27580700  | -1.86202200 |
| H                                                                                   | 0.24804000  | 1.64619400  | -2.21659600 | H                                                                                   | -2.99185300 | 1.67438600  | 1.69545400  |
| H                                                                                   | -0.15277600 | -1.33422200 | -2.34497700 | H                                                                                   | -1.25338900 | -2.19048300 | 2.23905600  |
| H                                                                                   | 2.57359100  | -2.70602700 | 0.67731700  | H                                                                                   | -0.38802800 | -2.38787200 | -1.64981800 |
| H                                                                                   | 0.17090000  | 2.48880400  | 1.82643100  | H                                                                                   | -0.45237600 | 2.91635300  | -1.49784800 |
| H                                                                                   | 3.40245400  | -0.19601300 | 2.17802000  | H                                                                                   | -2.21851100 | 2.63099500  | 0.73645700  |
| H                                                                                   | 0.91324600  | -2.39078000 | -1.95144600 | N                                                                                   | 2.11206600  | -0.84324600 | 0.19598700  |
| H                                                                                   | 1.35212100  | -2.99834000 | 1.59239800  | C                                                                                   | 2.21739000  | -2.14290000 | 0.50506800  |
| H                                                                                   | 0.95885400  | 3.05873400  | 0.61744600  | C                                                                                   | 3.25212700  | -0.18173700 | -0.07503200 |
| H                                                                                   | 2.87790900  | 1.26931500  | 2.12541000  | C                                                                                   | 3.43413600  | -2.82016700 | 0.54719100  |
| N                                                                                   | -2.05886400 | -0.70596600 | 0.21564100  | C                                                                                   | 4.50720700  | -0.77228000 | -0.06230800 |
| C                                                                                   | -2.28598600 | -2.03206300 | 0.19771600  | C                                                                                   | 4.59810700  | -2.12621700 | 0.25528400  |
| C                                                                                   | -3.13046000 | 0.10940800  | 0.20897700  | H                                                                                   | 3.45219700  | -3.87100200 | 0.80465700  |
| C                                                                                   | -3.55234000 | -2.59639800 | 0.17776100  | H                                                                                   | 5.38824900  | -0.19104800 | -0.29224900 |
| H                                                                                   | -1.40680900 | -2.66193000 | 0.17604600  | H                                                                                   | 5.56192100  | -2.61905700 | 0.27411000  |
| C                                                                                   | -4.44277200 | -0.37030000 | 0.19211100  | N                                                                                   | -3.41637200 | -0.61270900 | -0.68818000 |
| C                                                                                   | -4.65111800 | -1.74288900 | 0.17618600  | O                                                                                   | -4.52701600 | -0.93601800 | -1.02735400 |
| H                                                                                   | -3.66641800 | -3.67192500 | 0.15926600  | H                                                                                   | 1.29235000  | -2.65575100 | 0.72484000  |
| H                                                                                   | -5.28375900 | 0.30719700  | 0.19281500  | C                                                                                   | 3.12081900  | 1.29026200  | -0.40503800 |
| H                                                                                   | -5.66034100 | -2.13652300 | 0.16241000  | F                                                                                   | 2.50217200  | 1.97540000  | 0.58648000  |
| N                                                                                   | 3.35374100  | 0.38414600  | -1.20226300 | F                                                                                   | 4.30769200  | 1.87371000  | -0.61087500 |
| O                                                                                   | 4.38401600  | 0.60807600  | -1.78763700 | F                                                                                   | 2.37983900  | 1.49326400  | -1.52963700 |
| S                                                                                   | -2.73819100 | 1.85238800  | 0.22430500  | Cm(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>1</sub> ) <sup>2+</sup> |             |             |             |
| C                                                                                   | -4.31534600 | 2.66789400  | -0.18862300 |                                                                                     |             |             |             |
| H                                                                                   | -4.06598800 | 3.72369800  | -0.28854400 | O                                                                                   | -0.69937600 | 2.11762500  | 1.17898400  |
| H                                                                                   | -4.71042400 | 2.29788600  | -1.13320400 | H                                                                                   | -1.54692300 | 2.17587300  | 1.63482100  |
| H                                                                                   | -5.03808900 | 2.54818300  | 0.61645600  | O                                                                                   | -0.15557000 | -1.19837700 | -2.04463200 |
| Am(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>7</sub> ) <sup>2+</sup> |             |             |             | O                                                                                   | 2.60797800  | -0.97686700 | 0.61503500  |
|                                                                                     |             |             |             | O                                                                                   | -0.13580400 | -2.30760000 | 0.51670600  |
| Am                                                                                  | -0.67797200 | 0.10400900  | 0.12907700  | O                                                                                   | 0.71649900  | -0.31447700 | 2.53272200  |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| O                                                                                   | 0.68934100  | 2.09372800  | -1.50406200 | H                                                                                   | 0.06465000  | 3.12547800  | 0.42585900  |
| O                                                                                   | 2.42577500  | -0.12967200 | -1.36701900 | H                                                                                   | 2.94737800  | 0.52582900  | 2.25120100  |
| O                                                                                   | 1.98153800  | 1.91047500  | 0.96609200  | H                                                                                   | 0.66486500  | -3.10811400 | -0.51245100 |
| H                                                                                   | -0.06267300 | 2.66271200  | 1.65999000  | H                                                                                   | 0.68706000  | -1.88975500 | 2.61662800  |
| H                                                                                   | -0.98157500 | -1.14093600 | -2.54031500 | H                                                                                   | 1.30853700  | 2.95927800  | -0.48175100 |
| H                                                                                   | 0.55592300  | -1.27722400 | -2.69333800 | H                                                                                   | 2.30051000  | 1.87192100  | 1.80632000  |
| H                                                                                   | -0.20799100 | -2.85920600 | -0.27303300 | N                                                                                   | -2.28692100 | -0.42852900 | -0.22133500 |
| H                                                                                   | 1.48216300  | -0.77884100 | 2.89187800  | C                                                                                   | -2.73199500 | -1.68997400 | -0.04738800 |
| H                                                                                   | 0.06147100  | 2.81775100  | -1.61752600 | C                                                                                   | -3.20295500 | 0.52280200  | -0.36537900 |
| H                                                                                   | 2.69278400  | 1.71646500  | 1.58872500  | C                                                                                   | -4.07884500 | -2.01547900 | -0.00382500 |
| H                                                                                   | 0.27753300  | -2.84080900 | 1.20573600  | H                                                                                   | -1.96583300 | -2.44840900 | 0.04347200  |
| H                                                                                   | 0.09714300  | -0.17409700 | 3.25830100  | C                                                                                   | -4.57592900 | 0.30796000  | -0.33672800 |
| H                                                                                   | 1.16704400  | 2.00069500  | -2.33754700 | C                                                                                   | -5.01674900 | -0.99604600 | -0.14717600 |
| H                                                                                   | 2.34329300  | 2.50066300  | 0.29260900  | H                                                                                   | -4.38093600 | -3.04437600 | 0.13818400  |
| N                                                                                   | -2.33004600 | -0.13547800 | -0.10896800 | H                                                                                   | -5.26443900 | 1.13170100  | -0.46000700 |
| C                                                                                   | -3.00233700 | -1.02107800 | 0.64777100  | H                                                                                   | -6.07820000 | -1.20883100 | -0.11685700 |
| C                                                                                   | -3.04098000 | 0.68536200  | -0.90362600 | N                                                                                   | 3.36681000  | -0.01452800 | -0.95831200 |
| C                                                                                   | -4.38847400 | -1.11484800 | 0.64066500  | O                                                                                   | 4.48694500  | 0.01242400  | -1.40891900 |
| H                                                                                   | -2.39978000 | -1.67892200 | 1.26055100  | Cl                                                                                  | -2.62769600 | 2.16963300  | -0.62946700 |
| C                                                                                   | -4.42741800 | 0.65470300  | -0.97348400 | Cm                                                                                  | 0.59981800  | -0.03730900 | 0.13324900  |
| H                                                                                   | -2.47539400 | 1.38883000  | -1.50399000 |                                                                                     |             |             |             |
| C                                                                                   | -5.11596200 | -0.26191300 | -0.18406700 | Cm(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>3</sub> ) <sup>2+</sup> |             |             |             |
| H                                                                                   | -4.88070400 | -1.84531200 | 1.26949100  | O                                                                                   | -0.46284500 | 1.70108500  | -1.66186000 |
| H                                                                                   | -4.94843200 | 1.33714000  | -1.63225600 | H                                                                                   | 0.28281600  | 1.83258300  | -2.25990800 |
| H                                                                                   | -6.19777100 | -0.31106900 | -0.21273500 | O                                                                                   | 0.19623900  | 0.20638000  | 2.59582500  |
| N                                                                                   | 3.16003000  | -0.74391700 | -0.51230200 | O                                                                                   | -2.68553800 | -1.25889000 | -0.68612300 |
| O                                                                                   | 4.29663500  | -1.07385500 | -0.76076600 | O                                                                                   | -0.79672000 | -2.22405600 | 1.24141900  |
| Cm                                                                                  | 0.36677100  | 0.12331800  | 0.08278500  | O                                                                                   | -0.04292100 | -1.36201600 | -1.69432900 |
|                                                                                     |             |             |             | O                                                                                   | -1.01438200 | 2.42491800  | 1.06364500  |
| Cm(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>2</sub> ) <sup>2+</sup> |             |             |             | O                                                                                   | -2.47789000 | 0.00968400  | 2.12819500  |
| O                                                                                   | -0.48957300 | 0.37847100  | 2.37010700  | O                                                                                   | -2.92777500 | 0.89336100  | -0.71062700 |
| H                                                                                   | -1.40321400 | 0.59729600  | 2.58755600  | H                                                                                   | -1.26663300 | 1.87040600  | -2.17066100 |
| O                                                                                   | 0.00769600  | 0.13523900  | -2.33464300 | H                                                                                   | 1.02900400  | 0.56877800  | 2.91976900  |
| O                                                                                   | 2.95978900  | -0.93620700 | -0.17466800 | H                                                                                   | -0.44002800 | 0.22469500  | 3.32255600  |
| O                                                                                   | 0.29977000  | -2.30188300 | -0.89570000 | H                                                                                   | -0.29929400 | -2.51424500 | 2.01556000  |
| O                                                                                   | 1.12353000  | -1.89373900 | 1.75574800  | H                                                                                   | -0.74976200 | -1.87725300 | -2.10502500 |
| O                                                                                   | 0.81496000  | 2.54723300  | 0.23936700  | H                                                                                   | -1.30032500 | 3.15345700  | 0.49887300  |
| O                                                                                   | 2.49687100  | 0.89128200  | -1.23395500 | H                                                                                   | -2.91531300 | -0.82908300 | 2.32262500  |
| O                                                                                   | 2.12690000  | 0.93113700  | 1.94541700  | H                                                                                   | -1.19061100 | -3.00897900 | 0.84133700  |
| H                                                                                   | 0.08411800  | 0.83082600  | 3.00273600  | H                                                                                   | 0.57511300  | -1.12878600 | -2.39749600 |
| H                                                                                   | -0.86345100 | 0.31410900  | -2.70819700 | H                                                                                   | -0.90249900 | 2.77622700  | 1.95511500  |
| H                                                                                   | 0.65701900  | 0.55695200  | -2.91196100 | H                                                                                   | -3.15345900 | 0.69613000  | 2.19758300  |
| H                                                                                   | 0.25806400  | -2.41655700 | -1.85308500 | N                                                                                   | 1.89617400  | 0.60922700  | 0.13224000  |
| H                                                                                   | 1.99726200  | -2.28487600 | 1.87839400  | C                                                                                   | 2.94899600  | -0.24291800 | 0.16726300  |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| C                                                                                   | 2.14338300  | 1.93792400  | 0.12815600  | C                                                                                   | -3.50249300 | -1.33859000 | -0.22996700 |
| C                                                                                   | 4.25926400  | 0.24567100  | 0.20066800  | C                                                                                   | -3.51608300 | 1.02543500  | 0.04243100  |
| C                                                                                   | 3.41560800  | 2.48212400  | 0.15345300  | C                                                                                   | -4.24261800 | -0.16527100 | -0.04498900 |
| C                                                                                   | 4.50045800  | 1.61136400  | 0.19247600  | H                                                                                   | -3.98782500 | -2.30290000 | -0.31442900 |
| H                                                                                   | 5.08652200  | -0.45048100 | 0.23532900  | H                                                                                   | -4.02345300 | 1.97293200  | 0.17860700  |
| H                                                                                   | 3.54467600  | 3.55627000  | 0.14627400  | H                                                                                   | -1.53825300 | -2.17883600 | -0.45434600 |
| H                                                                                   | 5.51532900  | 1.98978600  | 0.21799700  | C                                                                                   | -5.75526800 | -0.18226300 | 0.06308700  |
| C                                                                                   | 2.68788800  | -1.73947300 | 0.20860700  | H                                                                                   | -6.07894800 | 0.85431900  | 0.19853800  |
| H                                                                                   | 1.63984000  | -1.89703300 | -0.05194500 | C                                                                                   | -6.40822800 | -0.71517400 | -1.22576000 |
| C                                                                                   | 2.92022300  | -2.29208100 | 1.62943400  | H                                                                                   | -7.49665000 | -0.66108800 | -1.14216400 |
| H                                                                                   | 2.66126100  | -3.35345000 | 1.66516700  | H                                                                                   | -6.10399300 | -0.12957900 | -2.09668000 |
| H                                                                                   | 3.96823200  | -2.19019900 | 1.92454000  | H                                                                                   | -6.13874500 | -1.75943700 | -1.40693000 |
| H                                                                                   | 2.31098700  | -1.76737500 | 2.36915100  | C                                                                                   | -6.21583700 | -0.98426800 | 1.29523900  |
| C                                                                                   | 3.52290600  | -2.51257900 | -0.82757900 | H                                                                                   | -5.77277000 | -0.59111500 | 2.21352000  |
| H                                                                                   | 3.21836300  | -3.56197400 | -0.83264500 | H                                                                                   | -7.30316900 | -0.93013200 | 1.39146200  |
| H                                                                                   | 3.38095500  | -2.11309500 | -1.83458800 | H                                                                                   | -5.93974600 | -2.03898700 | 1.20924300  |
| H                                                                                   | 4.59072800  | -2.48140400 | -0.59662800 | H                                                                                   | -1.55823300 | 1.92001900  | 0.03884100  |
| H                                                                                   | 1.27607100  | 2.58506600  | 0.11273400  | O                                                                                   | 3.55583400  | -1.17276900 | -0.63748200 |
| N                                                                                   | -3.42825600 | -0.25733900 | -0.97906300 | O                                                                                   | 3.13841500  | 0.88720400  | -1.15305000 |
| O                                                                                   | -4.52497800 | -0.38572500 | -1.46780100 | N                                                                                   | 3.97518800  | -0.08736600 | -1.16231000 |
| Cm                                                                                  | -0.74108700 | 0.07777600  | 0.26649000  | O                                                                                   | 5.08351500  | 0.02355900  | -1.63320300 |
| Cm(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>4</sub> ) <sup>2+</sup> |             |             |             | Cm                                                                                  | 1.24269000  | -0.28178100 | 0.01914200  |
| O                                                                                   | 0.25487800  | 0.15920000  | 2.30129600  | Cm(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>5</sub> ) <sup>2+</sup> |             |             |             |
| H                                                                                   | -0.56238700 | -0.18493400 | 2.68025900  | O                                                                                   | -0.68671200 | 1.88952100  | 1.39205700  |
| O                                                                                   | 0.61722500  | 0.58058500  | -2.28025900 | H                                                                                   | -1.61283100 | 2.14440000  | 1.46822800  |
| O                                                                                   | 0.69426400  | -2.21065300 | -1.50522800 | O                                                                                   | -0.12382400 | -1.49759600 | -1.77867100 |
| O                                                                                   | 1.97340100  | -2.34497900 | 1.24175700  | O                                                                                   | 2.76459700  | -0.88893000 | 0.69522000  |
| O                                                                                   | 0.90882900  | 2.16611900  | 0.39439300  | O                                                                                   | 0.04206900  | -2.42830400 | 0.84776100  |
| O                                                                                   | 2.90188900  | 0.43240100  | 1.85094100  | O                                                                                   | 0.85705700  | -0.21749900 | 2.67310300  |
| H                                                                                   | 0.91005500  | 0.21873000  | 3.00885400  | O                                                                                   | 0.28801500  | 1.64787100  | -1.61293700 |
| H                                                                                   | -0.25621100 | 0.87201700  | -2.56685900 | O                                                                                   | 2.36011500  | -0.33618500 | -1.35532200 |
| H                                                                                   | 1.27122100  | 1.07910400  | -2.78590700 | O                                                                                   | 1.91793100  | 1.98350200  | 0.65334000  |
| H                                                                                   | 0.59535500  | -2.02893600 | -2.44837200 | H                                                                                   | -0.14517300 | 2.67855700  | 1.52141300  |
| H                                                                                   | 2.78769400  | -2.81116300 | 1.01603900  | H                                                                                   | -0.95146900 | -1.49665800 | -2.27424000 |
| H                                                                                   | 0.63104800  | 2.51562800  | 1.25015300  | H                                                                                   | 0.59109400  | -1.63191100 | -2.41422900 |
| H                                                                                   | 3.57859700  | -0.19285000 | 2.13918700  | H                                                                                   | 0.03683400  | -3.11284600 | 0.16746400  |
| H                                                                                   | 1.06966700  | -3.09537700 | -1.42106700 | H                                                                                   | 1.70214800  | -0.48549900 | 3.05439100  |
| H                                                                                   | 1.48385700  | -2.89745700 | 1.86240500  | H                                                                                   | -0.64855100 | 1.86835400  | -1.78420700 |
| H                                                                                   | 1.24128500  | 2.90553300  | -0.12870200 | H                                                                                   | 2.74403300  | 1.96279400  | 1.15194100  |
| H                                                                                   | 3.32466900  | 1.30012200  | 1.82650100  | H                                                                                   | 0.25202200  | -2.84574400 | 1.69154400  |
| N                                                                                   | -1.42331800 | -0.12944700 | -0.20040100 | H                                                                                   | 0.44180100  | 0.39441200  | 3.29312500  |
| C                                                                                   | -2.12111500 | -1.27888700 | -0.30286300 | H                                                                                   | 0.71419400  | 1.48252600  | -2.46281300 |
| C                                                                                   | -2.13019600 | 1.00346400  | -0.03578000 | H                                                                                   | 2.06437900  | 2.54871100  | -0.11626700 |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| N                                                                                   | -2.32879300 | -0.02782700 | -0.31602600 | H                                                                                   | -1.36948100 | -2.70096100 | -0.15364100 |
| C                                                                                   | -2.95124900 | -1.09204000 | 0.23396500  | C                                                                                   | -4.44313000 | -0.45611700 | -0.24842400 |
| C                                                                                   | -3.09267100 | 0.88544700  | -0.93371700 | C                                                                                   | -4.62140100 | -1.83092100 | -0.31924400 |
| C                                                                                   | -4.32069700 | -1.28620800 | 0.18973600  | H                                                                                   | -3.59973100 | -3.74065900 | -0.33522600 |
| H                                                                                   | -2.31014500 | -1.81523900 | 0.72323600  | H                                                                                   | -5.29763300 | 0.20348000  | -0.27146900 |
| C                                                                                   | -4.48203900 | 0.77194800  | -1.03668100 | H                                                                                   | -5.62007700 | -2.24268500 | -0.40169700 |
| C                                                                                   | -5.09619600 | -0.33125500 | -0.46261300 | N                                                                                   | 3.35675100  | 0.21523000  | -1.18674800 |
| H                                                                                   | -4.76047900 | -2.15925400 | 0.65199900  | O                                                                                   | 4.41381200  | 0.34747900  | -1.75606400 |
| H                                                                                   | -5.06729600 | 1.52073600  | -1.54807300 | S                                                                                   | -2.79302300 | 1.80076800  | -0.04527000 |
| H                                                                                   | -6.17189900 | -0.44041800 | -0.52721000 | C                                                                                   | -4.39322400 | 2.59764100  | -0.40055100 |
| N                                                                                   | 3.20434300  | -0.78577000 | -0.49883900 | H                                                                                   | -4.17383200 | 3.66459600  | -0.41971200 |
| O                                                                                   | 4.33477900  | -1.08481300 | -0.80559100 | H                                                                                   | -4.77725700 | 2.29047300  | -1.37193200 |
| O                                                                                   | -2.39800200 | 1.93612400  | -1.43986600 | H                                                                                   | -5.11325200 | 2.39651500  | 0.39079500  |
| C                                                                                   | -3.11698100 | 3.03073900  | -2.05085800 | Cm                                                                                  | 0.73831600  | -0.05033700 | 0.21343000  |
| H                                                                                   | -3.81056700 | 3.47400500  | -1.33555400 |                                                                                     |             |             |             |
| H                                                                                   | -2.35636400 | 3.75673700  | -2.32490500 | Cm(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>7</sub> ) <sup>2+</sup> |             |             |             |
| H                                                                                   | -3.64521400 | 2.69161800  | -2.94295600 | O                                                                                   | -0.49493100 | 0.32895900  | 2.44083000  |
| Cm                                                                                  | 0.41498000  | -0.02496700 | 0.21792200  | H                                                                                   | -1.40617300 | 0.59443700  | 2.61296800  |
|                                                                                     |             |             |             | O                                                                                   | 0.10873300  | 0.22473300  | -2.37137400 |
| Cm(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>6</sub> ) <sup>2+</sup> |             |             |             | O                                                                                   | 2.86059300  | -1.08808500 | -0.15729600 |
| O                                                                                   | -0.17766400 | -0.14348700 | 2.55103300  | O                                                                                   | 0.18191700  | -2.14139600 | -1.06148800 |
| H                                                                                   | -1.07707500 | -0.01758200 | 2.87520900  | O                                                                                   | 1.08165500  | -1.85100000 | 1.76057300  |
| O                                                                                   | -0.20714100 | 1.01592400  | -1.93610400 | O                                                                                   | 0.89413000  | 2.55453500  | 0.05747100  |
| O                                                                                   | 3.02261000  | -0.86326500 | -0.59134000 | O                                                                                   | 2.58837900  | 0.77316100  | -1.21560600 |
| O                                                                                   | 0.48360700  | -1.64596800 | -1.72120800 | O                                                                                   | 2.12897200  | 0.96914100  | 1.92923400  |
| O                                                                                   | 1.47631400  | -2.22357600 | 1.24204200  | H                                                                                   | 0.07028900  | 0.82595700  | 3.04734900  |
| O                                                                                   | 0.95735500  | 2.44559400  | 0.78380900  | H                                                                                   | -0.67028000 | 0.69554400  | -2.69373000 |
| O                                                                                   | 2.48419900  | 1.15579900  | -1.13542800 | H                                                                                   | 0.86534100  | 0.56609200  | -2.86669400 |
| O                                                                                   | 2.43420100  | 0.47098100  | 2.01750100  | H                                                                                   | 0.08984600  | -2.04077000 | -2.01827600 |
| H                                                                                   | 0.43400800  | 0.12522200  | 3.24818700  | H                                                                                   | 1.90399000  | -2.35002200 | 1.83087600  |
| H                                                                                   | -1.04854500 | 1.49217400  | -1.83845300 | H                                                                                   | 0.15282600  | 3.17102600  | 0.11020800  |
| H                                                                                   | 0.39523900  | 1.60341200  | -2.41107300 | H                                                                                   | 2.89340200  | 0.52192500  | 2.31249900  |
| H                                                                                   | 0.09189400  | -1.20369900 | -2.48676300 | H                                                                                   | 0.62762200  | -2.97995200 | -0.89193100 |
| H                                                                                   | 2.13698200  | -2.82171700 | 0.87321000  | H                                                                                   | 0.64091800  | -1.87540100 | 2.61852300  |
| H                                                                                   | 0.23640800  | 2.97658200  | 1.14538400  | H                                                                                   | 1.50075200  | 2.89824900  | -0.61108800 |
| H                                                                                   | 3.21681700  | -0.07318900 | 2.16763600  | H                                                                                   | 2.36477500  | 1.89809100  | 1.80775000  |
| H                                                                                   | 1.22197000  | -2.17697000 | -2.04459700 | N                                                                                   | -2.30323200 | -0.38605900 | -0.10156000 |
| H                                                                                   | 0.96030300  | -2.72280100 | 1.88608800  | C                                                                                   | -2.67861500 | -1.65666200 | 0.09849000  |
| H                                                                                   | 1.42673900  | 3.00535200  | 0.15220400  | C                                                                                   | -3.27724900 | 0.52034700  | -0.30168700 |
| H                                                                                   | 2.69820900  | 1.39577700  | 2.10623900  | C                                                                                   | -4.01101500 | -2.06440700 | 0.10398600  |
| N                                                                                   | -2.05900600 | -0.74872600 | -0.10609400 | H                                                                                   | -1.88270200 | -2.37433200 | 0.24286800  |
| C                                                                                   | -2.25556900 | -2.07952000 | -0.17247900 | C                                                                                   | -4.62810400 | 0.20735300  | -0.32005200 |
| C                                                                                   | -3.14436700 | 0.04979100  | -0.14296300 | C                                                                                   | -5.00200000 | -1.11877400 | -0.11114700 |
| C                                                                                   | -3.50779900 | -2.66421800 | -0.28090000 | H                                                                                   | -4.25176200 | -3.10576700 | 0.27176800  |

|                                                                                                  |             |             |             |                                                                                                  |             |             |             |
|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                                | -5.36631200 | 0.97714600  | -0.49180800 | Am(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>2</sub> ) <sup>+</sup> |             |             |             |
| H                                                                                                | -6.04812200 | -1.39755800 | -0.11854400 | O                                                                                                | 0.65984300  | -0.08906500 | -2.82651300 |
| N                                                                                                | 3.36701400  | -0.20690800 | -0.92984300 | H                                                                                                | -0.10612200 | -0.27695700 | -3.38240700 |
| O                                                                                                | 4.49259900  | -0.28494900 | -1.36018000 | O                                                                                                | 0.14206200  | -0.21413700 | 2.35620800  |
| Cm                                                                                               | 0.59611500  | 0.00563600  | 0.15808100  | O                                                                                                | 0.68740900  | 1.64959900  | 1.41313100  |
| C                                                                                                | -2.83887300 | 1.95369000  | -0.51317100 | O                                                                                                | 1.59228400  | 1.75102600  | -1.16823500 |
| F                                                                                                | -2.15960700 | 2.43814800  | 0.55767000  | O                                                                                                | 1.34202700  | -2.38816400 | 1.17939100  |
| F                                                                                                | -2.00605600 | 2.07502100  | -1.57977500 | O                                                                                                | 2.99977600  | -0.11137400 | 0.63391600  |
| F                                                                                                | -3.87303700 | 2.77530100  | -0.72828600 | O                                                                                                | 2.72175900  | -1.16985700 | -1.23025600 |
| Am(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>1</sub> ) <sup>+</sup> |             |             |             | H                                                                                                | 1.41473500  | -0.51899000 | -3.24780900 |
| O                                                                                                | 0.61739900  | -0.09115200 | -2.79288500 | H                                                                                                | 1.52959400  | 2.60477900  | -0.72432500 |
| H                                                                                                | -0.07941300 | -0.36752200 | -3.39965100 | H                                                                                                | 0.98243600  | -3.22909200 | 0.86990700  |
| O                                                                                                | 0.31018600  | -0.32134200 | 2.38063400  | H                                                                                                | 1.29871300  | 1.86149000  | -2.08249200 |
| O                                                                                                | 0.58133500  | 1.62012300  | 1.47970000  | H                                                                                                | 1.23483900  | -2.35808700 | 2.13818000  |
| O                                                                                                | 1.45609900  | 1.81397300  | -1.12179600 | N                                                                                                | -2.22342200 | -0.92946300 | 0.02654100  |
| O                                                                                                | 1.44227100  | -2.43272600 | 1.07199900  | C                                                                                                | -2.58636600 | -1.89173500 | 0.90135900  |
| O                                                                                                | 2.96948200  | -0.06137300 | 0.59851800  | C                                                                                                | -3.20282800 | -0.29693100 | -0.61032200 |
| O                                                                                                | 2.66851000  | -1.09757300 | -1.27611300 | C                                                                                                | -3.90570500 | -2.23293800 | 1.15190000  |
| H                                                                                                | 1.44433700  | -0.45124900 | -3.13893000 | C                                                                                                | -4.55753600 | -0.55792700 | -0.43414900 |
| H                                                                                                | 1.36840600  | 2.63957500  | -0.63107600 | C                                                                                                | -4.91037300 | -1.55109800 | 0.47027100  |
| H                                                                                                | 0.97344200  | -3.22784900 | 0.78686900  | H                                                                                                | -4.13430100 | -3.01368400 | 1.86474800  |
| H                                                                                                | 1.13804400  | 1.96612200  | -2.02093200 | H                                                                                                | -5.30004500 | -0.00048300 | -0.98696600 |
| H                                                                                                | 1.38133500  | -2.39418800 | 2.03482000  | H                                                                                                | -5.95428900 | -1.78579600 | 0.63757900  |
| N                                                                                                | -2.11724400 | -0.96929500 | 0.13880600  | H                                                                                                | -1.78271800 | -2.40081900 | 1.41739500  |
| C                                                                                                | -2.57982000 | -1.81235000 | 1.07838000  | N                                                                                                | 3.53551600  | -0.73038400 | -0.34098900 |
| C                                                                                                | -3.00437400 | -0.40198600 | -0.69671500 | O                                                                                                | 4.73261000  | -0.89437700 | -0.43034500 |
| C                                                                                                | -3.92728600 | -2.12131800 | 1.21269800  | N                                                                                                | 0.35929300  | 1.04000400  | 2.48820600  |
| C                                                                                                | -4.36900300 | -0.65326400 | -0.62979000 | O                                                                                                | 0.26419800  | 1.60633500  | 3.55219800  |
| C                                                                                                | -4.83962200 | -1.53157500 | 0.34219000  | Cl                                                                                               | -2.74955800 | 0.96105700  | -1.75732700 |
| H                                                                                                | -4.24758400 | -2.81033600 | 1.98339100  | O                                                                                                | 0.26934600  | -2.63824400 | -1.30142700 |
| H                                                                                                | -5.04133100 | -0.17081800 | -1.32721200 | H                                                                                                | -0.53463200 | -2.88186900 | -1.77657600 |
| H                                                                                                | -5.89729200 | -1.75272900 | 0.41975100  | H                                                                                                | 1.00895100  | -2.93478000 | -1.84721500 |
| H                                                                                                | -1.84185000 | -2.25068100 | 1.73942500  | Am                                                                                               | 0.60394900  | -0.34356300 | -0.14320400 |
| N                                                                                                | 3.49154200  | -0.64861500 | -0.40078700 | Am(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>3</sub> ) <sup>+</sup> |             |             |             |
| O                                                                                                | 4.69159600  | -0.77896900 | -0.52635900 | O                                                                                                | 0.93997200  | -0.20591400 | -2.81504400 |
| N                                                                                                | 0.43115000  | 0.94311800  | 2.55087500  | H                                                                                                | 0.27409600  | -0.40661000 | -3.48271600 |
| O                                                                                                | 0.40777500  | 1.45211300  | 3.64765600  | O                                                                                                | 0.65474900  | -0.06871400 | 2.62348900  |
| O                                                                                                | 0.04963600  | -2.63609400 | -1.22965700 | O                                                                                                | 0.81607200  | 1.74058600  | 1.45643900  |
| H                                                                                                | -0.83236100 | -2.85234600 | -1.55641700 | O                                                                                                | 1.69301900  | 1.63552200  | -1.12042000 |
| H                                                                                                | 0.67148700  | -2.97398100 | -1.88698700 | O                                                                                                | 1.37715200  | -2.42945600 | 1.39568500  |
| H                                                                                                | -2.60013800 | 0.27254100  | -1.44382800 | O                                                                                                | 3.11598100  | -0.15161900 | 0.83431000  |
| Am                                                                                               | 0.53406200  | -0.35763900 | -0.12686000 | O                                                                                                | 2.81813600  | -1.20174800 | -1.02903500 |
|                                                                                                  |             |             |             | H                                                                                                | 1.74069700  | -0.67406700 | -3.08295500 |

|                                                                                                  |             |             |             |                                                                                                  |             |             |             |
|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                                | 1.54210900  | 2.53651000  | -0.81246200 | H                                                                                                | 1.29293800  | -3.21799900 | 0.86373200  |
| H                                                                                                | 0.99165300  | -3.27048400 | 1.12116300  | H                                                                                                | 0.79641200  | 1.85227500  | -2.05651000 |
| H                                                                                                | 1.45997400  | 1.57942600  | -2.05991200 | H                                                                                                | 1.43838700  | -2.34386200 | 2.13958900  |
| H                                                                                                | 1.32645800  | -2.38279500 | 2.35820200  | N                                                                                                | -2.05270600 | -1.14485800 | 0.01364400  |
| N                                                                                                | -2.16429600 | -0.88829900 | -0.09786100 | C                                                                                                | -2.48841100 | -2.11898400 | 0.83344700  |
| C                                                                                                | -2.50987600 | -1.89784000 | 0.72914100  | C                                                                                                | -2.97739300 | -0.38422300 | -0.59488700 |
| C                                                                                                | -3.14765300 | -0.25264000 | -0.77076500 | C                                                                                                | -3.83104800 | -2.36129400 | 1.07053200  |
| C                                                                                                | -3.81248100 | -2.32461400 | 0.92779200  | C                                                                                                | -4.34160000 | -0.56095600 | -0.40471200 |
| C                                                                                                | -4.48707600 | -0.63568100 | -0.61998300 | C                                                                                                | -4.80260000 | -1.56645900 | 0.44965500  |
| C                                                                                                | -4.82743600 | -1.67514900 | 0.23164500  | H                                                                                                | -4.10665200 | -3.16267000 | 1.74442300  |
| H                                                                                                | -4.01740700 | -3.14132300 | 1.60761900  | H                                                                                                | -5.03899200 | 0.08959000  | -0.91861400 |
| H                                                                                                | -5.25762500 | -0.11506800 | -1.17350700 | H                                                                                                | -1.72817100 | -2.71633800 | 1.32279600  |
| H                                                                                                | -5.86247100 | -1.97298700 | 0.35080700  | N                                                                                                | 3.50273300  | -0.50551100 | -0.46513400 |
| H                                                                                                | -1.70523200 | -2.39172200 | 1.26104200  | O                                                                                                | 4.70657400  | -0.55352300 | -0.60187800 |
| N                                                                                                | 3.64307600  | -0.76749600 | -0.14585900 | N                                                                                                | 0.15512900  | 0.81727000  | 2.57035000  |
| O                                                                                                | 4.83782900  | -0.93626100 | -0.24702300 | O                                                                                                | -0.00370800 | 1.32019700  | 3.65943000  |
| N                                                                                                | 0.75299400  | 1.20172700  | 2.61767700  | O                                                                                                | 0.39082100  | -2.77038700 | -1.21046200 |
| O                                                                                                | 0.78854100  | 1.85928400  | 3.63390600  | H                                                                                                | -0.42358400 | -3.10224200 | -1.60829800 |
| O                                                                                                | 0.38099500  | -2.64225200 | -1.11675500 | H                                                                                                | 1.10643700  | -3.01087300 | -1.81295200 |
| H                                                                                                | -0.37513200 | -2.80534900 | -1.69388600 | Am                                                                                               | 0.53715300  | -0.44273000 | -0.10939100 |
| H                                                                                                | 1.16091100  | -2.95487300 | -1.59359500 | H                                                                                                | -2.60701200 | 0.39725400  | -1.25004500 |
| C                                                                                                | -2.79672600 | 0.87748800  | -1.72488500 | C                                                                                                | -6.28422600 | -1.77690900 | 0.69828000  |
| H                                                                                                | -1.73499000 | 1.09737800  | -1.61674400 | H                                                                                                | -6.81809400 | -1.02782400 | 0.10540300  |
| C                                                                                                | -3.03568300 | 0.45004100  | -3.18631100 | C                                                                                                | -6.74399300 | -3.16798800 | 0.22443000  |
| H                                                                                                | -4.09559600 | 0.25813600  | -3.37510000 | H                                                                                                | -7.82320000 | -3.27123300 | 0.36316800  |
| H                                                                                                | -2.71017800 | 1.24014300  | -3.86780100 | H                                                                                                | -6.52053700 | -3.32080300 | -0.83418700 |
| H                                                                                                | -2.48172600 | -0.46096600 | -3.42834700 | H                                                                                                | -6.25601300 | -3.96410900 | 0.79362700  |
| C                                                                                                | -3.55787200 | 2.17388400  | -1.39126700 | C                                                                                                | -6.64018200 | -1.54544600 | 2.17918500  |
| H                                                                                                | -3.37971300 | 2.48320400  | -0.35831100 | H                                                                                                | -6.33500900 | -0.54984200 | 2.51047600  |
| H                                                                                                | -3.22262200 | 2.97936100  | -2.04956700 | H                                                                                                | -7.71997000 | -1.63565300 | 2.32207300  |
| H                                                                                                | -4.63592900 | 2.05953300  | -1.53121300 | H                                                                                                | -6.15468300 | -2.28221200 | 2.82531200  |
| Am                                                                                               | 0.71276500  | -0.35606100 | 0.05571900  |                                                                                                  |             |             |             |
| Am(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>4</sub> ) <sup>+</sup> |             |             |             | Am(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>5</sub> ) <sup>+</sup> |             |             |             |
| O                                                                                                | 0.58267700  | -0.18648600 | -2.81491100 | O                                                                                                | 0.53336000  | -0.11706100 | -2.85771700 |
| H                                                                                                | -0.09794200 | -0.52687900 | -3.40758100 | H                                                                                                | -0.21165400 | -0.35566000 | -3.42231800 |
| O                                                                                                | -0.04460500 | -0.43005100 | 2.35764500  | O                                                                                                | 0.03244700  | -0.23398000 | 2.32962500  |
| O                                                                                                | 0.53381200  | 1.48825400  | 1.55259300  | O                                                                                                | 0.53750900  | 1.64535600  | 1.39446900  |
| O                                                                                                | 1.06118200  | 1.80086800  | -1.12847200 | O                                                                                                | 1.39015000  | 1.77931500  | -1.22263700 |
| O                                                                                                | 1.60824200  | -2.36449700 | 1.18915800  | O                                                                                                | 1.34876500  | -2.38378500 | 1.17314200  |
| O                                                                                                | 2.94788200  | 0.09995200  | 0.50651800  | O                                                                                                | 2.88125600  | -0.02549800 | 0.56987100  |
| O                                                                                                | 2.70310300  | -1.06341500 | -1.29862700 | O                                                                                                | 2.61256300  | -1.11318500 | -1.27861000 |
| H                                                                                                | 1.42778400  | -0.50962200 | -3.15328200 | H                                                                                                | 1.31730500  | -0.51688900 | -3.25506400 |
| H                                                                                                | 0.86054800  | 2.64258200  | -0.70343900 | H                                                                                                | 1.27027400  | 2.63158900  | -0.78758100 |
|                                                                                                  |             |             |             | H                                                                                                | 1.00576300  | -3.23147300 | 0.86330500  |

|                                                                                                  |             |             |             |                                                                                                  |             |             |             |
|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                                | 1.07335800  | 1.85856600  | -2.13248300 | C                                                                                                | -4.61149700 | -0.52995500 | -0.40341500 |
| H                                                                                                | 1.23128200  | -2.35503700 | 2.13059900  | C                                                                                                | -4.92456800 | -1.54708400 | 0.48665100  |
| N                                                                                                | -2.20927700 | -1.02430300 | 0.08670900  | H                                                                                                | -4.08949700 | -3.05840600 | 1.79631800  |
| C                                                                                                | -2.57708300 | -1.99309100 | 0.94631600  | H                                                                                                | -5.39986100 | 0.02551000  | -0.88877500 |
| C                                                                                                | -3.17334400 | -0.33639900 | -0.54202900 | H                                                                                                | -5.96135700 | -1.78187200 | 0.69632600  |
| C                                                                                                | -3.89642700 | -2.31521300 | 1.21352300  | H                                                                                                | -1.76873400 | -2.43476400 | 1.25647400  |
| C                                                                                                | -4.53559000 | -0.58721300 | -0.33271100 | N                                                                                                | 3.54785100  | -0.73931700 | -0.28556100 |
| C                                                                                                | -4.88987800 | -1.59085300 | 0.55662400  | O                                                                                                | 4.74584900  | -0.90619000 | -0.35058400 |
| H                                                                                                | -4.13396300 | -3.10422900 | 1.91388300  | N                                                                                                | 0.38088100  | 1.08387600  | 2.46573400  |
| H                                                                                                | -5.29398500 | -0.01719200 | -0.84803600 | O                                                                                                | 0.29788600  | 1.67675600  | 3.51678900  |
| H                                                                                                | -5.93704500 | -1.80411800 | 0.73498500  | O                                                                                                | 0.40388400  | -2.71175600 | -1.27960000 |
| H                                                                                                | -1.77278900 | -2.52461000 | 1.44002200  | H                                                                                                | -0.33560400 | -2.95660000 | -1.84936900 |
| N                                                                                                | 3.42273100  | -0.62933400 | -0.40973900 | H                                                                                                | 1.20800400  | -2.97557000 | -1.74553800 |
| O                                                                                                | 4.62488900  | -0.74109700 | -0.52330300 | Am                                                                                               | 0.61343200  | -0.35303700 | -0.14334200 |
| N                                                                                                | 0.23011500  | 1.02318100  | 2.46745600  | S                                                                                                | -2.74631800 | 1.02752200  | -1.79255200 |
| O                                                                                                | 0.13522300  | 1.57999500  | 3.53703100  | C                                                                                                | -4.30567500 | 1.77388800  | -2.36845800 |
| O                                                                                                | 0.25142300  | -2.68388700 | -1.29364800 | H                                                                                                | -4.86184100 | 2.21139300  | -1.54057200 |
| H                                                                                                | -0.54291500 | -2.96317400 | -1.76542100 | H                                                                                                | -3.99854900 | 2.56670000  | -3.04986700 |
| H                                                                                                | 1.00155300  | -2.93253800 | -1.84882900 | H                                                                                                | -4.91430600 | 1.05274500  | -2.91208200 |
| Am                                                                                               | 0.46765600  | -0.35626400 | -0.16473500 |                                                                                                  |             |             |             |
| O                                                                                                | -2.69664000 | 0.60369400  | -1.37959500 | Am(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>7</sub> ) <sup>+</sup> |             |             |             |
| C                                                                                                | -3.62116900 | 1.45138600  | -2.07949900 | O                                                                                                | 0.71144300  | -0.09047100 | -2.85191900 |
| H                                                                                                | -4.22956900 | 2.02467900  | -1.37658000 | H                                                                                                | -0.08321100 | -0.20167000 | -3.38724100 |
| H                                                                                                | -3.00555300 | 2.12684000  | -2.66738900 | O                                                                                                | 0.16769700  | -0.16373100 | 2.33600400  |
| H                                                                                                | -4.26105400 | 0.86510700  | -2.74252000 | O                                                                                                | 0.72279200  | 1.67737500  | 1.35676600  |
|                                                                                                  |             |             |             | O                                                                                                | 1.65521700  | 1.73351100  | -1.17924400 |
| Am(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>6</sub> ) <sup>+</sup> |             |             |             | O                                                                                                | 1.27538000  | -2.39977500 | 1.18877400  |
| O                                                                                                | 0.66952500  | -0.12559700 | -2.84155400 | O                                                                                                | 2.99222400  | -0.14676500 | 0.68410900  |
| H                                                                                                | -0.12815900 | -0.24405700 | -3.37233700 | O                                                                                                | 2.76394900  | -1.18451300 | -1.19765700 |
| O                                                                                                | 0.15390500  | -0.17011500 | 2.36453700  | H                                                                                                | 1.42268000  | -0.55336400 | -3.31105600 |
| O                                                                                                | 0.70653400  | 1.66676700  | 1.37468000  | H                                                                                                | 1.60772700  | 2.58906500  | -0.73698900 |
| O                                                                                                | 1.60836800  | 1.71815500  | -1.19957600 | H                                                                                                | 0.90669000  | -3.23307900 | 0.86968200  |
| O                                                                                                | 1.29793600  | -2.39129400 | 1.22888800  | H                                                                                                | 1.40525200  | 1.85049800  | -2.10527500 |
| O                                                                                                | 2.99271700  | -0.12316400 | 0.68010700  | H                                                                                                | 1.16570000  | -2.37319600 | 2.14705200  |
| O                                                                                                | 2.75113400  | -1.17264900 | -1.19341500 | N                                                                                                | -2.28794600 | -0.88617300 | 0.02195200  |
| H                                                                                                | 1.37321100  | -0.60602000 | -3.29500800 | C                                                                                                | -2.60228400 | -1.86454300 | 0.88141700  |
| H                                                                                                | 1.49912800  | 2.59130400  | -0.80504500 | C                                                                                                | -3.30367100 | -0.26958700 | -0.60489300 |
| H                                                                                                | 0.95352100  | -3.23610600 | 0.91279400  | C                                                                                                | -3.91143700 | -2.26076800 | 1.14390800  |
| H                                                                                                | 1.34510400  | 1.76754000  | -2.12888900 | C                                                                                                | -4.63926100 | -0.59033800 | -0.40563600 |
| H                                                                                                | 1.17233400  | -2.35797800 | 2.18517400  | C                                                                                                | -4.94818200 | -1.61220600 | 0.48976300  |
| N                                                                                                | -2.25916400 | -0.91563900 | -0.06362000 | H                                                                                                | -4.09891500 | -3.06099900 | 1.84760600  |
| C                                                                                                | -2.58991500 | -1.90281100 | 0.79106700  | H                                                                                                | -5.41531400 | -0.05701600 | -0.93510300 |
| C                                                                                                | -3.26534800 | -0.24259400 | -0.65785500 | H                                                                                                | -5.97958000 | -1.88968800 | 0.66718100  |
| C                                                                                                | -3.89469500 | -2.25550000 | 1.09813100  | H                                                                                                | -1.77813600 | -2.35444500 | 1.38478100  |

|                                                                                                  |             |             |             |                                                                                                  |             |             |             |
|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| N                                                                                                | 3.55238400  | -0.77208500 | -0.27324600 | H                                                                                                | -2.68770100 | 0.49303000  | -1.23265200 |
| O                                                                                                | 4.74729200  | -0.96512400 | -0.31544100 | Cm                                                                                               | 0.50037400  | -0.35313200 | -0.15587100 |
| N                                                                                                | 0.39920100  | 1.08816500  | 2.44528100  |                                                                                                  |             |             |             |
| O                                                                                                | 0.32214500  | 1.67392700  | 3.50077300  | Cm(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>2</sub> ) <sup>+</sup> |             |             |             |
| O                                                                                                | 0.38140000  | -2.67222000 | -1.31449100 | O                                                                                                | 0.67592200  | -0.07420300 | -2.84714200 |
| H                                                                                                | -0.35221200 | -2.90666700 | -1.89627300 | H                                                                                                | -0.08842300 | -0.25617300 | -3.40727800 |
| H                                                                                                | 1.18861400  | -2.93882300 | -1.77397100 | O                                                                                                | 0.24510300  | -0.14671100 | 2.32447700  |
| Am                                                                                               | 0.62536000  | -0.33499200 | -0.17417200 | O                                                                                                | 0.68367500  | 1.73637300  | 1.36668800  |
| C                                                                                                | -2.93019400 | 0.83311400  | -1.57394700 | O                                                                                                | 1.64579500  | 1.72929300  | -1.16513300 |
| F                                                                                                | -2.14671600 | 0.37098100  | -2.58345000 | O                                                                                                | 1.26964000  | -2.40163100 | 1.15706500  |
| F                                                                                                | -4.01106400 | 1.38880700  | -2.14437700 | O                                                                                                | 2.96390000  | -0.11746000 | 0.68403700  |
| F                                                                                                | -2.24201300 | 1.82553600  | -0.97089100 | O                                                                                                | 2.70854800  | -1.15652700 | -1.19380500 |
|                                                                                                  |             |             |             | H                                                                                                | 1.43076400  | -0.50484500 | -3.26750800 |
| Cm(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>1</sub> ) <sup>+</sup> |             |             |             | H                                                                                                | 1.59419900  | 2.55961800  | -0.67692300 |
| O                                                                                                | 0.59331800  | -0.13070400 | -2.82948500 | H                                                                                                | 0.90091100  | -3.23166800 | 0.82971600  |
| H                                                                                                | -0.11724800 | -0.40788600 | -3.42004700 | H                                                                                                | 1.36186900  | 1.89123200  | -2.07428300 |
| O                                                                                                | 0.29840900  | -0.21212800 | 2.37753500  | H                                                                                                | 1.17164800  | -2.38874100 | 2.11670600  |
| O                                                                                                | 0.58207500  | 1.69436300  | 1.40652600  | N                                                                                                | -2.26077700 | -0.89712800 | 0.06741900  |
| O                                                                                                | 1.48550700  | 1.74298100  | -1.17308100 | C                                                                                                | -2.60208700 | -1.88034300 | 0.92542600  |
| O                                                                                                | 1.39097400  | -2.39210400 | 1.13948000  | C                                                                                                | -3.24706100 | -0.28449800 | -0.57484800 |
| O                                                                                                | 2.91594100  | -0.04310300 | 0.64102400  | C                                                                                                | -3.91392600 | -2.26430800 | 1.15377100  |
| O                                                                                                | 2.63414100  | -1.10813700 | -1.21886300 | C                                                                                                | -4.59594300 | -0.58536100 | -0.41848400 |
| H                                                                                                | 1.40532300  | -0.51942700 | -3.17926300 | C                                                                                                | -4.92915500 | -1.60195600 | 0.46797300  |
| H                                                                                                | 1.41914400  | 2.57190400  | -0.68441500 | H                                                                                                | -4.12928300 | -3.06259400 | 1.85123100  |
| H                                                                                                | 0.99881800  | -3.21877700 | 0.83024200  | H                                                                                                | -5.34851100 | -0.04277600 | -0.97249900 |
| H                                                                                                | 1.17640100  | 1.89770900  | -2.07507800 | H                                                                                                | -5.96749000 | -1.87076800 | 0.61800600  |
| H                                                                                                | 1.27504700  | -2.35381900 | 2.09693000  | H                                                                                                | -1.78598000 | -2.37006100 | 1.44158500  |
| N                                                                                                | -2.16144700 | -0.98394800 | 0.11670600  | N                                                                                                | 3.51238400  | -0.73007600 | -0.28562200 |
| C                                                                                                | -2.59875100 | -1.94635500 | 0.94649100  | O                                                                                                | 4.70856500  | -0.90326100 | -0.35931600 |
| C                                                                                                | -3.07238800 | -0.27781400 | -0.57372600 | N                                                                                                | 0.43563600  | 1.11324400  | 2.44966900  |
| C                                                                                                | -3.94609000 | -2.24008200 | 1.11260200  | O                                                                                                | 0.38656700  | 1.66800500  | 3.52616800  |
| C                                                                                                | -4.43895500 | -0.50417800 | -0.46538500 | Cl                                                                                               | -2.80277900 | 0.99369700  | -1.70294000 |
| C                                                                                                | -4.88443300 | -1.50543700 | 0.39305600  | O                                                                                                | 0.28331100  | -2.68181500 | -1.33339000 |
| H                                                                                                | -4.24648200 | -3.02723200 | 1.79191900  | H                                                                                                | -0.50458200 | -2.91582100 | -1.83921600 |
| H                                                                                                | -5.13269800 | 0.09298900  | -1.04274900 | H                                                                                                | 1.03823100  | -2.95970000 | -1.86775600 |
| H                                                                                                | -5.94309600 | -1.70901100 | 0.50003100  | Cm                                                                                               | 0.59077500  | -0.32856100 | -0.18342200 |
| H                                                                                                | -1.84018600 | -2.49442100 | 1.49303000  |                                                                                                  |             |             |             |
| N                                                                                                | 3.44956000  | -0.65120800 | -0.33638000 | Cm(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>3</sub> ) <sup>+</sup> |             |             |             |
| O                                                                                                | 4.64887800  | -0.79720000 | -0.44287100 | O                                                                                                | 0.96034300  | -0.15994000 | -2.69517000 |
| N                                                                                                | 0.44264000  | 1.05365600  | 2.49938100  | H                                                                                                | 0.28605200  | -0.46290400 | -3.31428500 |
| O                                                                                                | 0.44940700  | 1.60069500  | 3.58123200  | O                                                                                                | 0.77043300  | -0.06951800 | 2.57204000  |
| O                                                                                                | 0.23975600  | -2.73147500 | -1.27004200 | O                                                                                                | 0.90976900  | 1.77499600  | 1.46199500  |
| H                                                                                                | -0.56267200 | -3.00447500 | -1.73132900 | O                                                                                                | 1.90889700  | 1.67059800  | -1.04644500 |
| H                                                                                                | 0.97721100  | -2.99467500 | -1.83523100 | O                                                                                                | 1.44734300  | -2.40141600 | 1.35423700  |

|                                                                                                  |             |             |             |                                                                                                  |             |             |             |
|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| O                                                                                                | 3.20800900  | -0.13575700 | 0.84939600  | O                                                                                                | 2.70877700  | -0.99197300 | -1.25920000 |
| O                                                                                                | 2.92710800  | -1.20785400 | -1.00384700 | H                                                                                                | 1.43210600  | -0.39203400 | -3.21885500 |
| H                                                                                                | 1.79208300  | -0.55183700 | -2.99242300 | H                                                                                                | 1.20849300  | 2.63078600  | -0.57221800 |
| H                                                                                                | 1.88078500  | 2.49946100  | -0.55345000 | H                                                                                                | 1.12879200  | -3.28307300 | 0.63576600  |
| H                                                                                                | 1.05230100  | -3.21682900 | 1.02004100  | H                                                                                                | 1.03636100  | 1.98610100  | -1.98582800 |
| H                                                                                                | 1.62037600  | 1.84385600  | -1.95175800 | H                                                                                                | 1.34102200  | -2.49956000 | 1.96633400  |
| H                                                                                                | 1.32029300  | -2.37504200 | 2.31025000  | N                                                                                                | -2.10412300 | -1.04216500 | 0.10644300  |
| N                                                                                                | -2.13529800 | -0.79704200 | -0.06054000 | C                                                                                                | -2.51971200 | -2.06777900 | 0.87140400  |
| C                                                                                                | -2.47482700 | -1.76095000 | 0.81888700  | C                                                                                                | -3.04547100 | -0.26588900 | -0.45447400 |
| C                                                                                                | -3.10575800 | -0.26042300 | -0.83026000 | C                                                                                                | -3.85712500 | -2.34833700 | 1.09876200  |
| C                                                                                                | -3.76393500 | -2.24815300 | 0.96782700  | C                                                                                                | -4.40551100 | -0.47730000 | -0.27039500 |
| C                                                                                                | -4.42957100 | -0.70833300 | -0.73488300 | C                                                                                                | -4.84544600 | -1.53931300 | 0.52453200  |
| C                                                                                                | -4.76489100 | -1.70949000 | 0.16398800  | H                                                                                                | -4.11530600 | -3.19261400 | 1.72546000  |
| H                                                                                                | -3.97117000 | -3.02638900 | 1.69074100  | H                                                                                                | -5.11629200 | 0.18874400  | -0.74472700 |
| H                                                                                                | -5.19045400 | -0.26860100 | -1.36706700 | H                                                                                                | -1.74547000 | -2.67925800 | 1.31984700  |
| H                                                                                                | -5.78731300 | -2.06086800 | 0.23863200  | N                                                                                                | 3.48736400  | -0.54370100 | -0.34056800 |
| H                                                                                                | -1.67362500 | -2.16060000 | 1.43147800  | O                                                                                                | 4.69311300  | -0.63071500 | -0.42842800 |
| N                                                                                                | 3.74138700  | -0.78312300 | -0.10271200 | N                                                                                                | 0.27408000  | 0.78631900  | 2.57307000  |
| O                                                                                                | 4.93235500  | -0.99462100 | -0.16922400 | O                                                                                                | 0.18607100  | 1.24550900  | 3.69163200  |
| N                                                                                                | 0.86845900  | 1.20084900  | 2.60225900  | O                                                                                                | 0.35068400  | -2.73242800 | -1.39268700 |
| O                                                                                                | 0.92315000  | 1.82348800  | 3.64246700  | H                                                                                                | -0.45657400 | -3.01444300 | -1.84033500 |
| O                                                                                                | 0.56947700  | -2.72966800 | -1.14025400 | H                                                                                                | 1.07610000  | -2.93941000 | -1.99554900 |
| H                                                                                                | -0.18608600 | -2.99868600 | -1.67660200 | H                                                                                                | -2.69373400 | 0.55775700  | -1.06619000 |
| H                                                                                                | 1.35880600  | -2.99275000 | -1.63038900 | C                                                                                                | -6.32347200 | -1.80100400 | 0.74471900  |
| Cm                                                                                               | 0.80987400  | -0.34062500 | -0.00394900 | H                                                                                                | -6.86804000 | -0.98993300 | 0.25135700  |
| C                                                                                                | -2.75594400 | 0.84528500  | -1.81358100 | C                                                                                                | -6.75505700 | -3.12523900 | 0.08644900  |
| H                                                                                                | -1.69878300 | 1.07534700  | -1.69197700 | H                                                                                                | -7.83148200 | -3.27067300 | 0.20880500  |
| C                                                                                                | -2.96900800 | 0.39309600  | -3.27093400 | H                                                                                                | -6.53031700 | -3.12816300 | -0.98293700 |
| H                                                                                                | -4.02575700 | 0.20711800  | -3.48118100 | H                                                                                                | -6.24618500 | -3.97879800 | 0.54324600  |
| H                                                                                                | -2.62273200 | 1.16929000  | -3.95832300 | C                                                                                                | -6.69223100 | -1.77297300 | 2.23923300  |
| H                                                                                                | -2.41851500 | -0.52606700 | -3.48839300 | H                                                                                                | -6.39767100 | -0.82851800 | 2.70320200  |
| C                                                                                                | -3.53273800 | 2.14157800  | -1.51494800 | H                                                                                                | -7.77255600 | -1.88845400 | 2.35811200  |
| H                                                                                                | -3.36585800 | 2.47553100  | -0.48781500 | H                                                                                                | -6.20868000 | -2.58633800 | 2.78739600  |
| H                                                                                                | -3.20054800 | 2.93609300  | -2.18833600 | Cm                                                                                               | 0.53261500  | -0.39995100 | -0.17731500 |
| H                                                                                                | -4.60841300 | 2.01079900  | -1.66014800 |                                                                                                  |             |             |             |
|                                                                                                  |             |             |             | Cm(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>5</sub> ) <sup>+</sup> |             |             |             |
| Cm(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>4</sub> ) <sup>+</sup> |             |             |             | O                                                                                                | 0.52538100  | -0.08599400 | -2.84010900 |
| O                                                                                                | 0.60183700  | -0.09062400 | -2.82881900 | H                                                                                                | -0.21335200 | -0.32733700 | -3.41164100 |
| H                                                                                                | -0.09943600 | -0.36205700 | -3.43284400 | O                                                                                                | 0.26001100  | -0.19656700 | 2.36607200  |
| O                                                                                                | 0.18880800  | -0.47037200 | 2.34488800  | O                                                                                                | 0.53002400  | 1.71537400  | 1.40182100  |
| O                                                                                                | 0.46035800  | 1.51750600  | 1.54546300  | O                                                                                                | 1.43518000  | 1.76190500  | -1.17659800 |
| O                                                                                                | 1.33317300  | 1.82128800  | -1.08150900 | O                                                                                                | 1.34298200  | -2.38715900 | 1.11144100  |
| O                                                                                                | 1.49296000  | -2.47184500 | 1.01356000  | O                                                                                                | 2.86237600  | -0.02489900 | 0.62813500  |
| O                                                                                                | 2.90865700  | -0.00671300 | 0.65528000  | O                                                                                                | 2.57717700  | -1.07143500 | -1.24131600 |

|                                                                                                  |             |             |             |                                                                                                  |             |             |             |
|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                                | 1.31382100  | -0.48715000 | -3.22697500 | C                                                                                                | -2.59172200 | -1.85494000 | 0.84283800  |
| H                                                                                                | 1.35049600  | 2.59261100  | -0.69380500 | C                                                                                                | -3.28467300 | -0.24793000 | -0.65756400 |
| H                                                                                                | 0.96442500  | -3.21477500 | 0.78818100  | C                                                                                                | -3.89252900 | -2.22954200 | 1.14131700  |
| H                                                                                                | 1.11969300  | 1.90167500  | -2.07917100 | C                                                                                                | -4.62754100 | -0.55964100 | -0.41497900 |
| H                                                                                                | 1.24482100  | -2.37365400 | 2.07135100  | C                                                                                                | -4.92922900 | -1.56208600 | 0.49584300  |
| N                                                                                                | -2.24589100 | -1.00032400 | 0.11485900  | H                                                                                                | -4.07957100 | -3.01809700 | 1.85777400  |
| C                                                                                                | -2.61207600 | -1.96364600 | 0.98017300  | H                                                                                                | -5.42148000 | -0.03540100 | -0.92545300 |
| C                                                                                                | -3.20687500 | -0.34180500 | -0.54799800 | H                                                                                                | -5.96312500 | -1.81746100 | 0.69557900  |
| C                                                                                                | -3.93087900 | -2.31142900 | 1.21821300  | H                                                                                                | -1.76313300 | -2.35237500 | 1.33247200  |
| C                                                                                                | -4.56808700 | -0.62078200 | -0.37121600 | N                                                                                                | 3.53127500  | -0.74454800 | -0.24159400 |
| C                                                                                                | -4.92229800 | -1.61994900 | 0.52366000  | O                                                                                                | 4.72696700  | -0.93143400 | -0.29214700 |
| H                                                                                                | -4.16998000 | -3.09537500 | 1.92371000  | N                                                                                                | 0.42565800  | 1.09735800  | 2.45083300  |
| H                                                                                                | -5.32554100 | -0.07660300 | -0.91520100 | O                                                                                                | 0.36731800  | 1.65631100  | 3.52480300  |
| H                                                                                                | -5.96870800 | -1.85552500 | 0.67666800  | O                                                                                                | 0.37266600  | -2.72369900 | -1.32141100 |
| H                                                                                                | -1.80622700 | -2.46864100 | 1.49918800  | H                                                                                                | -0.37489600 | -2.97154200 | -1.87899300 |
| N                                                                                                | 3.39490600  | -0.61678700 | -0.36017100 | H                                                                                                | 1.16736800  | -2.99179500 | -1.80028300 |
| O                                                                                                | 4.59468000  | -0.74920700 | -0.47719900 | S                                                                                                | -2.77139300 | 1.00700300  | -1.81087000 |
| N                                                                                                | 0.39846200  | 1.06993200  | 2.49237100  | C                                                                                                | -4.33552200 | 1.73878400  | -2.39330100 |
| O                                                                                                | 0.40750700  | 1.61197800  | 3.57660000  | H                                                                                                | -4.89846100 | 2.16943500  | -1.56634300 |
| O                                                                                                | 0.20195900  | -2.70855200 | -1.30435700 | H                                                                                                | -4.03419100 | 2.53578200  | -3.07236700 |
| H                                                                                                | -0.60325800 | -2.97524600 | -1.76449300 | H                                                                                                | -4.93562200 | 1.01264700  | -2.93968400 |
| H                                                                                                | 0.93573000  | -2.95510900 | -1.88157100 | Cm                                                                                               | 0.60611700  | -0.33688800 | -0.18429400 |
| O                                                                                                | -2.72713700 | 0.59685400  | -1.38574000 | Cm(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>7</sub> ) <sup>+</sup> |             |             |             |
| C                                                                                                | -3.64926100 | 1.40735900  | -2.13121300 | O                                                                                                | 0.72344300  | -0.07321500 | -2.86771700 |
| H                                                                                                | -4.29451900 | 1.97813500  | -1.45980100 | H                                                                                                | -0.06552900 | -0.17015800 | -3.41417000 |
| H                                                                                                | -3.03181700 | 2.08738500  | -2.71197400 | O                                                                                                | 0.21862400  | -0.15028300 | 2.29635100  |
| H                                                                                                | -4.25234700 | 0.79264900  | -2.80298300 | O                                                                                                | 0.70493000  | 1.72770300  | 1.35065400  |
| Cm                                                                                               | 0.44830800  | -0.33428000 | -0.16179400 | O                                                                                                | 1.70877000  | 1.72655700  | -1.16449600 |
| Cm(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>6</sub> ) <sup>+</sup> |             |             |             | O                                                                                                | 1.25615600  | -2.38958600 | 1.15026100  |
| O                                                                                                | 0.68981900  | -0.09690100 | -2.85233600 | O                                                                                                | 2.96141600  | -0.13580700 | 0.71406800  |
| H                                                                                                | -0.10259000 | -0.22897300 | -3.38772000 | O                                                                                                | 2.74797200  | -1.17435400 | -1.16875200 |
| O                                                                                                | 0.22743800  | -0.16141300 | 2.32717200  | H                                                                                                | 1.43785200  | -0.53161000 | -3.32637100 |
| O                                                                                                | 0.69213000  | 1.71645100  | 1.36929000  | H                                                                                                | 1.67829700  | 2.55645100  | -0.67391100 |
| O                                                                                                | 1.66386000  | 1.71208900  | -1.17089000 | H                                                                                                | 0.88484600  | -3.22044600 | 0.82793500  |
| O                                                                                                | 1.27737100  | -2.40341400 | 1.17300700  | H                                                                                                | 1.47096800  | 1.90336500  | -2.08361300 |
| O                                                                                                | 2.97201700  | -0.12075900 | 0.71419300  | H                                                                                                | 1.14471100  | -2.36276600 | 2.10810300  |
| O                                                                                                | 2.74015600  | -1.16752100 | -1.16235700 | N                                                                                                | -2.30603200 | -0.87204600 | 0.04049200  |
| H                                                                                                | 1.40416700  | -0.56596700 | -3.30105700 | C                                                                                                | -2.60836300 | -1.84619100 | 0.90757300  |
| H                                                                                                | 1.60829100  | 2.55575700  | -0.70690700 | C                                                                                                | -3.32545400 | -0.27405200 | -0.59601300 |
| H                                                                                                | 0.91511800  | -3.23357100 | 0.83855800  | C                                                                                                | -3.91365200 | -2.25660200 | 1.16860000  |
| H                                                                                                | 1.40340800  | 1.85007300  | -2.09115400 | C                                                                                                | -4.65784100 | -0.60701700 | -0.39760900 |
| H                                                                                                | 1.15437800  | -2.38639400 | 2.12973500  | C                                                                                                | -4.95611000 | -1.62493700 | 0.50627200  |
| N                                                                                                | -2.27372900 | -0.88531600 | -0.03505600 | H                                                                                                | -4.09459400 | -3.05493300 | 1.87613900  |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                   | -5.43842300 | -0.08819700 | -0.93497900 | O                                                                                   | -1.05069600 | 4.22857900  | -0.31066700 |
| H                                                                                   | -5.98452300 | -1.91410400 | 0.68244300  | H                                                                                   | 2.36096500  | 0.68762200  | 1.56565400  |
| H                                                                                   | -1.77510800 | -2.31982700 | 1.41186400  | Am                                                                                  | -0.68086300 | 0.08762100  | 0.09992500  |
| N                                                                                   | 3.52803800  | -0.77120600 | -0.22970400 |                                                                                     |             |             |             |
| O                                                                                   | 4.71961800  | -0.98596100 | -0.25322300 | Am(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>2</sub> ) |             |             |             |
| N                                                                                   | 0.43144800  | 1.10461900  | 2.42813300  | O                                                                                   | -0.71146600 | 2.30301900  | -1.15523600 |
| O                                                                                   | 0.37982400  | 1.65699700  | 3.50612800  | O                                                                                   | -1.85827400 | 0.03340800  | 2.30002700  |
| O                                                                                   | 0.37542500  | -2.69473300 | -1.34561800 | O                                                                                   | 0.06441800  | -2.10846200 | -0.91124600 |
| H                                                                                   | -0.35033700 | -2.93469300 | -1.93474700 | O                                                                                   | -0.21198200 | -2.07492100 | 1.23154000  |
| H                                                                                   | 1.18735800  | -2.95503300 | -1.79984900 | O                                                                                   | -1.17886500 | -0.17160300 | -2.48093100 |
| C                                                                                   | -2.95182900 | 0.80998700  | -1.58417700 | O                                                                                   | -1.13725000 | 2.41748200  | 0.96214800  |
| F                                                                                   | -2.16954900 | 0.32141800  | -2.58288900 | O                                                                                   | -2.80040400 | -1.43747900 | -0.19212400 |
| F                                                                                   | -4.03063900 | 1.35733600  | -2.16563200 | O                                                                                   | -3.21404600 | 0.67971300  | -0.35763300 |
| F                                                                                   | -2.25911600 | 1.81160000  | -1.00217900 | H                                                                                   | -1.66330600 | -0.67084500 | 2.93003400  |
| Cm                                                                                  | 0.61041300  | -0.31953300 | -0.21959000 | H                                                                                   | -1.93983700 | 0.85118400  | 2.80552100  |
|                                                                                     |             |             |             | H                                                                                   | -1.40757600 | -1.04110900 | -2.83064700 |
| Am(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>1</sub> ) |             |             |             | H                                                                                   | -1.72693700 | 0.47471600  | -2.94175900 |
| O                                                                                   | -0.53927500 | 2.28742100  | -1.16261800 | N                                                                                   | 2.09396800  | 0.41037800  | -0.28262300 |
| O                                                                                   | -1.81958100 | 0.09824600  | 2.36229100  | C                                                                                   | 2.54221900  | 0.41911000  | -1.55544900 |
| O                                                                                   | 0.12023800  | -2.17863400 | -0.68228900 | C                                                                                   | 2.99026600  | 0.59947500  | 0.67673400  |
| O                                                                                   | -0.12359700 | -2.00909500 | 1.45873200  | C                                                                                   | 3.87372100  | 0.61068800  | -1.88749400 |
| O                                                                                   | -0.82275700 | -0.21191900 | -2.39411400 | C                                                                                   | 4.34962700  | 0.79842700  | 0.45672100  |
| O                                                                                   | -1.13144600 | 2.42528700  | 0.91296500  | C                                                                                   | 4.79386200  | 0.80311400  | -0.85961600 |
| O                                                                                   | -2.69770200 | -1.45973800 | -0.20295400 | H                                                                                   | 4.17712800  | 0.60887500  | -2.92586700 |
| O                                                                                   | -3.11477200 | 0.64899500  | -0.45173800 | H                                                                                   | 5.02591000  | 0.94493500  | 1.28678100  |
| H                                                                                   | -1.63778700 | -0.59312300 | 3.00989200  | H                                                                                   | 5.84393500  | 0.95602800  | -1.07622500 |
| H                                                                                   | -1.96671500 | 0.91611300  | 2.85185900  | H                                                                                   | 1.79444700  | 0.26624100  | -2.32409100 |
| H                                                                                   | -1.03258900 | -1.07123000 | -2.77959800 | N                                                                                   | -3.67056900 | -0.51161000 | -0.31570200 |
| H                                                                                   | -1.22960500 | 0.46205700  | -2.95189000 | O                                                                                   | -4.85997800 | -0.74993400 | -0.38886200 |
| N                                                                                   | 1.91205400  | 0.27655900  | -0.41299300 | N                                                                                   | 0.10429900  | -2.75132900 | 0.19452300  |
| C                                                                                   | 2.39289600  | 0.12163000  | -1.65849300 | O                                                                                   | 0.41922100  | -3.91852500 | 0.25228100  |
| C                                                                                   | 2.77915700  | 0.56867200  | 0.57185700  | N                                                                                   | -0.99991500 | 3.03679000  | -0.14608300 |
| C                                                                                   | 3.74195200  | 0.25043700  | -1.96268200 | O                                                                                   | -1.13526400 | 4.23629400  | -0.23966700 |
| C                                                                                   | 4.14361000  | 0.71421000  | 0.35409000  | Cl                                                                                  | 2.40600600  | 0.59981000  | 2.34013900  |
| C                                                                                   | 4.63489100  | 0.55232500  | -0.93822700 | Am                                                                                  | -0.76349200 | 0.07713500  | 0.02065700  |
| H                                                                                   | 4.07868000  | 0.11719000  | -2.98270800 |                                                                                     |             |             |             |
| H                                                                                   | 4.80003400  | 0.94994500  | 1.18162400  | Am(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>3</sub> ) |             |             |             |
| H                                                                                   | 5.69323900  | 0.66009300  | -1.14323800 | O                                                                                   | -0.52303800 | 2.33579000  | -1.02370300 |
| H                                                                                   | 1.66328900  | -0.10869600 | -2.42515300 | O                                                                                   | -1.90203300 | 0.05269200  | 2.33136900  |
| N                                                                                   | -3.56274600 | -0.54583600 | -0.41340300 | O                                                                                   | 0.14407400  | -2.09371600 | -0.76656500 |
| O                                                                                   | -4.74225000 | -0.79716600 | -0.56908300 | O                                                                                   | -0.44997700 | -2.14625100 | 1.31182100  |
| N                                                                                   | 0.17436300  | -2.74782700 | 0.45971500  | O                                                                                   | -0.81535200 | -0.04960800 | -2.39696500 |
| O                                                                                   | 0.48937300  | -3.91194300 | 0.58660700  | O                                                                                   | -1.16731200 | 2.42625500  | 1.03691800  |
| N                                                                                   | -0.91204000 | 3.03117700  | -0.19368900 | O                                                                                   | -2.78344000 | -1.35329900 | -0.40838200 |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| O                                                                                   | -3.11603600 | 0.78143300  | -0.51732900 | H                                                                                   | -0.99093700 | -1.16021400 | -2.72255000 |
| H                                                                                   | -1.83826300 | -0.68093900 | 2.95402100  | H                                                                                   | -1.20211200 | 0.36469200  | -2.94329400 |
| H                                                                                   | -2.08550200 | 0.85129300  | 2.83982700  | N                                                                                   | 1.92719500  | 0.23134800  | -0.42109300 |
| H                                                                                   | -0.97899100 | -0.88562500 | -2.85019700 | C                                                                                   | 2.40756100  | 0.10593900  | -1.67122000 |
| H                                                                                   | -1.21274400 | 0.65280500  | -2.92597100 | C                                                                                   | 2.81299900  | 0.45824700  | 0.56313400  |
| N                                                                                   | 1.97521600  | 0.51320700  | -0.23028400 | C                                                                                   | 3.75682400  | 0.20134000  | -1.97380700 |
| C                                                                                   | 2.30901100  | 0.51610500  | -1.53712800 | C                                                                                   | 4.17914800  | 0.56529500  | 0.34162400  |
| C                                                                                   | 2.94932800  | 0.70667200  | 0.68467000  | C                                                                                   | 4.68680100  | 0.43810600  | -0.95387800 |
| C                                                                                   | 3.60133500  | 0.70776700  | -1.99720300 | H                                                                                   | 4.07033700  | 0.09118100  | -3.00452700 |
| C                                                                                   | 4.27702700  | 0.90668000  | 0.28655100  | H                                                                                   | 4.84112500  | 0.74888300  | 1.17952900  |
| C                                                                                   | 4.61026400  | 0.90818700  | -1.05926700 | H                                                                                   | 1.67301100  | -0.07614700 | -2.44617700 |
| H                                                                                   | 3.80515900  | 0.69934300  | -3.06004700 | N                                                                                   | -3.55004600 | -0.49468600 | -0.44702600 |
| H                                                                                   | 5.04300200  | 1.06039000  | 1.03560000  | O                                                                                   | -4.72861300 | -0.72510300 | -0.64103900 |
| H                                                                                   | 5.63660100  | 1.06257500  | -1.37093500 | N                                                                                   | 0.08714200  | -2.75768300 | 0.58244500  |
| H                                                                                   | 1.49797600  | 0.35714500  | -2.23717600 | O                                                                                   | 0.35065200  | -3.92899700 | 0.75340800  |
| N                                                                                   | -3.60000600 | -0.39550800 | -0.61874800 | N                                                                                   | -0.86146100 | 3.02669600  | -0.26184700 |
| O                                                                                   | -4.76653500 | -0.59132100 | -0.89935900 | O                                                                                   | -0.98840800 | 4.22144900  | -0.41691700 |
| N                                                                                   | -0.00174700 | -2.78420700 | 0.30135900  | H                                                                                   | 2.40966600  | 0.55701100  | 1.56551200  |
| O                                                                                   | 0.26797900  | -3.96455300 | 0.34628100  | C                                                                                   | 6.17355300  | 0.55812900  | -1.23120400 |
| N                                                                                   | -0.90243700 | 3.05961100  | -0.04020200 | H                                                                                   | 6.66517900  | 0.71904100  | -0.26671200 |
| O                                                                                   | -1.00357100 | 4.26372200  | -0.12584100 | C                                                                                   | 6.74318300  | -0.73694300 | -1.83845200 |
| Am                                                                                  | -0.73539700 | 0.09425200  | 0.11040300  | H                                                                                   | 6.30640400  | -0.94327600 | -2.81956400 |
| C                                                                                   | 2.60103700  | 0.70559800  | 2.16454400  | H                                                                                   | 7.82479500  | -0.64501800 | -1.96664000 |
| H                                                                                   | 1.52802100  | 0.54471400  | 2.26110800  | H                                                                                   | 6.54907200  | -1.59670300 | -1.19246800 |
| C                                                                                   | 3.29737900  | -0.45081000 | 2.90665100  | C                                                                                   | 6.47902100  | 1.77674300  | -2.12220700 |
| H                                                                                   | 4.38528900  | -0.34393500 | 2.88727100  | H                                                                                   | 6.10481200  | 2.69981700  | -1.67265400 |
| H                                                                                   | 2.98169100  | -0.46478200 | 3.95309500  | H                                                                                   | 7.55862300  | 1.87825900  | -2.26004400 |
| H                                                                                   | 3.04139800  | -1.41574400 | 2.46211600  | H                                                                                   | 6.02292300  | 1.67123300  | -3.11061500 |
| C                                                                                   | 2.91092800  | 2.06471100  | 2.81992600  | Am                                                                                  | -0.66451600 | 0.09112900  | 0.12492200  |
| H                                                                                   | 2.38520400  | 2.87664700  | 2.31135700  | Am(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>5</sub> ) |             |             |             |
| H                                                                                   | 2.59059400  | 2.05470900  | 3.86497300  | Am                                                                                  | -0.50981600 | -0.02766800 | -0.00353400 |
| H                                                                                   | 3.98128500  | 2.28650000  | 2.80086200  | O                                                                                   | 0.01560900  | 2.12312100  | -1.29430000 |
| Am(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>4</sub> ) |             |             |             | O                                                                                   | -0.91405800 | 0.25085900  | 2.48123700  |
| O                                                                                   | -0.48921200 | 2.25025000  | -1.20441200 | O                                                                                   | -0.26637000 | -2.45439300 | -0.67361500 |
| O                                                                                   | -1.83185800 | 0.17497000  | 2.37047800  | O                                                                                   | 0.19999900  | -2.04368300 | 1.39725900  |
| O                                                                                   | 0.09885000  | -2.21900500 | -0.57464200 | O                                                                                   | -0.41130600 | -0.34561300 | -2.50845500 |
| O                                                                                   | -0.21960800 | -1.97999000 | 1.54961100  | O                                                                                   | -0.80727300 | 2.38927400  | 0.68711400  |
| O                                                                                   | -0.78996800 | -0.28734800 | -2.36384700 | O                                                                                   | -2.77098900 | -1.07450400 | 0.48925100  |
| O                                                                                   | -1.09402700 | 2.45805900  | 0.86172200  | O                                                                                   | -2.80716400 | 0.58529300  | -0.90287400 |
| O                                                                                   | -2.71506700 | -1.42007300 | -0.17657400 | H                                                                                   | -1.11543100 | -0.55321700 | 2.97562300  |
| O                                                                                   | -3.07418200 | 0.68835200  | -0.50375800 | H                                                                                   | -1.51320800 | 0.93552200  | 2.80274200  |
| H                                                                                   | -1.68264200 | -0.51972100 | 3.02269700  | H                                                                                   | -0.78848300 | -1.13293200 | -2.91948900 |
| H                                                                                   | -1.96918100 | 0.99796800  | 2.85391500  | H                                                                                   | -0.67745900 | 0.40757500  | -3.05008600 |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| N                                                                                   | 2.06363500  | -0.29532800 | -0.62125800 | H                                                                                   | 1.88660100  | -0.82199900 | -1.95652300 |
| C                                                                                   | 2.78473500  | -0.83306800 | -1.61375300 | N                                                                                   | -3.69175100 | -0.60655500 | -0.38206600 |
| C                                                                                   | 2.69860400  | 0.32902800  | 0.37104700  | O                                                                                   | -4.87390400 | -0.86458700 | -0.48393100 |
| C                                                                                   | 4.17061800  | -0.76779200 | -1.63930600 | N                                                                                   | 0.12713300  | -2.76967100 | 0.21587200  |
| C                                                                                   | 4.08407400  | 0.45365900  | 0.44228600  | O                                                                                   | 0.49108800  | -3.92419200 | 0.26044100  |
| C                                                                                   | 4.82058100  | -0.11421800 | -0.59231700 | N                                                                                   | -0.97661600 | 3.01688700  | -0.12716700 |
| H                                                                                   | 4.72363600  | -1.21338800 | -2.45497300 | O                                                                                   | -1.06481400 | 4.22445900  | -0.15485700 |
| H                                                                                   | 4.56810700  | 0.96868200  | 1.25917200  | S                                                                                   | 2.25552100  | 1.33984700  | 2.20020300  |
| H                                                                                   | 5.90144700  | -0.04192700 | -0.57918900 | C                                                                                   | 3.64804300  | 2.11047200  | 3.08861300  |
| H                                                                                   | 2.21832200  | -1.31638600 | -2.40024500 | H                                                                                   | 3.21225900  | 2.49655100  | 4.00971700  |
| O                                                                                   | 1.80309700  | 0.81252700  | 1.26870600  | H                                                                                   | 4.41418100  | 1.37742900  | 3.33772100  |
| C                                                                                   | 2.25294800  | 1.50343300  | 2.44883400  | H                                                                                   | 4.07010600  | 2.93848900  | 2.52048200  |
| H                                                                                   | 1.35087800  | 1.71282000  | 3.01529300  | Am                                                                                  | -0.81417800 | 0.04393500  | -0.00311300 |
| H                                                                                   | 2.91858600  | 0.86355300  | 3.03042300  | Am(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>7</sub> ) |             |             |             |
| H                                                                                   | 2.75457900  | 2.43304000  | 2.17471700  | O                                                                                   | -0.98282100 | 2.36428400  | -1.45574900 |
| N                                                                                   | -3.46304000 | -0.30412100 | -0.25990000 | O                                                                                   | -1.62417000 | 0.24849000  | 2.27158800  |
| O                                                                                   | -4.66820600 | -0.41010800 | -0.35486400 | O                                                                                   | -0.02394000 | -2.07176600 | -0.86464200 |
| N                                                                                   | 0.09841800  | -2.90959400 | 0.46359200  | O                                                                                   | 0.04296800  | -1.76997900 | 1.27410100  |
| O                                                                                   | 0.33616600  | -4.08526100 | 0.64150100  | O                                                                                   | -1.20717000 | -0.24069800 | -2.55305200 |
| N                                                                                   | -0.38837700 | 2.93184800  | -0.39262800 | O                                                                                   | -1.28941000 | 2.47827500  | 0.68295800  |
| O                                                                                   | -0.37337400 | 4.13443100  | -0.54559000 | O                                                                                   | -2.79846500 | -1.45627200 | 0.00423700  |
| Am(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>6</sub> ) |             |             |             | O                                                                                   | -3.34986600 | 0.59612700  | -0.39675400 |
| O                                                                                   | -0.56489800 | 2.33648600  | -1.12564400 | H                                                                                   | -1.33877700 | -0.42013700 | 2.90591800  |
| O                                                                                   | -1.90103300 | -0.01404400 | 2.27934300  | H                                                                                   | -1.73071100 | 1.07806600  | 2.75216600  |
| O                                                                                   | -0.00369300 | -2.14373800 | -0.89664700 | H                                                                                   | -1.28932400 | -1.11719100 | -2.94688500 |
| O                                                                                   | -0.15045800 | -2.09597200 | 1.26061200  | H                                                                                   | -1.65540200 | 0.38504400  | -3.13402500 |
| O                                                                                   | -1.13711300 | -0.10132300 | -2.49005600 | N                                                                                   | 2.11676400  | 0.22211100  | -0.22432900 |
| O                                                                                   | -1.29330300 | 2.33607100  | 0.90992100  | C                                                                                   | 2.58944500  | 0.03210900  | -1.46543200 |
| O                                                                                   | -2.80797200 | -1.51553300 | -0.23158200 | C                                                                                   | 2.99648700  | 0.58987000  | 0.71566900  |
| O                                                                                   | -3.25325000 | 0.59271100  | -0.41872800 | C                                                                                   | 3.92789200  | 0.20225500  | -1.80612600 |
| H                                                                                   | -1.68756800 | -0.71228500 | 2.91010300  | C                                                                                   | 4.35083000  | 0.78601600  | 0.47514700  |
| H                                                                                   | -1.99779600 | 0.80295800  | 2.78356300  | C                                                                                   | 4.82480900  | 0.58860300  | -0.81884500 |
| H                                                                                   | -1.38177400 | -0.92730000 | -2.92432000 | H                                                                                   | 4.24760300  | 0.03762800  | -2.82681800 |
| H                                                                                   | -1.58440200 | 0.61295800  | -2.95947300 | H                                                                                   | 5.01146500  | 1.08848400  | 1.27561800  |
| N                                                                                   | 2.12348400  | 0.15220100  | -0.15366600 | H                                                                                   | 5.87294800  | 0.73640100  | -1.04664300 |
| C                                                                                   | 2.60826300  | -0.34292500 | -1.30635400 | H                                                                                   | 1.86697500  | -0.26369200 | -2.21694400 |
| C                                                                                   | 2.98997200  | 0.74030000  | 0.69267900  | N                                                                                   | -3.73232900 | -0.60581400 | -0.19288000 |
| C                                                                                   | 3.94384600  | -0.27076000 | -1.67330600 | O                                                                                   | -4.90362200 | -0.91991100 | -0.18658600 |
| C                                                                                   | 4.35486500  | 0.85609800  | 0.40441700  | N                                                                                   | 0.26329400  | -2.54960500 | 0.28912200  |
| C                                                                                   | 4.83068500  | 0.34603500  | -0.79567600 | O                                                                                   | 0.71606700  | -3.66383500 | 0.42838800  |
| H                                                                                   | 4.27133300  | -0.68582900 | -2.61719500 | N                                                                                   | -1.24076800 | 3.09376100  | -0.44443200 |
| H                                                                                   | 5.03263100  | 1.33199200  | 1.09717400  | O                                                                                   | -1.43034500 | 4.28638000  | -0.52750500 |
| H                                                                                   | 5.88368400  | 0.42869400  | -1.03775600 | Am                                                                                  | -0.87344300 | 0.16324200  | -0.10828200 |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| C                                                                                   | 2.45775600  | 0.73949900  | 2.12131200  | O                                                                                   | -2.76798400 | -1.42352200 | -0.15543100 |
| F                                                                                   | 1.17811700  | 1.18569600  | 2.12574100  | O                                                                                   | -3.18600200 | 0.68693300  | -0.36679800 |
| F                                                                                   | 2.46431900  | -0.43430700 | 2.78571200  | H                                                                                   | -1.69041900 | -0.67348700 | 2.88652000  |
| F                                                                                   | 3.18407800  | 1.60905400  | 2.84653200  | H                                                                                   | -1.92412500 | 0.85815700  | 2.77669200  |
| Cm(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>1</sub> ) |             |             |             | H                                                                                   | -1.36523500 | -1.07325900 | -2.82626900 |
| O                                                                                   | -0.79328000 | 2.33612100  | -1.31017900 | H                                                                                   | -1.76677200 | 0.42238500  | -2.96097000 |
| O                                                                                   | -1.41494100 | 0.10980600  | 2.28550400  | N                                                                                   | 2.07480800  | 0.41762600  | -0.28083200 |
| O                                                                                   | 0.01449200  | -2.15726900 | -1.08740900 | C                                                                                   | 2.52520700  | 0.43006800  | -1.55314200 |
| O                                                                                   | 0.11920100  | -2.03080400 | 1.07120400  | C                                                                                   | 2.97182500  | 0.59151400  | 0.68185500  |
| O                                                                                   | -1.32973500 | -0.11130800 | -2.50039100 | C                                                                                   | 3.85892600  | 0.61000700  | -1.88193700 |
| O                                                                                   | -1.05032600 | 2.51289400  | 0.83322400  | C                                                                                   | 4.33357100  | 0.77512000  | 0.46411600  |
| O                                                                                   | -2.67519700 | -1.41916900 | -0.05357700 | C                                                                                   | 4.77976000  | 0.78389300  | -0.85146900 |
| O                                                                                   | -3.16270300 | 0.68275300  | -0.20143600 | H                                                                                   | 4.16341400  | 0.61303500  | -2.91994000 |
| H                                                                                   | -1.66661500 | -0.69790400 | 2.74875100  | H                                                                                   | 5.01032300  | 0.90742900  | 1.29615100  |
| H                                                                                   | -1.97328200 | 0.82098500  | 2.62202600  | H                                                                                   | 5.83187900  | 0.92589000  | -1.06545400 |
| H                                                                                   | -1.55674000 | -0.94935000 | -2.91968600 | H                                                                                   | 1.77703400  | 0.28928900  | -2.32356500 |
| H                                                                                   | -1.81417000 | 0.58707400  | -2.95588900 | N                                                                                   | -3.64334500 | -0.50379600 | -0.29754800 |
| N                                                                                   | 2.01712000  | 0.26048600  | -0.37771400 | O                                                                                   | -4.83034400 | -0.74575900 | -0.36295300 |
| C                                                                                   | 2.61535700  | 0.10846900  | -1.57064500 | N                                                                                   | 0.13784500  | -2.76098900 | 0.18329300  |
| C                                                                                   | 2.78564400  | 0.52130500  | 0.69303800  | O                                                                                   | 0.45809700  | -3.92957000 | 0.24283000  |
| C                                                                                   | 3.99092000  | 0.20927900  | -1.73740700 | N                                                                                   | -1.00744100 | 3.07747400  | -0.13554800 |
| C                                                                                   | 4.16759000  | 0.63755800  | 0.61508900  | O                                                                                   | -1.13922100 | 4.28039200  | -0.22567300 |
| C                                                                                   | 4.78210700  | 0.47863700  | -0.62391000 | Cl                                                                                  | 2.38548800  | 0.59312000  | 2.34263300  |
| H                                                                                   | 4.42646100  | 0.07913800  | -2.71957100 | Cm                                                                                  | -0.76114000 | 0.09032700  | 0.01071700  |
| H                                                                                   | 4.74281600  | 0.84838200  | 1.50729500  | Cm(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>3</sub> ) |             |             |             |
| H                                                                                   | 5.85790500  | 0.56338300  | -0.71988400 | O                                                                                   | -0.89570300 | 2.35599100  | -1.21785900 |
| H                                                                                   | 1.96551400  | -0.10088800 | -2.41250100 | O                                                                                   | -1.87889900 | 0.05000800  | 2.21394200  |
| N                                                                                   | -3.58070400 | -0.52002300 | -0.14112900 | O                                                                                   | 0.17053300  | -2.09699800 | -0.86186800 |
| O                                                                                   | -4.76283400 | -0.79828900 | -0.16506500 | O                                                                                   | -0.00457300 | -1.92428700 | 1.28766200  |
| N                                                                                   | 0.26645300  | -2.74033700 | 0.01896900  | O                                                                                   | -1.06301100 | -0.18803700 | -2.50220200 |
| O                                                                                   | 0.62510500  | -3.89996000 | 0.07012200  | O                                                                                   | -1.20831200 | 2.48441500  | 0.92302100  |
| N                                                                                   | -1.03714800 | 3.08884800  | -0.30223200 | O                                                                                   | -2.70033100 | -1.49562900 | -0.23701600 |
| O                                                                                   | -1.24454600 | 4.27872400  | -0.42883300 | O                                                                                   | -3.24227800 | 0.58925900  | -0.42973000 |
| Cm                                                                                  | -0.66499800 | 0.11105800  | -0.09784500 | H                                                                                   | -1.63245500 | -0.62450200 | 2.85840400  |
| H                                                                                   | 2.27086000  | 0.63936800  | 1.63975900  | H                                                                                   | -2.00660900 | 0.87538400  | 2.69728200  |
| Cm(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>2</sub> ) |             |             |             | H                                                                                   | -1.16874900 | -1.05021800 | -2.92136500 |
| O                                                                                   | -0.72791700 | 2.34963200  | -1.15131600 | H                                                                                   | -1.44583000 | 0.47393900  | -3.08985700 |
| O                                                                                   | -1.87313700 | 0.04164300  | 2.26484300  | N                                                                                   | 2.00569300  | 0.36255200  | -0.19144000 |
| O                                                                                   | 0.05135600  | -2.13660700 | -0.92835800 | C                                                                                   | 2.41216600  | 0.04307400  | -1.43798500 |
| O                                                                                   | -0.13445700 | -2.07630500 | 1.22681900  | C                                                                                   | 2.93936600  | 0.72873500  | 0.71319400  |
| O                                                                                   | -1.20117800 | -0.18975000 | -2.47569100 | C                                                                                   | 3.73458200  | 0.06263300  | -1.84722300 |
| O                                                                                   | -1.14095100 | 2.46011500  | 0.97226900  | C                                                                                   | 4.29629600  | 0.76478500  | 0.36642800  |
|                                                                                     |             |             |             | C                                                                                   | 4.70187000  | 0.43112900  | -0.91658600 |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                   | 3.99192900  | -0.20475900 | -2.86377200 | N                                                                                   | -3.55625300 | -0.45947100 | -0.40801300 |
| H                                                                                   | 5.02918100  | 1.05665000  | 1.10742300  | O                                                                                   | -4.73951600 | -0.68469000 | -0.55912700 |
| H                                                                                   | 5.75100700  | 0.45895100  | -1.18641200 | N                                                                                   | 0.17983800  | -2.79927200 | 0.36107500  |
| H                                                                                   | 1.63407400  | -0.24172000 | -2.13673900 | O                                                                                   | 0.50331000  | -3.96424000 | 0.47793000  |
| N                                                                                   | -3.62694800 | -0.62689500 | -0.38689500 | N                                                                                   | -0.87914700 | 3.06466900  | -0.06981000 |
| O                                                                                   | -4.79488100 | -0.94093300 | -0.48411000 | O                                                                                   | -1.00261700 | 4.26849900  | -0.17269900 |
| N                                                                                   | 0.33003600  | -2.63978100 | 0.28340600  | H                                                                                   | 2.35412100  | 0.80661100  | 1.51800100  |
| O                                                                                   | 0.77345500  | -3.76198000 | 0.40924300  | C                                                                                   | 6.14999000  | 0.60663700  | -1.23053300 |
| N                                                                                   | -1.15645100 | 3.08856400  | -0.19957300 | H                                                                                   | 6.61749300  | 0.95781600  | -0.30534700 |
| O                                                                                   | -1.34335700 | 4.28281000  | -0.30141500 | C                                                                                   | 6.77554700  | -0.75566300 | -1.58397000 |
| C                                                                                   | 2.51963300  | 1.10398500  | 2.12534400  | H                                                                                   | 6.36137800  | -1.15436500 | -2.51435400 |
| H                                                                                   | 1.43486000  | 1.03671700  | 2.19013300  | H                                                                                   | 7.85521000  | -0.64829200 | -1.71690700 |
| C                                                                                   | 3.09895000  | 0.12023400  | 3.15980000  | H                                                                                   | 6.60114400  | -1.48916900 | -0.79298700 |
| H                                                                                   | 4.19158500  | 0.15534000  | 3.17987900  | C                                                                                   | 6.43071400  | 1.65307100  | -2.32451200 |
| H                                                                                   | 2.73795600  | 0.37505600  | 4.15961000  | H                                                                                   | 6.00671000  | 2.62524700  | -2.06127700 |
| H                                                                                   | 2.79448000  | -0.90584700 | 2.93948500  | H                                                                                   | 7.50876800  | 1.77639100  | -2.45572100 |
| C                                                                                   | 2.89850200  | 2.56002100  | 2.45706200  | H                                                                                   | 6.00986200  | 1.34807000  | -3.28665900 |
| H                                                                                   | 2.45817000  | 3.25537700  | 1.73804400  | Cm                                                                                  | -0.67790400 | 0.06784800  | 0.09944000  |
| H                                                                                   | 2.52951100  | 2.82213100  | 3.45199200  |                                                                                     |             |             |             |
| H                                                                                   | 3.98185900  | 2.70700600  | 2.45366300  |                                                                                     |             |             |             |
| Cm                                                                                  | -0.78240100 | 0.11681500  | -0.04284500 | Cm(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>5</sub> ) |             |             |             |
|                                                                                     |             |             |             | O                                                                                   | -0.01570600 | 2.13318400  | -1.27375400 |
|                                                                                     |             |             |             | O                                                                                   | -0.86609200 | 0.26418000  | 2.50045700  |
|                                                                                     |             |             |             | O                                                                                   | -0.23550300 | -2.47872200 | -0.69963600 |
| Cm(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>4</sub> ) |             |             |             | O                                                                                   | 0.18590300  | -2.02278400 | 1.37199000  |
| O                                                                                   | -0.56245500 | 2.33038100  | -1.06805100 | O                                                                                   | -0.39586600 | -0.36539600 | -2.52204900 |
| O                                                                                   | -1.82476400 | 0.04784800  | 2.33772800  | O                                                                                   | -0.81161300 | 2.44872900  | 0.71291900  |
| O                                                                                   | 0.07501500  | -2.23332300 | -0.77469300 | O                                                                                   | -2.75111900 | -1.04059800 | 0.50502600  |
| O                                                                                   | -0.07509000 | -2.06365600 | 1.37716100  | O                                                                                   | -2.78274500 | 0.57951900  | -0.93361800 |
| O                                                                                   | -0.80634700 | -0.13088100 | -2.38880700 | H                                                                                   | -1.03931600 | -0.54948900 | 2.98985300  |
| O                                                                                   | -1.05748100 | 2.45626600  | 1.03675100  | H                                                                                   | -1.48505800 | 0.92601400  | 2.83175000  |
| O                                                                                   | -2.70429800 | -1.39657700 | -0.23125500 | H                                                                                   | -0.72489400 | -1.19235400 | -2.89475000 |
| O                                                                                   | -3.08161900 | 0.72481500  | -0.41713500 | H                                                                                   | -0.72495800 | 0.34385700  | -3.08750600 |
| H                                                                                   | -1.67651200 | -0.65655900 | 2.97988500  | N                                                                                   | 2.05055700  | -0.27303400 | -0.63276300 |
| H                                                                                   | -1.94336900 | 0.86752200  | 2.83235700  | C                                                                                   | 2.76874000  | -0.81443700 | -1.62585600 |
| H                                                                                   | -1.01248400 | -0.96522100 | -2.82723500 | C                                                                                   | 2.68806400  | 0.33697800  | 0.36674700  |
| H                                                                                   | -1.15867800 | 0.58125200  | -2.93618300 | C                                                                                   | 4.15516300  | -0.76693300 | -1.64161100 |
| N                                                                                   | 1.90892700  | 0.23140200  | -0.42072600 | C                                                                                   | 4.07367800  | 0.44276100  | 0.44791700  |
| C                                                                                   | 2.40814700  | -0.02275600 | -1.64392400 | C                                                                                   | 4.80775400  | -0.12915700 | -0.58633700 |
| C                                                                                   | 2.77344000  | 0.60506400  | 0.53785700  | H                                                                                   | 4.70730500  | -1.21466000 | -2.45661500 |
| C                                                                                   | 3.75631500  | 0.08477500  | -1.94494800 | H                                                                                   | 4.55913400  | 0.94608400  | 1.27118600  |
| C                                                                                   | 4.13719700  | 0.73576400  | 0.31477800  | H                                                                                   | 5.88939200  | -0.07238900 | -0.56655200 |
| C                                                                                   | 4.66447600  | 0.47453600  | -0.95285400 | H                                                                                   | 2.19973100  | -1.28455300 | -2.41799300 |
| H                                                                                   | 4.08565900  | -0.13484300 | -2.95299300 | O                                                                                   | 1.78923700  | 0.82452300  | 1.25925500  |
| H                                                                                   | 4.78239900  | 1.04222700  | 1.12940400  | C                                                                                   | 2.23396700  | 1.49086500  | 2.45699600  |
| H                                                                                   | 1.68991200  | -0.31450600 | -2.39982000 |                                                                                     |             |             |             |

|                                                                                     |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                   | 1.32821700  | 1.69660100  | 3.01825700  | H                                                                                   | 4.30141300  | 2.42067900  | 2.94639800  |
| H                                                                                   | 2.88849000  | 0.83343300  | 3.03122900  | Cm                                                                                  | -0.77205600 | 0.11038400  | -0.02653000 |
| H                                                                                   | 2.74611300  | 2.41988400  | 2.20207100  |                                                                                     |             |             |             |
| N                                                                                   | -3.44068800 | -0.29413500 | -0.27093000 | Cm(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>7</sub> ) |             |             |             |
| O                                                                                   | -4.64455400 | -0.40747700 | -0.37215900 | O                                                                                   | -1.01382700 | 2.33606200  | -1.48764800 |
| N                                                                                   | 0.10056300  | -2.90888900 | 0.45055500  | O                                                                                   | -1.66919200 | 0.28592400  | 2.21953800  |
| O                                                                                   | 0.33013800  | -4.08112100 | 0.66515600  | O                                                                                   | 0.02920500  | -2.13750100 | -0.84299200 |
| N                                                                                   | -0.41060600 | 2.96345300  | -0.38155600 | O                                                                                   | 0.01101100  | -1.73086800 | 1.28156200  |
| O                                                                                   | -0.39838300 | 4.16193400  | -0.57032900 | O                                                                                   | -1.23796600 | -0.28287800 | -2.56144300 |
| Cm                                                                                  | -0.48555700 | -0.00440600 | -0.00492700 | O                                                                                   | -1.23744600 | 2.56151800  | 0.65500600  |
|                                                                                     |             |             |             | O                                                                                   | -2.77122500 | -1.45033800 | -0.04611000 |
| Cm(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>6</sub> ) |             |             |             | O                                                                                   | -3.33187700 | 0.61407400  | -0.35521200 |
| O                                                                                   | -0.83469600 | 2.34462200  | -1.20941100 | H                                                                                   | -1.37891800 | -0.35321200 | 2.88138900  |
| O                                                                                   | -1.87887400 | 0.05411100  | 2.23195400  | H                                                                                   | -1.82207300 | 1.12483100  | 2.67049500  |
| O                                                                                   | 0.12283000  | -2.10103900 | -0.89930300 | H                                                                                   | -1.36687000 | -1.16997500 | -2.91781200 |
| O                                                                                   | -0.10610400 | -2.02901500 | 1.25233300  | H                                                                                   | -1.70362700 | 0.33304000  | -3.13962800 |
| O                                                                                   | -1.18331100 | -0.19573300 | -2.49616400 | N                                                                                   | 2.11959500  | 0.22264600  | -0.21570200 |
| O                                                                                   | -1.17099800 | 2.47872600  | 0.92644200  | C                                                                                   | 2.58376500  | 0.09389800  | -1.46924200 |
| O                                                                                   | -2.73963000 | -1.45318300 | -0.19624100 | C                                                                                   | 3.00773100  | 0.55293300  | 0.73095200  |
| O                                                                                   | -3.21987400 | 0.64629900  | -0.38592900 | C                                                                                   | 3.91659600  | 0.28865000  | -1.81603100 |
| H                                                                                   | -1.65831200 | -0.64156500 | 2.86331600  | C                                                                                   | 4.35819200  | 0.77072500  | 0.48391600  |
| H                                                                                   | -1.95917600 | 0.87637600  | 2.73062300  | C                                                                                   | 4.82096200  | 0.63740300  | -0.82183300 |
| H                                                                                   | -1.37480200 | -1.06952400 | -2.85686400 | H                                                                                   | 4.22526900  | 0.17249400  | -2.84673700 |
| H                                                                                   | -1.69168200 | 0.44571300  | -3.00645900 | H                                                                                   | 5.02490300  | 1.04211000  | 1.29043900  |
| N                                                                                   | 2.07971600  | 0.37175800  | -0.24803000 | H                                                                                   | 5.86530900  | 0.80485900  | -1.05337300 |
| C                                                                                   | 2.54972500  | 0.01309400  | -1.45847100 | H                                                                                   | 1.85727500  | -0.16979300 | -2.22880600 |
| C                                                                                   | 2.96916400  | 0.79108800  | 0.67410100  | N                                                                                   | -3.71213600 | -0.59354100 | -0.17868500 |
| C                                                                                   | 3.89171800  | 0.04231700  | -1.80246300 | O                                                                                   | -4.88159800 | -0.90621700 | -0.13895700 |
| C                                                                                   | 4.34337500  | 0.84615000  | 0.41186200  | N                                                                                   | 0.27141700  | -2.55486200 | 0.33712700  |
| C                                                                                   | 4.80429300  | 0.46535500  | -0.84024600 | O                                                                                   | 0.72268000  | -3.65933600 | 0.55525200  |
| H                                                                                   | 4.20499900  | -0.25935800 | -2.79297200 | N                                                                                   | -1.23334000 | 3.11460900  | -0.49808800 |
| H                                                                                   | 5.03969700  | 1.18462600  | 1.16420100  | O                                                                                   | -1.42798400 | 4.30279300  | -0.64250600 |
| H                                                                                   | 5.86451700  | 0.50441900  | -1.06042600 | C                                                                                   | 2.49657300  | 0.62893800  | 2.15329600  |
| H                                                                                   | 1.81082800  | -0.31674100 | -2.18029600 | F                                                                                   | 1.20351100  | 1.02244700  | 2.21259100  |
| N                                                                                   | -3.64166200 | -0.55714200 | -0.32748300 | F                                                                                   | 2.57137400  | -0.56849900 | 2.77019600  |
| O                                                                                   | -4.82137100 | -0.83368000 | -0.39340300 | F                                                                                   | 3.21009000  | 1.49909500  | 2.89248600  |
| N                                                                                   | 0.21464300  | -2.70992400 | 0.22166500  | Cm                                                                                  | -0.86612500 | 0.16615600  | -0.13516000 |
| O                                                                                   | 0.58384700  | -3.86337800 | 0.29751200  |                                                                                     |             |             |             |
| N                                                                                   | -1.09388900 | 3.08222800  | -0.19421800 | Am(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup>                                     |             |             |             |
| O                                                                                   | -1.25705100 | 4.27994800  | -0.29760700 | Am                                                                                  | -0.02826000 | -0.03654200 | 0.00559900  |
| S                                                                                   | 2.25922300  | 1.28805100  | 2.23115700  | O                                                                                   | 1.83276100  | 0.50437600  | -1.72299200 |
| C                                                                                   | 3.70965200  | 1.57649600  | 3.29736800  | H                                                                                   | 2.56380900  | -0.10307400 | -1.89478500 |
| H                                                                                   | 3.29261400  | 1.81725100  | 4.27488000  | O                                                                                   | 0.36336600  | -0.27060100 | 2.47497800  |
| H                                                                                   | 4.32040700  | 0.67844800  | 3.38150800  | O                                                                                   | -2.12593600 | -0.48705200 | -1.29071600 |

|                                                 |             |             |             |                                                     |             |             |             |
|-------------------------------------------------|-------------|-------------|-------------|-----------------------------------------------------|-------------|-------------|-------------|
| O                                               | -1.23145100 | -2.08783800 | 0.94468000  | H                                                   | -0.61410200 | 1.43610400  | 2.79280700  |
| O                                               | 0.39140700  | -2.11132900 | -1.36523500 | H                                                   | -1.93782900 | -1.51303300 | -2.06090300 |
| O                                               | 1.56573800  | 1.90105700  | 0.60109800  | H                                                   | 0.50060400  | -3.15305800 | -0.60929900 |
| O                                               | -2.04650000 | 0.72442500  | 1.31956500  |                                                     |             |             |             |
| O                                               | -0.76452200 | 2.20971000  | -0.72582200 | Am(H <sub>2</sub> O) <sub>9</sub> <sup>3+</sup> -ts |             |             |             |
| H                                               | 1.63488700  | 0.93342500  | -2.56558500 | Am                                                  | -0.08209400 | 0.06911500  | -0.08845300 |
| H                                               | 1.21310000  | -0.45147700 | 2.89646600  | O                                                   | 1.89605100  | 0.79179000  | -1.53765400 |
| H                                               | -0.14956100 | 0.27363600  | 3.08564700  | O                                                   | 2.76168200  | -0.62459500 | 0.59379200  |
| H                                               | -2.18168100 | -0.91962500 | -2.15145400 | H                                                   | 2.67143900  | 0.29431500  | -1.23303100 |
| H                                               | -2.97885900 | -0.06944000 | -1.12025900 | H                                                   | 3.53506800  | -0.23679900 | 1.02300900  |
| H                                               | -1.12659900 | -2.35392500 | 1.86634200  | H                                                   | 2.99399600  | -1.54065900 | 0.39397400  |
| H                                               | 0.64710300  | -2.23335600 | -2.28692500 | O                                                   | 0.53435500  | -0.42530700 | 2.28533500  |
| H                                               | 2.34258200  | 1.89416400  | 0.02494800  | O                                                   | -2.04968400 | -0.73813700 | -1.43354100 |
| H                                               | -2.68831600 | 0.20772300  | 1.82081700  | O                                                   | -0.87765400 | -2.26178700 | 0.73255700  |
| H                                               | -1.32188500 | 2.46977400  | -1.46920300 | O                                                   | 0.92070600  | -1.93569600 | -1.25249400 |
| H                                               | -2.09715500 | -2.39490700 | 0.64916400  | O                                                   | 1.12809700  | 2.13763800  | 0.67689500  |
| H                                               | 0.02621300  | -2.94681800 | -1.04870400 | O                                                   | -2.22333800 | 0.24737900  | 1.21686100  |
| H                                               | 1.86705100  | 2.12431600  | 1.49021200  | O                                                   | -1.40528700 | 2.18975500  | -0.48290300 |
| H                                               | -2.37831500 | 1.62837100  | 1.25469100  | H                                                   | 1.92242300  | 0.84631200  | -2.50070500 |
| H                                               | -0.14363000 | 2.92775000  | -0.54302500 | H                                                   | 1.48874300  | -0.56867700 | 2.36845200  |
|                                                 |             |             |             | H                                                   | 0.22493600  | 0.01325700  | 3.08732000  |
| Cm(H <sub>2</sub> O) <sub>8</sub> <sup>3+</sup> |             |             |             | H                                                   | -2.10097800 | -0.87142500 | -2.38783400 |
| Cm                                              | 0.01299300  | -0.04195900 | -0.01579800 | H                                                   | -2.94655500 | -0.58275000 | -1.11162100 |
| O                                               | 1.53712500  | 1.96967600  | 0.23171000  | H                                                   | -0.68984600 | -2.51111700 | 1.64601100  |
| O                                               | 1.92652300  | -0.85781400 | 1.47378500  | H                                                   | 1.24251500  | -2.02641700 | -2.15729000 |
| H                                               | 2.43086900  | 2.08056700  | -0.11679500 | H                                                   | 1.85919500  | 2.40277300  | 0.10256400  |
| H                                               | 2.82468100  | -0.50398500 | 1.45443800  | H                                                   | -2.54157800 | -0.29605600 | 1.94748700  |
| H                                               | 1.52933400  | 2.34687800  | 1.12101400  | H                                                   | -1.99082800 | 2.35749700  | -1.23198300 |
| O                                               | -1.68309900 | 1.76773300  | 0.12487900  | H                                                   | -1.70793300 | -2.68380500 | 0.47975400  |
| O                                               | 0.03500300  | 0.90811400  | 2.31272300  | H                                                   | 0.51660300  | -2.77436600 | -0.99369800 |
| O                                               | -1.94725700 | -0.73492000 | -1.48950200 | H                                                   | 1.33677700  | 2.42748100  | 1.57335700  |
| O                                               | 0.01808500  | -2.53675600 | -0.04525300 | H                                                   | -2.58807400 | 1.13508600  | 1.32549600  |
| O                                               | -0.08199200 | 1.47703000  | -2.06524800 | H                                                   | -0.90637000 | 3.00106500  | -0.31904500 |
| O                                               | -1.92934000 | -0.99124000 | 1.26408900  |                                                     |             |             |             |
| H                                               | -2.51850500 | 1.81618000  | 0.60411800  | Cm(H <sub>2</sub> O) <sub>9</sub> <sup>3+</sup> -ts |             |             |             |
| H                                               | 0.59232000  | 0.45644100  | 2.95975200  | Cm                                                  | -0.03703900 | -0.09696900 | -0.03952600 |
| H                                               | -2.62170600 | -0.14000700 | -1.83914300 | O                                                   | 1.61300500  | 1.78407200  | -0.02924800 |
| H                                               | -0.66054300 | -3.03457700 | 0.42708000  | O                                                   | 1.94501100  | -1.09818200 | 1.15372900  |
| H                                               | 2.01035900  | -1.81702000 | 1.55185700  | H                                                   | 2.40481700  | 1.44804200  | -0.49498000 |
| H                                               | 0.59750600  | 2.14871700  | -2.20461900 | H                                                   | 2.65786200  | -0.68407100 | 1.65517000  |
| H                                               | -0.31292800 | 1.13134200  | -2.93665000 | H                                                   | 1.88588200  | 2.21785900  | 0.78781500  |
| H                                               | -2.12694100 | -0.91461600 | 2.20483100  | O                                                   | -1.68386200 | 1.77277100  | 0.23109800  |
| H                                               | -2.75115100 | -1.19638200 | 0.80109700  | O                                                   | 0.05952900  | 0.97873700  | 2.22119800  |
| H                                               | -1.72795600 | 2.38463000  | -0.61689400 | O                                                   | 2.73415600  | -0.02360300 | -1.53517100 |

|                                                                       |             |             |             |                                                                       |             |             |             |
|-----------------------------------------------------------------------|-------------|-------------|-------------|-----------------------------------------------------------------------|-------------|-------------|-------------|
| O                                                                     | -1.99633300 | -0.78974300 | -1.47377600 | H                                                                     | -2.59828600 | -2.33672700 | -1.03325400 |
| O                                                                     | -0.22355900 | -2.62981900 | -0.08610700 | H                                                                     | -3.18937300 | -0.65820500 | 2.02326900  |
| O                                                                     | -0.15330500 | 1.42692000  | -2.05941200 | N                                                                     | 2.47341000  | -0.30745700 | -0.08533700 |
| O                                                                     | -2.01055500 | -0.81633300 | 1.35542700  | C                                                                     | 3.13048300  | 0.84685200  | -0.29456300 |
| H                                                                     | -2.54930000 | 1.58839300  | 0.61808300  | C                                                                     | 3.20317700  | -1.40307300 | 0.18123800  |
| H                                                                     | 0.42068900  | 0.63546300  | 3.04720900  | C                                                                     | 4.51536500  | 0.95244000  | -0.24825600 |
| H                                                                     | 2.89598300  | 0.02644600  | -2.48456400 | H                                                                     | 2.51909400  | 1.71497500  | -0.51323800 |
| H                                                                     | -2.60562300 | -0.24083900 | -1.98172600 | C                                                                     | 4.59242700  | -1.39057900 | 0.24863100  |
| H                                                                     | -0.74001500 | -3.14814200 | 0.54253500  | H                                                                     | 2.64762400  | -2.31999400 | 0.34089600  |
| H                                                                     | 1.96730700  | -2.04150700 | 1.35613500  | C                                                                     | 5.26162600  | -0.18992500 | 0.02856900  |
| H                                                                     | 0.48940600  | 2.14803500  | -2.07812400 | H                                                                     | 4.99158100  | 1.90774600  | -0.42883100 |
| H                                                                     | -0.28829600 | 1.14069100  | -2.97116700 | H                                                                     | 5.13183700  | -2.30367800 | 0.46544300  |
| H                                                                     | -2.07080500 | -0.86686400 | 2.31666200  | H                                                                     | 6.34337000  | -0.14508800 | 0.06956600  |
| H                                                                     | -2.79280200 | -1.24341300 | 0.98528500  |                                                                       |             |             |             |
| H                                                                     | -1.82170000 | 2.36924700  | -0.51617600 | Cm(H <sub>2</sub> O) <sub>9</sub> (L <sub>1</sub> ) <sup>3+</sup> -ts |             |             |             |
| H                                                                     | -0.51865700 | 1.72013200  | 2.43904100  | O                                                                     | 0.35152200  | -0.36720900 | 2.16404300  |
| H                                                                     | 3.31909200  | -0.71342400 | -1.19997400 | H                                                                     | 1.31388300  | -0.34930300 | 2.23967600  |
| H                                                                     | -2.02850300 | -1.67637500 | -1.85397200 | O                                                                     | 0.33743500  | -0.61350700 | -2.13133500 |
| H                                                                     | 0.26993100  | -3.25214200 | -0.63437100 | O                                                                     | -2.83903000 | 1.28818200  | -0.83323600 |
|                                                                       |             |             |             | O                                                                     | -0.28513700 | 2.03193100  | -1.58464300 |
| Am(H <sub>2</sub> O) <sub>9</sub> (L <sub>1</sub> ) <sup>3+</sup> -ts |             |             |             | O                                                                     | -0.91043400 | 2.18791600  | 1.40149800  |
| Am                                                                    | -0.80425600 | 0.04396500  | -0.01411400 | O                                                                     | -0.10039800 | -2.35107500 | 0.19827600  |
| O                                                                     | 0.29775500  | -0.39979500 | 2.23106800  | O                                                                     | -2.44184600 | -1.40915900 | -1.10589700 |
| H                                                                     | 1.25637900  | -0.32605700 | 2.32324900  | O                                                                     | -2.66070000 | 0.06926700  | 1.69519900  |
| O                                                                     | 0.34985900  | -0.61921200 | -2.12070800 | H                                                                     | -0.01011400 | -0.36998900 | 3.05878000  |
| O                                                                     | -2.82563800 | 1.26473000  | -0.86316100 | H                                                                     | 1.27367000  | -0.79343700 | -1.95086200 |
| O                                                                     | -0.28532500 | 2.02809500  | -1.53935900 | H                                                                     | 0.02665100  | -1.23919800 | -2.79716000 |
| O                                                                     | -0.90618500 | 2.17316000  | 1.42451800  | H                                                                     | -2.75174800 | 2.03350100  | -1.44032300 |
| O                                                                     | -0.11707100 | -2.36567400 | 0.30196400  | H                                                                     | -3.61387300 | 1.43877900  | -0.27784400 |
| O                                                                     | -2.38990000 | -1.41680600 | -1.23789000 | H                                                                     | 0.16456400  | 1.77752000  | -2.40133800 |
| O                                                                     | -2.72826600 | 0.10034300  | 1.64356400  | H                                                                     | -1.37200600 | 3.01052500  | 1.19649500  |
| H                                                                     | -0.07856600 | -0.37890900 | 3.11952600  | H                                                                     | 0.05206000  | -2.74168900 | 1.06755700  |
| H                                                                     | 1.28732500  | -0.82144500 | -1.98625400 | H                                                                     | -3.25928400 | -1.02882400 | -1.45123500 |
| H                                                                     | -0.01098300 | -1.26124500 | -2.74526300 | H                                                                     | -2.64162500 | 0.75944300  | 2.37019200  |
| H                                                                     | -2.70673200 | 2.03496900  | -1.43299600 | H                                                                     | 0.01326000  | 2.92080100  | -1.35718800 |
| H                                                                     | -3.59319700 | 1.41746700  | -0.29775900 | H                                                                     | -0.20156400 | 2.41446100  | 2.01631500  |
| H                                                                     | 0.17382700  | 1.79445900  | -2.35720800 | H                                                                     | 0.04329500  | -3.04263600 | -0.45827600 |
| H                                                                     | -1.34592500 | 3.01094500  | 1.23373600  | H                                                                     | -2.60603100 | -2.33771100 | -0.90163900 |
| H                                                                     | 0.09607800  | -2.67115800 | 1.19259500  | H                                                                     | -3.14793200 | -0.68101300 | 2.05696800  |
| H                                                                     | -3.18947400 | -1.00219700 | -1.58709400 | N                                                                     | 2.48374600  | -0.32633300 | -0.16917600 |
| H                                                                     | -2.68898500 | 0.78521000  | 2.32357000  | C                                                                     | 3.14410100  | 0.82958500  | -0.35909000 |
| H                                                                     | 0.02813000  | 2.90166000  | -1.27516000 | C                                                                     | 3.20205600  | -1.40874300 | 0.17359200  |
| H                                                                     | -0.22788200 | 2.36326900  | 2.08458600  | C                                                                     | 4.52116000  | 0.95004900  | -0.21651100 |
| H                                                                     | 0.00709200  | -3.10986100 | -0.29894200 | H                                                                     | 2.54174100  | 1.68552100  | -0.64117200 |

|                                                                   |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| C                                                                 | 4.58243100  | -1.38017700 | 0.34052400  | H                                                                                   | -0.07363200 | 1.90823100  | -2.45747300 |
| H                                                                 | 2.64380200  | -2.32694700 | 0.31481500  | H                                                                                   | -1.56047900 | 2.88697400  | 1.39695800  |
| C                                                                 | 5.25513900  | -0.17785200 | 0.14074100  | H                                                                                   | -0.36004300 | -2.82063000 | 1.28780900  |
| H                                                                 | 5.00122700  | 1.90554000  | -0.38525900 | H                                                                                   | -3.26408600 | -0.77547100 | -1.55101300 |
| H                                                                 | 5.11264500  | -2.28223600 | 0.61776900  | H                                                                                   | -2.84377600 | 0.26197000  | 2.28831000  |
| H                                                                 | 6.33059200  | -0.12087700 | 0.25903900  | H                                                                                   | 0.75038100  | 2.33307700  | -1.20090300 |
| Cm                                                                | -0.79417700 | 0.07187000  | -0.01748800 | H                                                                                   | -0.59861600 | 2.12250700  | 2.35323700  |
|                                                                   |             |             |             | H                                                                                   | -0.27527700 | -3.04364000 | -0.24692200 |
| L <sub>8</sub>                                                    |             |             |             | H                                                                                   | -2.78715000 | -2.15330400 | -1.00622700 |
| N                                                                 | 2.06158100  | 0.07439500  | -0.13932800 | H                                                                                   | -3.20643000 | -1.13152600 | 1.70130200  |
| C                                                                 | 2.89485900  | 1.11792800  | -0.21597300 | N                                                                                   | 2.04287100  | 0.06645300  | -0.05001700 |
| C                                                                 | 2.61638800  | -1.13150400 | -0.00341300 | C                                                                                   | 2.88230500  | 1.11538700  | -0.15539600 |
| C                                                                 | 4.28310400  | 1.00504600  | -0.16031600 | C                                                                                   | 2.61395600  | -1.15126600 | 0.04365600  |
| C                                                                 | 3.98380300  | -1.37779300 | 0.06348000  | C                                                                                   | 4.26274800  | 0.99524400  | -0.17412000 |
| H                                                                 | 1.92422900  | -1.96676700 | 0.05699900  | C                                                                                   | 3.97490900  | -1.38736800 | 0.03845800  |
| C                                                                 | 4.83765400  | -0.27187700 | -0.01764200 | H                                                                                   | 1.93014300  | -1.98395400 | 0.13606300  |
| H                                                                 | 4.94498900  | 1.85618700  | -0.22283300 | C                                                                                   | 4.82868100  | -0.28140700 | -0.07523800 |
| H                                                                 | 4.34721300  | -2.38870800 | 0.17331800  | H                                                                                   | 4.91583500  | 1.84918200  | -0.26581600 |
| O                                                                 | 2.24491200  | 2.29981800  | -0.35365300 | H                                                                                   | 4.33963800  | -2.39961400 | 0.12268100  |
| C                                                                 | 3.01633300  | 3.50010300  | -0.44936600 | O                                                                                   | 2.24734600  | 2.31505800  | -0.24210100 |
| H                                                                 | 3.67112300  | 3.48213900  | -1.32524800 | C                                                                                   | 3.03124300  | 3.52788000  | -0.27119400 |
| H                                                                 | 2.29326200  | 4.30597200  | -0.55431900 | H                                                                                   | 3.65677600  | 3.55895900  | -1.16473300 |
| H                                                                 | 3.61261900  | 3.66154300  | 0.45318800  | H                                                                                   | 2.30672000  | 4.33718400  | -0.29720500 |
| O                                                                 | 6.18582400  | -0.32864500 | 0.03035300  | H                                                                                   | 3.64087900  | 3.60402200  | 0.62965000  |
| C                                                                 | 6.81506600  | -1.60814100 | 0.17653700  | Am                                                                                  | -0.74885100 | 0.10744100  | 0.01209700  |
| H                                                                 | 7.88391100  | -1.40781600 | 0.19046300  | O                                                                                   | 6.16491400  | -0.33780300 | -0.09978700 |
| H                                                                 | 6.51967700  | -2.08614600 | 1.11404900  | C                                                                                   | 6.81235100  | -1.61931700 | -0.00623300 |
| H                                                                 | 6.57579900  | -2.26209600 | -0.66599900 | H                                                                                   | 7.87706900  | -1.40760500 | -0.05639500 |
|                                                                   |             |             |             | H                                                                                   | 6.57625700  | -2.10346800 | 0.94369200  |
| Am(H <sub>2</sub> O) <sub>8</sub> (L <sub>8</sub> ) <sup>3+</sup> |             |             |             | H                                                                                   | 6.52354500  | -2.26115500 | -0.84124900 |
| O                                                                 | 0.24731600  | -0.22188000 | 2.34221200  |                                                                                     |             |             |             |
| H                                                                 | 1.18369100  | -0.28393300 | 2.56421100  | Am(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>8</sub> ) <sup>2+</sup> |             |             |             |
| O                                                                 | 0.08203000  | -1.02286900 | -2.05950800 | O                                                                                   | -0.66999700 | 1.97148000  | 1.24136900  |
| O                                                                 | -2.75397500 | 1.45546200  | -0.78194300 | H                                                                                   | -1.40151500 | 2.36976000  | 0.74763100  |
| O                                                                 | -0.13087300 | 2.02842300  | -1.50096200 | O                                                                                   | -0.10069800 | -1.72390300 | -1.66018300 |
| O                                                                 | -1.20462000 | 2.01550700  | 1.60890100  | O                                                                                   | 2.75332400  | -0.81827300 | 0.69878500  |
| O                                                                 | -0.42259300 | -2.37571400 | 0.43390100  | O                                                                                   | 0.01623800  | -2.31372100 | 1.19139600  |
| O                                                                 | -2.49549300 | -1.25934300 | -1.22248300 | O                                                                                   | 0.81523400  | -0.01664700 | 2.67294600  |
| O                                                                 | -2.52383300 | -0.45062700 | 1.72034800  | O                                                                                   | 0.24383200  | 1.55742200  | -1.74900100 |
| H                                                                 | -0.25185700 | -0.56622400 | 3.09325500  | O                                                                                   | 2.36267400  | -0.47863200 | -1.39951200 |
| H                                                                 | 0.90462300  | -0.87432400 | -2.54060400 | O                                                                                   | 1.97004100  | 2.00865200  | 0.47837600  |
| H                                                                 | -0.57704500 | -1.34677100 | -2.68697400 | H                                                                                   | 0.00297000  | 2.66011300  | 1.34037100  |
| H                                                                 | -2.56892500 | 2.26152500  | -1.28105200 | H                                                                                   | -0.91059600 | -1.75369200 | -2.18344800 |
| H                                                                 | -3.58563500 | 1.59647000  | -0.31266300 | H                                                                                   | 0.63030100  | -1.93237800 | -2.25649000 |

|                                                                                                  |             |             |             |                                                                                     |             |             |             |
|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                                | 0.21442700  | -3.14724500 | 0.74692100  | H                                                                                   | 1.40626400  | -2.35993800 | 2.04131300  |
| H                                                                                                | 1.67512000  | -0.14358400 | 3.09261800  | N                                                                                   | -2.13083300 | -1.07379800 | 0.08690700  |
| H                                                                                                | -0.66635900 | 1.87836300  | -1.87092400 | C                                                                                   | -2.50299400 | -2.03355000 | 0.95096600  |
| H                                                                                                | 2.81786900  | 1.99183500  | 0.93931500  | C                                                                                   | -3.11246700 | -0.39891200 | -0.54275600 |
| H                                                                                                | 0.18283300  | -2.43675300 | 2.13440100  | C                                                                                   | -3.81429800 | -2.37093500 | 1.23062400  |
| H                                                                                                | 0.32492400  | 0.61088800  | 3.21848600  | C                                                                                   | -4.46229300 | -0.65125700 | -0.33344600 |
| H                                                                                                | 0.61695900  | 1.38608600  | -2.62237400 | C                                                                                   | -4.82453000 | -1.65667200 | 0.56962400  |
| H                                                                                                | 2.09496600  | 2.53947700  | -0.31910200 | H                                                                                   | -4.02449700 | -3.15738100 | 1.93942300  |
| N                                                                                                | -2.24735900 | -0.07820000 | -0.34836800 | H                                                                                   | -5.23837400 | -0.09944500 | -0.84168200 |
| C                                                                                                | -2.83695600 | -1.23889900 | 0.00703100  | H                                                                                   | -1.69989700 | -2.55923000 | 1.45312300  |
| C                                                                                                | -3.06367400 | 0.89956100  | -0.78273800 | N                                                                                   | 3.46222400  | -0.50846700 | -0.45492900 |
| C                                                                                                | -4.19527900 | -1.48087300 | -0.05403400 | O                                                                                   | 4.66845900  | -0.57682500 | -0.56476600 |
| H                                                                                                | -2.17408300 | -2.01096800 | 0.37651800  | N                                                                                   | 0.11731700  | 0.88725000  | 2.49318400  |
| C                                                                                                | -4.43653300 | 0.76483000  | -0.89533600 | O                                                                                   | -0.04536700 | 1.40708800  | 3.57357700  |
| C                                                                                                | -5.02366800 | -0.45047800 | -0.51937900 | O                                                                                   | 0.33816500  | -2.72675800 | -1.30644700 |
| H                                                                                                | -4.57790700 | -2.44057600 | 0.25829200  | H                                                                                   | -0.47655400 | -3.03766800 | -1.72050300 |
| H                                                                                                | -5.07040700 | 1.56448500  | -1.24562700 | H                                                                                   | 1.05404100  | -2.95051500 | -1.91489600 |
| N                                                                                                | 3.20670500  | -0.82829600 | -0.49899000 | Am                                                                                  | 0.49678800  | -0.38781000 | -0.17508600 |
| O                                                                                                | 4.34212000  | -1.13968300 | -0.76145000 | O                                                                                   | -2.64671200 | 0.54126100  | -1.38781000 |
| Am                                                                                               | 0.43393200  | -0.05273200 | 0.15537900  | C                                                                                   | -3.57783000 | 1.37344400  | -2.09517900 |
| O                                                                                                | -2.40472100 | 2.06027900  | -1.07272400 | H                                                                                   | -4.19134800 | 1.94822700  | -1.39776300 |
| C                                                                                                | -3.16641200 | 3.19758900  | -1.54696500 | H                                                                                   | -2.96821200 | 2.04855000  | -2.68998700 |
| H                                                                                                | -3.89449900 | 3.50361700  | -0.79526700 | H                                                                                   | -4.21308700 | 0.77515200  | -2.75210600 |
| H                                                                                                | -2.43596200 | 3.98721200  | -1.69908300 | O                                                                                   | -6.14062500 | -1.85616000 | 0.73204200  |
| H                                                                                                | -3.65968300 | 2.95645800  | -2.48899500 | C                                                                                   | -6.58432800 | -2.87041000 | 1.64850600  |
| O                                                                                                | -6.35389600 | -0.52125800 | -0.63126900 | H                                                                                   | -6.24847800 | -2.65004100 | 2.66423700  |
| C                                                                                                | -7.02697000 | -1.72716100 | -0.22575400 | H                                                                                   | -7.67011100 | -2.84176300 | 1.60695400  |
| H                                                                                                | -6.85284700 | -1.92880200 | 0.83323600  | H                                                                                   | -6.22935200 | -3.85586900 | 1.33894200  |
| H                                                                                                | -8.08340300 | -1.53715800 | -0.39508800 |                                                                                     |             |             |             |
| H                                                                                                | -6.70156300 | -2.57463500 | -0.83236300 | Am(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>8</sub> ) |             |             |             |
|                                                                                                  |             |             |             | Am                                                                                  | -0.90914600 | 0.25669300  | 2.49212300  |
| Am(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>8</sub> ) <sup>+</sup> |             |             |             | O                                                                                   | -0.31709500 | -2.46065300 | -0.66385200 |
| O                                                                                                | 0.53419700  | -0.11606900 | -2.85261100 | O                                                                                   | 0.16719500  | -2.05187800 | 1.40322100  |
| H                                                                                                | -0.18965400 | -0.39664800 | -3.42510600 | O                                                                                   | -0.47458900 | -0.35538100 | -2.50749000 |
| O                                                                                                | -0.05032000 | -0.36679800 | 2.30420300  | O                                                                                   | -0.79066700 | 2.39153600  | 0.70098200  |
| O                                                                                                | 0.46906100  | 1.55041200  | 1.45891000  | O                                                                                   | -2.80398500 | -1.05448200 | 0.49985400  |
| O                                                                                                | 1.24573500  | 1.83393800  | -1.17493200 | O                                                                                   | -2.82297000 | 0.61967600  | -0.87528300 |
| O                                                                                                | 1.53074500  | -2.36020800 | 1.08388200  | H                                                                                   | -1.11766500 | -0.54245400 | 2.99137000  |
| O                                                                                                | 2.89788500  | 0.07151000  | 0.52670800  | H                                                                                   | -1.48854800 | 0.95406200  | 2.82215400  |
| O                                                                                                | 2.67294300  | -1.01697600 | -1.32780500 | H                                                                                   | -0.87243500 | -1.14085500 | -2.90239500 |
| H                                                                                                | 1.34661400  | -0.45775000 | -3.24699800 | H                                                                                   | -0.76197800 | 0.39828600  | -3.03759400 |
| H                                                                                                | 1.08657500  | 2.66475200  | -0.71196000 | N                                                                                   | 2.01126100  | -0.30842600 | -0.65334900 |
| H                                                                                                | 1.18265200  | -3.19770300 | 0.75017600  | C                                                                                   | 2.71733300  | -0.83897200 | -1.65856900 |
| H                                                                                                | 0.93181000  | 1.93104600  | -2.08361200 | C                                                                                   | 2.68472400  | 0.29917100  | 0.33114800  |

|                                                                   |             |             |             |                                                                                     |             |             |             |
|-------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| C                                                                 | 4.10037500  | -0.79636300 | -1.72305100 | H                                                                                   | -0.51262200 | 2.51481500  | 2.00063400  |
| C                                                                 | 4.06199100  | 0.40777800  | 0.37941600  | H                                                                                   | -0.36494800 | -3.17632800 | 0.09799000  |
| C                                                                 | 4.78938200  | -0.15981200 | -0.67826100 | H                                                                                   | -2.76223100 | -2.27996300 | -0.80886300 |
| H                                                                 | 4.61071800  | -1.24446900 | -2.56194500 | H                                                                                   | -3.17716900 | -0.89849100 | 1.84846100  |
| H                                                                 | 4.58484100  | 0.90491300  | 1.18288800  | N                                                                                   | 2.01877700  | 0.00753900  | -0.09990900 |
| H                                                                 | 2.13910300  | -1.30976500 | -2.44413900 | C                                                                                   | 2.84793300  | 1.07041800  | -0.05258800 |
| O                                                                 | 1.81546900  | 0.78621300  | 1.25295000  | C                                                                                   | 2.60087600  | -1.20795700 | -0.14814100 |
| C                                                                 | 2.30120200  | 1.46536400  | 2.42430200  | C                                                                                   | 4.22978900  | 0.96403900  | -0.04517200 |
| H                                                                 | 1.41541800  | 1.68938900  | 3.01072100  | C                                                                                   | 3.96364700  | -1.42933200 | -0.14287000 |
| H                                                                 | 2.96825500  | 0.81274200  | 2.99016600  | H                                                                                   | 1.92493800  | -2.05123900 | -0.18302900 |
| H                                                                 | 2.81371100  | 2.38673500  | 2.14216400  | C                                                                                   | 4.80726200  | -0.31065500 | -0.08669200 |
| N                                                                 | -3.48828200 | -0.26546200 | -0.23596200 | H                                                                                   | 4.87474300  | 1.82848700  | -0.01109300 |
| O                                                                 | -4.69604300 | -0.35045700 | -0.32312000 | H                                                                                   | 4.33799200  | -2.44090100 | -0.17788600 |
| N                                                                 | 0.05282200  | -2.91722900 | 0.47071300  | Cm                                                                                  | -0.70999800 | 0.06385000  | -0.03310900 |
| O                                                                 | 0.28413000  | -4.09470400 | 0.64769900  | O                                                                                   | 2.19690100  | 2.26092900  | -0.01366900 |
| N                                                                 | -0.40176700 | 2.93366600  | -0.39026600 | C                                                                                   | 2.95957900  | 3.47489900  | 0.15686900  |
| O                                                                 | -0.38842000 | 4.13677300  | -0.54226200 | H                                                                                   | 3.61393700  | 3.64112900  | -0.70040500 |
| O                                                                 | 6.12240000  | -0.03943800 | -0.60005700 | H                                                                                   | 2.22204200  | 4.27024000  | 0.22005300  |
| C                                                                 | 6.93748100  | -0.59657500 | -1.64454100 | H                                                                                   | 3.53885600  | 3.43020700  | 1.07981400  |
| H                                                                 | 6.71438100  | -0.12622600 | -2.60473900 | O                                                                                   | 6.14382600  | -0.35400900 | -0.07102000 |
| H                                                                 | 7.96272900  | -0.37701200 | -1.35798100 | C                                                                                   | 6.80263500  | -1.63298000 | -0.10025800 |
| H                                                                 | 6.79677200  | -1.67762300 | -1.71195800 | H                                                                                   | 7.86577300  | -1.40906000 | -0.07783500 |
| Cm(H <sub>2</sub> O) <sub>8</sub> (L <sub>8</sub> ) <sup>3+</sup> |             |             |             | H                                                                                   | 6.53169000  | -2.22750800 | 0.77481200  |
|                                                                   |             |             |             | H                                                                                   | 6.55833300  | -2.17399800 | -1.01678000 |
|                                                                   |             |             |             |                                                                                     |             |             |             |
| O                                                                 | 0.25836000  | -0.26897600 | 2.29126400  | Cm(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>8</sub> ) <sup>2+</sup> |             |             |             |
| H                                                                 | 1.16523200  | -0.09060800 | 2.56756700  |                                                                                     |             |             |             |
| O                                                                 | 0.05409900  | -0.92000200 | -2.20765800 |                                                                                     |             |             |             |
| O                                                                 | -2.78651000 | 1.35084800  | -0.83133000 | O                                                                                   | -0.68061500 | 1.98489000  | 1.17882900  |
| O                                                                 | -0.08320400 | 1.96926400  | -1.55340400 | H                                                                                   | -1.40328200 | 2.34230200  | 0.63929600  |
| O                                                                 | -1.16593600 | 2.16193800  | 1.38331900  | O                                                                                   | -0.03604000 | -1.64407300 | -1.66495500 |
| O                                                                 | -0.34923000 | -2.34039500 | 0.57923000  | O                                                                                   | 2.82531700  | -0.78900600 | 0.77811600  |
| O                                                                 | -2.44171000 | -1.42839400 | -1.12979400 | O                                                                                   | -0.00231800 | -2.30916100 | 1.12247700  |
| O                                                                 | -2.49849700 | -0.22616100 | 1.71620500  | O                                                                                   | 0.86077800  | 0.00754500  | 2.66967300  |
| H                                                                 | -0.29415400 | -0.25467400 | 3.08297200  | O                                                                                   | 0.23143800  | 1.52291500  | -1.75707700 |
| H                                                                 | 0.91486100  | -0.93588600 | -2.64160400 | O                                                                                   | 2.43531100  | -0.47911200 | -1.32787800 |
| H                                                                 | -0.52947700 | -1.52868800 | -2.67779300 | O                                                                                   | 1.99431800  | 2.02043400  | 0.45344600  |
| H                                                                 | -2.72569600 | 2.06298700  | -1.48019200 | H                                                                                   | -0.05733400 | 2.70967800  | 1.32625300  |
| H                                                                 | -3.64893900 | 1.42447600  | -0.40526500 | H                                                                                   | -0.84624800 | -1.67859200 | -2.18736600 |
| H                                                                 | 0.05170200  | 1.77797500  | -2.49025400 | H                                                                                   | 0.69701300  | -1.85677000 | -2.25706200 |
| H                                                                 | -1.59396100 | 2.92251600  | 0.97099900  | H                                                                                   | 0.14573200  | -3.10885700 | 0.60269900  |
| H                                                                 | -0.05269000 | -2.52505600 | 1.47975200  | H                                                                                   | 1.71586300  | -0.16706500 | 3.08198900  |
| H                                                                 | -3.20067800 | -0.96520400 | -1.50746400 | H                                                                                   | -0.68489300 | 1.83003400  | -1.87135800 |
| H                                                                 | -2.77162600 | 0.56771900  | 2.19403600  | H                                                                                   | 2.84023300  | 2.00601300  | 0.91815200  |
| H                                                                 | 0.75237100  | 2.34472600  | -1.21792200 | H                                                                                   | 0.15897800  | -2.52718700 | 2.04870500  |
|                                                                   |             |             |             | H                                                                                   | 0.35535400  | 0.55805700  | 3.28003300  |

|                                                                                                  |             |             |             |                                                                                     |             |             |             |
|--------------------------------------------------------------------------------------------------|-------------|-------------|-------------|-------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                                | 0.58462000  | 1.32247000  | -2.63251400 | C                                                                                   | -4.87282600 | -1.71610800 | 0.52837900  |
| H                                                                                                | 2.11837300  | 2.55522800  | -0.34146800 | H                                                                                   | -4.04386400 | -3.17037000 | 1.93121000  |
| N                                                                                                | -2.27143200 | -0.10121200 | -0.34523200 | H                                                                                   | -5.31934500 | -0.18347600 | -0.89936200 |
| C                                                                                                | -2.86776100 | -1.25598700 | 0.01360400  | H                                                                                   | -1.73876100 | -2.45516900 | 1.51949300  |
| C                                                                                                | -3.08282800 | 0.87905100  | -0.77866700 | N                                                                                   | 3.42068700  | -0.58351700 | -0.37727000 |
| C                                                                                                | -4.22890200 | -1.48891500 | -0.04501500 | O                                                                                   | 4.62113000  | -0.70744300 | -0.49924800 |
| H                                                                                                | -2.20872800 | -2.03053100 | 0.38364400  | N                                                                                   | 0.43776100  | 1.07551900  | 2.49357500  |
| C                                                                                                | -4.45655400 | 0.75641600  | -0.88973300 | O                                                                                   | 0.45402300  | 1.61770700  | 3.57791200  |
| C                                                                                                | -5.05130700 | -0.45402100 | -0.50969100 | O                                                                                   | 0.23326300  | -2.69639000 | -1.30647600 |
| H                                                                                                | -4.61806800 | -2.44524900 | 0.26982400  | H                                                                                   | -0.57460100 | -2.96215800 | -1.76256000 |
| H                                                                                                | -5.08533100 | 1.56058000  | -1.23896000 | H                                                                                   | 0.96331600  | -2.93808500 | -1.89041800 |
| N                                                                                                | 3.27346300  | -0.82429000 | -0.41908400 | O                                                                                   | -2.74342000 | 0.59216600  | -1.35800300 |
| O                                                                                                | 4.40587200  | -1.15513400 | -0.67998300 | C                                                                                   | -3.69355800 | 1.36697200  | -2.10436000 |
| O                                                                                                | -2.41574700 | 2.03882700  | -1.06987700 | H                                                                                   | -4.36455300 | 1.90872700  | -1.43380700 |
| C                                                                                                | -3.17034600 | 3.18050400  | -1.54634400 | H                                                                                   | -3.10236900 | 2.07353800  | -2.68088900 |
| H                                                                                                | -3.89550800 | 3.49317500  | -0.79458500 | H                                                                                   | -4.26965200 | 0.73072900  | -2.78003500 |
| H                                                                                                | -2.43464400 | 3.96468700  | -1.70164000 | Cm                                                                                  | 0.47020300  | -0.31899600 | -0.16814900 |
| H                                                                                                | -3.66589700 | 2.93966800  | -2.48708800 | O                                                                                   | -6.18075500 | -1.99132100 | 0.64122600  |
| O                                                                                                | -6.38318200 | -0.51390800 | -0.61687200 | C                                                                                   | -6.59490600 | -3.04631800 | 1.52538100  |
| C                                                                                                | -7.06503000 | -1.71114300 | -0.20190800 | H                                                                                   | -6.30926400 | -2.82504500 | 2.55612300  |
| H                                                                                                | -6.88570900 | -1.91043700 | 0.85672500  | H                                                                                   | -7.67818900 | -3.08271800 | 1.44467500  |
| H                                                                                                | -8.12078400 | -1.51149400 | -0.36465900 | H                                                                                   | -6.16941600 | -4.00280100 | 1.21356500  |
| H                                                                                                | -6.75237400 | -2.56451000 | -0.80707300 |                                                                                     |             |             |             |
| Cm                                                                                               | 0.47768400  | -0.01225400 | 0.19123400  | Cm(H <sub>2</sub> O) <sub>2</sub> (NO <sub>3</sub> ) <sub>3</sub> (L <sub>8</sub> ) |             |             |             |
|                                                                                                  |             |             |             | O                                                                                   | -0.03430000 | 2.12757100  | -1.27832300 |
| Cm(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>8</sub> ) <sup>+</sup> |             |             |             | O                                                                                   | -0.87082800 | 0.26309500  | 2.50063200  |
| O                                                                                                | 0.54980400  | -0.07549600 | -2.84264300 | O                                                                                   | -0.29965000 | -2.48640300 | -0.70528900 |
| H                                                                                                | -0.18239300 | -0.32070800 | -3.42081400 | O                                                                                   | 0.13435300  | -2.04682300 | 1.36756100  |
| O                                                                                                | 0.31438800  | -0.19197400 | 2.36837100  | O                                                                                   | -0.47069500 | -0.35216100 | -2.52500700 |
| O                                                                                                | 0.54646700  | 1.72380600  | 1.40181500  | O                                                                                   | -0.78078500 | 2.44809600  | 0.72668400  |
| O                                                                                                | 1.44302500  | 1.78804800  | -1.18345300 | O                                                                                   | -2.77989300 | -1.02970000 | 0.51273100  |
| O                                                                                                | 1.38911500  | -2.37703900 | 1.09772800  | O                                                                                   | -2.80568500 | 0.63862300  | -0.86919600 |
| O                                                                                                | 2.88813800  | 0.00199800  | 0.61454000  | H                                                                                   | -1.07480200 | -0.54023000 | 2.99496500  |
| O                                                                                                | 2.60304400  | -1.04151500 | -1.25651100 | H                                                                                   | -1.45451900 | 0.95396000  | 2.83642400  |
| H                                                                                                | 1.34474700  | -0.47007100 | -3.22296800 | H                                                                                   | -0.83072200 | -1.16211300 | -2.90618600 |
| H                                                                                                | 1.34997400  | 2.61769600  | -0.70032800 | H                                                                                   | -0.78854600 | 0.37676200  | -3.07157600 |
| H                                                                                                | 1.00848100  | -3.20477400 | 0.77743400  | N                                                                                   | 2.00354900  | -0.32247600 | -0.65253000 |
| H                                                                                                | 1.12499300  | 1.92545000  | -2.08548500 | C                                                                                   | 2.71307400  | -0.88131100 | -1.64046400 |
| H                                                                                                | 1.30199000  | -2.36546600 | 2.05868000  | C                                                                                   | 2.67431100  | 0.28433300  | 0.33426000  |
| N                                                                                                | -2.19984600 | -0.99319600 | 0.13681800  | C                                                                                   | 4.09709200  | -0.86709500 | -1.68195800 |
| C                                                                                                | -2.55091600 | -1.96893600 | 0.99205800  | C                                                                                   | 4.05134800  | 0.36725500  | 0.40374600  |
| C                                                                                                | -3.19101800 | -0.36811900 | -0.52582400 | C                                                                                   | 4.78310500  | -0.23044500 | -0.63462500 |
| C                                                                                                | -3.85118200 | -2.37408100 | 1.22854300  | H                                                                                   | 4.61158900  | -1.33728700 | -2.50599700 |
| C                                                                                                | -4.53288900 | -0.69121700 | -0.36193700 | H                                                                                   | 4.57068600  | 0.86425100  | 1.20950900  |

|                                                         |             |             |             |                                                                       |             |             |             |
|---------------------------------------------------------|-------------|-------------|-------------|-----------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                       | 2.13771800  | -1.35190600 | -2.42796700 | H                                                                     | -2.71543000 | -1.81212600 | 0.99707900  |
| O                                                       | 1.79637200  | 0.79544400  | 1.23526400  | Na                                                                    | 4.16780400  | 0.25126000  | 2.39496500  |
| C                                                       | 2.27052100  | 1.47955800  | 2.41008100  | Am                                                                    | -0.35169300 | -0.04554700 | 0.05576200  |
| H                                                       | 1.37769300  | 1.71899800  | 2.97879700  |                                                                       |             |             |             |
| H                                                       | 2.91941100  | 0.82243200  | 2.99124900  | Am(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> -Na |             |             |             |
| H                                                       | 2.79911700  | 2.39098200  | 2.12636500  | O                                                                     | 0.65727000  | -0.03775900 | -2.79743000 |
| N                                                       | -3.46832000 | -0.24361900 | -0.22290400 | H                                                                     | -0.10459300 | -0.07717500 | -3.38850500 |
| O                                                       | -4.67644800 | -0.32864400 | -0.30333700 | O                                                                     | 0.31819900  | -0.07530500 | 2.52776000  |
| N                                                       | 0.03463300  | -2.92637700 | 0.44165200  | O                                                                     | 0.73189200  | 1.73121200  | 1.41871100  |
| O                                                       | 0.25026800  | -4.10290700 | 0.64928100  | O                                                                     | 1.66824200  | 1.74897500  | -1.11084100 |
| N                                                       | -0.40050600 | 2.96001800  | -0.37625300 | O                                                                     | 1.20798900  | -2.38455300 | 1.13881500  |
| O                                                       | -0.38149400 | 4.15888400  | -0.56409700 | O                                                                     | 3.04062300  | -0.18063300 | 0.68836600  |
| Cm                                                      | -0.50058100 | -0.01124000 | -0.00324600 | O                                                                     | 2.72552700  | -1.12455400 | -1.23002500 |
| O                                                       | 6.11603300  | -0.13790400 | -0.53610900 | H                                                                     | 1.37924900  | -0.48417900 | -3.25711700 |
| C                                                       | 6.93732100  | -0.73062100 | -1.55640000 | H                                                                     | 1.66986400  | 2.60716600  | -0.67095200 |
| H                                                       | 6.74342200  | -0.26999900 | -2.52747500 | H                                                                     | 0.77529800  | -3.17101700 | 0.78109400  |
| H                                                       | 7.96173500  | -0.53068700 | -1.25317100 | H                                                                     | 1.43748800  | 1.87938100  | -2.04021500 |
| H                                                       | 6.77192100  | -1.80889200 | -1.60952800 | H                                                                     | 1.17949300  | -2.43627100 | 2.10160900  |
|                                                         |             |             |             | N                                                                     | 3.54439000  | -0.73973800 | -0.34278400 |
| Am(H <sub>2</sub> O) <sub>7</sub> (NO <sub>3</sub> )-Na |             |             |             | O                                                                     | 4.75005100  | -0.88730800 | -0.45757100 |
| O                                                       | -2.09414100 | 1.70986600  | -0.09802800 | N                                                                     | 0.52603600  | 1.18162500  | 2.54184100  |
| H                                                       | -3.01141600 | 1.71663200  | 0.19947300  | O                                                                     | 0.52882500  | 1.81311800  | 3.58744800  |
| O                                                       | -0.20592500 | -2.23864000 | -1.10802900 | O                                                                     | 0.07914400  | -2.53352700 | -1.26732700 |
| O                                                       | 2.05140100  | 0.17363200  | 0.98389300  | H                                                                     | -0.85708600 | -2.50043000 | -1.51577300 |
| O                                                       | -0.35366400 | -1.75962300 | 1.89908900  | H                                                                     | 0.56648900  | -2.90743500 | -2.01114500 |
| O                                                       | -0.26228900 | 1.10571600  | 2.28045900  | O                                                                     | -1.98543000 | -0.92976400 | -0.72824200 |
| O                                                       | -0.51217500 | 0.72498500  | -2.39213100 | H                                                                     | -2.47965200 | -0.29975500 | -1.26851500 |
| O                                                       | 1.94465500  | -0.36017200 | -1.11192100 | H                                                                     | -2.55047500 | -1.11810900 | 0.03245300  |
| O                                                       | 0.52938000  | 2.33174400  | -0.41032400 | Na                                                                    | 5.37146800  | 0.22102600  | 1.75136900  |
| H                                                       | -1.77380300 | 2.62132600  | -0.11516300 | Na                                                                    | 0.13923200  | -0.15053000 | 5.12298900  |
| H                                                       | -0.97948200 | -2.78030200 | -1.30755000 | Am                                                                    | 0.60707600  | -0.30293300 | -0.12036900 |
| H                                                       | 0.50712700  | -2.51285800 | -1.69781700 |                                                                       |             |             |             |
| H                                                       | 0.03960200  | -2.63686300 | 1.81114600  | Am(H <sub>2</sub> O) <sub>3</sub> (NO <sub>3</sub> ) <sub>3</sub> -Na |             |             |             |
| H                                                       | 0.56289500  | 1.35855100  | 2.71288100  | O                                                                     | 2.42463700  | -0.22820800 | 1.08243000  |
| H                                                       | -0.08637900 | 0.26810300  | -3.12810400 | O                                                                     | -2.28361600 | -0.32134600 | -0.93694900 |
| H                                                       | 1.18487100  | 2.81550500  | 0.10625400  | O                                                                     | -0.53276600 | 2.08728800  | -1.02105300 |
| H                                                       | -0.23025600 | -1.48077100 | 2.81496500  | O                                                                     | 0.16257500  | -0.50276300 | -2.45308700 |
| H                                                       | -0.95372600 | 1.68223600  | 2.62835300  | O                                                                     | 2.39774600  | 0.58902800  | -0.91959800 |
| H                                                       | -1.35947900 | 1.05056100  | -2.72177600 | O                                                                     | -1.91419400 | -1.54642400 | 0.80897500  |
| H                                                       | 0.71669600  | 2.50143000  | -1.34284000 | O                                                                     | -1.38094500 | 1.74444600  | 0.94185100  |
| N                                                       | 2.66717200  | -0.13081300 | -0.10006500 | O                                                                     | 0.05179800  | -0.41339300 | 2.51337200  |
| O                                                       | 3.88459100  | -0.18933100 | -0.13069900 | H                                                                     | -0.66111400 | -0.38421300 | -2.94357100 |
| O                                                       | -2.55976500 | -1.24547700 | 0.23147000  | H                                                                     | 0.79694000  | -0.30977400 | 3.11698000  |
| H                                                       | -3.39155400 | -1.15833000 | -0.24884100 | H                                                                     | 0.86541600  | -0.11298800 | -2.98863300 |

|                                                                          |             |             |             |                                                                                        |             |             |             |
|--------------------------------------------------------------------------|-------------|-------------|-------------|----------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                        | -0.72779600 | -0.63200800 | 3.03699100  | H                                                                                      | -4.85620500 | -1.91262100 | 1.12950800  |
| N                                                                        | -1.27134900 | 2.50347600  | -0.08617600 | H                                                                                      | -4.93341400 | 1.44580200  | -1.56286600 |
| O                                                                        | -1.86358700 | 3.57126300  | -0.13577800 | N                                                                                      | 3.17002700  | -0.70999400 | -0.66427800 |
| N                                                                        | -2.73977300 | -1.14337800 | -0.09322300 | O                                                                                      | 4.30324900  | -1.01697900 | -0.98243500 |
| O                                                                        | -3.88837900 | -1.54365300 | -0.10857100 | Am                                                                                     | 0.36418300  | 0.06412900  | 0.10372800  |
| N                                                                        | 3.07940200  | 0.24941200  | 0.10869100  | Na                                                                                     | 4.77288800  | -2.09858000 | 1.35576300  |
| O                                                                        | 4.29011000  | 0.38221000  | 0.13366000  | C                                                                                      | -6.64764200 | -0.26564700 | -0.23396700 |
| O                                                                        | 1.11057900  | -2.37349200 | -0.68908200 | C                                                                                      | -7.23761600 | -0.08256700 | 1.17628600  |
| H                                                                        | 1.20771100  | -3.17632200 | -0.16303500 | C                                                                                      | -7.16671600 | -1.55637500 | -0.89552200 |
| H                                                                        | 0.88023000  | -2.63932300 | -1.58853500 | H                                                                                      | -6.97755700 | 0.57918700  | -0.84635300 |
| Am                                                                       | 0.11616900  | -0.17521100 | 0.05223100  | H                                                                                      | -6.88151500 | 0.84125500  | 1.63869500  |
| Na                                                                       | -2.84724900 | 3.29898800  | 2.20693400  | H                                                                                      | -8.32809500 | -0.03647200 | 1.12016000  |
| Na                                                                       | -3.32949500 | -3.22070300 | 1.91902400  | H                                                                                      | -6.97259300 | -0.91597000 | 1.83276200  |
| Na                                                                       | 4.41617500  | 1.38309000  | -2.22504700 | H                                                                                      | -6.77906800 | -1.66514000 | -1.91133000 |
| Am(H <sub>2</sub> O) <sub>6</sub> (NO <sub>3</sub> )(L <sub>4</sub> )-Na |             |             |             | H                                                                                      | -6.87384000 | -2.44093000 | -0.32300300 |
| O                                                                        | -0.77896000 | 1.83493200  | 1.49124500  | H                                                                                      | -8.25827400 | -1.53602000 | -0.94764700 |
| H                                                                        | -1.70727900 | 2.08725100  | 1.55245600  | Am(H <sub>2</sub> O) <sub>4</sub> (NO <sub>3</sub> ) <sub>2</sub> (L <sub>4</sub> )-Na |             |             |             |
| O                                                                        | -0.13243000 | -1.29700500 | -1.96538100 | O                                                                                      | 0.53551900  | -0.22015100 | -2.81316500 |
| O                                                                        | 2.72268200  | -0.94825800 | 0.51027600  | H                                                                                      | -0.21493400 | -0.46836300 | -3.36686000 |
| O                                                                        | -0.04026200 | -2.33687800 | 0.68636200  | O                                                                                      | -0.00990000 | -0.34692000 | 2.37379400  |
| O                                                                        | 0.73902800  | -0.36238300 | 2.56909200  | O                                                                                      | 0.55355600  | 1.55040700  | 1.50737000  |
| O                                                                        | 0.71099600  | 2.07762900  | -1.49624400 | O                                                                                      | 1.12342400  | 1.77902700  | -1.17385100 |
| O                                                                        | 2.36354000  | -0.14093000 | -1.46223700 | O                                                                                      | 1.63923800  | -2.31216000 | 1.14668500  |
| O                                                                        | 1.91551000  | 1.92170600  | 0.96381300  | O                                                                                      | 2.96294100  | 0.10788800  | 0.49307800  |
| H                                                                        | -0.24305500 | 2.59193500  | 1.76097600  | O                                                                                      | 2.73296500  | -1.07271200 | -1.30324500 |
| H                                                                        | -1.00426500 | -1.40229600 | -2.36499800 | H                                                                                      | 1.32537900  | -0.55264500 | -3.25792900 |
| H                                                                        | 0.52095000  | -1.36908900 | -2.67240200 | H                                                                                      | 1.02188900  | 2.63742200  | -0.74685300 |
| H                                                                        | -0.03180200 | -3.02589600 | 0.01067300  | H                                                                                      | 1.31515800  | -3.18015400 | 0.87180900  |
| H                                                                        | 1.56724900  | -0.63304300 | 2.98400900  | H                                                                                      | 0.87571100  | 1.86507800  | -2.10348600 |
| H                                                                        | 0.06062500  | 2.76330100  | -1.69252900 | H                                                                                      | 1.59490500  | -2.28253500 | 2.11045400  |
| H                                                                        | 2.66842600  | 1.81881500  | 1.55796500  | N                                                                                      | -2.03956100 | -1.16325600 | 0.07871300  |
| H                                                                        | 0.20008300  | -2.74109500 | 1.52866700  | C                                                                                      | -2.48464500 | -2.11927500 | 0.91521900  |
| H                                                                        | 0.28411100  | 0.21531300  | 3.19485400  | C                                                                                      | -2.95845800 | -0.41412100 | -0.55466500 |
| H                                                                        | 1.21783500  | 1.93642400  | -2.30593800 | C                                                                                      | -3.83106400 | -2.35076100 | 1.14594500  |
| H                                                                        | 2.17212600  | 2.55178400  | 0.27767100  | C                                                                                      | -4.32339300 | -0.57974200 | -0.37029100 |
| N                                                                        | -2.31273300 | -0.14722900 | -0.17831400 | C                                                                                      | -4.79514100 | -1.56427300 | 0.50198500  |
| C                                                                        | -2.99499000 | -1.06940400 | 0.52786000  | H                                                                                      | -4.11525700 | -3.13925800 | 1.83130100  |
| C                                                                        | -3.02965900 | 0.72363200  | -0.91195100 | H                                                                                      | -5.01329000 | 0.06265300  | -0.90391000 |
| C                                                                        | -4.37856500 | -1.14352100 | 0.53545200  | H                                                                                      | -1.72925400 | -2.71187600 | 1.41800200  |
| H                                                                        | -2.39865800 | -1.77204700 | 1.09586300  | N                                                                                      | 3.51086900  | -0.54097300 | -0.45920900 |
| C                                                                        | -4.41629100 | 0.71317500  | -0.95510300 | O                                                                                      | 4.72741300  | -0.63506200 | -0.53680600 |
| H                                                                        | -2.47004700 | 1.45695000  | -1.48141700 | N                                                                                      | 0.17806900  | 0.91490000  | 2.53105800  |
| C                                                                        | -5.13153400 | -0.23230300 | -0.21450500 | O                                                                                      | -0.00353900 | 1.44181500  | 3.61388600  |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| O  | 0.36617000  | -2.77518100 | -1.20020700 | N  | -0.97802900 | 2.98053100  | 0.06618800  |
| H  | -0.47032100 | -3.12184500 | -1.53549600 | O  | -1.13350100 | 4.17178400  | -0.15323700 |
| H  | 1.04520800  | -3.04716600 | -1.83095100 | H  | 2.19694900  | 0.88084500  | 2.17937700  |
| Am | 0.50991400  | -0.43663800 | -0.15473100 | C  | 6.27337300  | 0.99235400  | -0.13632200 |
| H  | -2.58270800 | 0.34957800  | -1.22800400 | H  | 6.62663800  | 1.26663300  | 0.86257200  |
| C  | -6.28178200 | -1.76781900 | 0.72340200  | C  | 6.98540600  | -0.31105900 | -0.54419500 |
| H  | -6.79560600 | -0.96499900 | 0.18562000  | H  | 6.68853500  | -0.63137900 | -1.54678500 |
| C  | -6.75010300 | -3.10768900 | 0.12418100  | H  | 8.06783300  | -0.15959100 | -0.54814800 |
| H  | -7.83162200 | -3.21159300 | 0.24339900  | H  | 6.75781500  | -1.12180200 | 0.15224300  |
| H  | -6.51740200 | -3.16805600 | -0.94172500 | C  | 6.62633900  | 2.14695100  | -1.09213400 |
| H  | -6.27273100 | -3.95415100 | 0.62592000  | H  | 6.14314400  | 3.07770700  | -0.78488200 |
| C  | -6.66212300 | -1.65505100 | 2.21048100  | H  | 7.70704000  | 2.31012000  | -1.09674900 |
| H  | -6.33810400 | -0.70029600 | 2.63198700  | H  | 6.31700100  | 1.92507900  | -2.11730500 |
| H  | -7.74697400 | -1.72501400 | 2.32232100  | Na | -4.97404400 | 1.75597400  | -1.29053600 |
| H  | -6.21456800 | -2.45851500 | 2.80185700  | Na | -0.06386600 | 4.08328300  | -2.46432400 |
| Na | 5.14899500  | 0.72726700  | 1.56142700  | Na | -0.84242200 | -4.18673400 | 3.36600100  |
| Na | -0.81114000 | -0.85296100 | 4.65471800  | Am | -0.60662500 | 0.01719200  | 0.47022900  |

Am(H<sub>2</sub>O)<sub>2</sub>(NO<sub>3</sub>)<sub>3</sub>(L<sub>4</sub>)-Na

TEDGA

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| O | -0.39976200 | 2.22810600  | -0.79737800 | O | -0.35476000 | 1.83523000  | 1.81380300  |
| O | -2.16379100 | 0.05071400  | 2.44737900  | N | -1.07204400 | -0.33427800 | 4.64384600  |
| O | 0.29619800  | -2.27260400 | -0.16689400 | C | -0.67932000 | 1.59777500  | 3.16598700  |
| O | -0.60591300 | -2.22386400 | 1.79797400  | H | -1.66699700 | 2.01371900  | 3.40582500  |
| O | -0.40066400 | -0.30450200 | -2.00610000 | H | 0.05065400  | 2.08276200  | 3.83134000  |
| O | -1.36577800 | 2.42154500  | 1.12730400  | O | -0.28127200 | -0.69200500 | 2.54471000  |
| O | -2.60716800 | -1.50916500 | -0.26140900 | N | 0.24329800  | 4.66959600  | -0.38498600 |
| O | -2.92477400 | 0.60876900  | -0.54963700 | C | -0.66100600 | 0.08424300  | 3.41574400  |
| H | -2.54025500 | -0.73512300 | 2.86038500  | O | 0.09368300  | 2.42669200  | -0.71353600 |
| H | -2.73338300 | 0.79588600  | 2.67197900  | C | -1.53983900 | 0.55579300  | 5.71476700  |
| H | -0.45120400 | -1.17369700 | -2.42281900 | H | -1.07492400 | 1.53531500  | 5.60646000  |
| H | -0.71334200 | 0.34366900  | -2.64894900 | C | -1.05190200 | -1.77565000 | 4.93171000  |
| N | 1.98862000  | 0.40959200  | 0.17271100  | H | -1.27568900 | -2.30485900 | 4.00588600  |
| C | 2.62855500  | 0.25750200  | -1.00163500 | C | -0.32173500 | 3.21492800  | 1.52146800  |
| C | 2.72758800  | 0.75759700  | 1.24106100  | H | 0.41727200  | 3.72541000  | 2.15304800  |
| C | 3.99493700  | 0.43820100  | -1.14407900 | H | -1.29941900 | 3.67850400  | 1.72189800  |
| C | 4.09980300  | 0.95447000  | 1.17857700  | C | 0.02715400  | 3.39422900  | 0.03808300  |
| C | 4.77305700  | 0.79341900  | -0.03535200 | C | 0.17393500  | 5.85660800  | 0.47760900  |
| H | 4.44025800  | 0.29738000  | -2.12101200 | H | -0.50858200 | 5.66767900  | 1.30570100  |
| H | 4.63834100  | 1.23040200  | 2.07715600  | H | -0.28371900 | 6.65789200  | -0.10833800 |
| H | 2.01241400  | -0.01816200 | -1.84809500 | C | 0.56622300  | 4.88985400  | -1.80176800 |
| N | -3.38151200 | -0.58543200 | -0.62785700 | H | 1.12324600  | 4.02269400  | -2.15490700 |
| O | -4.51609000 | -0.79163800 | -1.03722500 | H | 1.22810500  | 5.75672400  | -1.85964300 |
| N | -0.03202200 | -2.90476700 | 0.87933000  | H | -1.16622500 | 0.15184600  | 6.65926900  |
| O | 0.17952700  | -4.09761600 | 1.02057200  | H | -1.85942900 | -1.98352600 | 5.63702900  |

|                                                                                                         |             |             |             |                                                                                                         |             |             |             |
|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| C                                                                                                       | 1.53785700  | 6.31123100  | 1.00497600  | H                                                                                                       | 0.33375300  | -4.47744600 | -1.85776200 |
| H                                                                                                       | 1.42198600  | 7.21611200  | 1.60731100  | H                                                                                                       | -1.32614100 | -4.33855900 | -1.23192900 |
| H                                                                                                       | 1.99773000  | 5.54185200  | 1.62971900  | O                                                                                                       | 0.32569600  | -2.68413800 | 0.73780700  |
| H                                                                                                       | 2.22375000  | 6.53814800  | 0.18535900  | N                                                                                                       | -0.77622500 | -0.65606000 | -4.76109200 |
| C                                                                                                       | -0.67391200 | 5.10743600  | -2.67114100 | C                                                                                                       | 0.20296400  | -3.80951300 | 0.20034200  |
| H                                                                                                       | -0.37829800 | 5.29550400  | -3.70700700 | O                                                                                                       | 0.11901800  | -0.24205000 | -2.72390900 |
| H                                                                                                       | -1.31496800 | 4.22348300  | -2.65349700 | C                                                                                                       | 0.38777100  | -6.27415700 | 0.22656900  |
| H                                                                                                       | -1.25783900 | 5.96518000  | -2.32675500 | H                                                                                                       | -0.40832200 | -6.25733400 | -0.51676100 |
| C                                                                                                       | -3.06390700 | 0.69286600  | 5.77373100  | C                                                                                                       | 1.04177100  | -4.86849600 | 2.21438400  |
| H                                                                                                       | -3.34937800 | 1.33293600  | 6.61270700  | H                                                                                                       | 1.57056200  | -3.92366600 | 2.32277000  |
| H                                                                                                       | -3.45722800 | 1.13676300  | 4.85616600  | C                                                                                                       | -0.70092600 | -2.46224400 | -3.09581700 |
| H                                                                                                       | -3.54302900 | -0.27911700 | 5.91311400  | H                                                                                                       | -1.74402500 | -2.74210200 | -3.26587900 |
| C                                                                                                       | 0.28727200  | -2.25198800 | 5.49791700  | H                                                                                                       | -0.05731000 | -3.14209100 | -3.66495200 |
| H                                                                                                       | 0.24220600  | -3.32136100 | 5.72184100  | C                                                                                                       | -0.43166500 | -1.02804500 | -3.53216500 |
| H                                                                                                       | 1.08824300  | -2.08684500 | 4.77435400  | C                                                                                                       | -1.41899100 | -1.56069200 | -5.73628700 |
| H                                                                                                       | 0.54017000  | -1.72436900 | 6.42136700  | H                                                                                                       | -1.11887400 | -2.58709200 | -5.52953900 |
|                                                                                                         |             |             |             | H                                                                                                       | -1.00183900 | -1.31474100 | -6.71409700 |
| Am(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>1</sub> ) <sup>+</sup> |             |             |             | C                                                                                                       | -0.51663400 | 0.73067600  | -5.20120600 |
| O                                                                                                       | 0.18397800  | -0.30659500 | 2.26821700  | H                                                                                                       | -0.63566900 | 1.38362400  | -4.33830900 |
| O                                                                                                       | 0.29006800  | 1.60895700  | 1.27556500  | H                                                                                                       | -1.29670700 | 0.98530500  | -5.91961900 |
| O                                                                                                       | 1.54587900  | 1.53447400  | -1.25925100 | H                                                                                                       | 0.04942900  | -6.94654900 | 1.01666100  |
| O                                                                                                       | 2.68223500  | -0.46455200 | 0.70658100  | H                                                                                                       | 1.77030900  | -5.67405700 | 2.31663700  |
| O                                                                                                       | 2.46484400  | -1.53500700 | -1.15990200 | C                                                                                                       | -2.94257300 | -1.43181200 | -5.75843300 |
| H                                                                                                       | 1.53793100  | 2.36641700  | -0.77067700 | H                                                                                                       | -3.35184800 | -2.09936700 | -6.51995300 |
| H                                                                                                       | 1.28159000  | 1.72861400  | -2.16718000 | H                                                                                                       | -3.38105900 | -1.70289900 | -4.79558000 |
| N                                                                                                       | -2.28492100 | -0.65599400 | 0.35911400  | H                                                                                                       | -3.25259200 | -0.41327500 | -6.00091300 |
| C                                                                                                       | -2.72328500 | -1.38864300 | 1.39655200  | C                                                                                                       | 0.86841100  | 0.89913300  | -5.82456100 |
| C                                                                                                       | -3.19520400 | -0.02100000 | -0.39914200 | H                                                                                                       | 0.99479500  | 1.93141000  | -6.15940300 |
| C                                                                                                       | -4.07110500 | -1.51849700 | 1.70784000  | H                                                                                                       | 1.65241900  | 0.67484000  | -5.09886800 |
| C                                                                                                       | -4.56138300 | -0.09522600 | -0.15700900 | H                                                                                                       | 0.99782800  | 0.24507800  | -6.69000700 |
| C                                                                                                       | -5.00846600 | -0.86081700 | 0.91624500  | C                                                                                                       | 1.69428800  | -6.78379700 | -0.38308000 |
| H                                                                                                       | -4.37280600 | -2.12222200 | 2.55405700  | H                                                                                                       | 1.54209200  | -7.79152900 | -0.77597600 |
| H                                                                                                       | -5.25322900 | 0.43654500  | -0.79730800 | H                                                                                                       | 2.03068500  | -6.14540400 | -1.20299700 |
| H                                                                                                       | -6.06694200 | -0.94141300 | 1.13297500  | H                                                                                                       | 2.48994100  | -6.82933000 | 0.36335400  |
| H                                                                                                       | -1.96064400 | -1.87548200 | 1.99141600  | C                                                                                                       | -0.05724600 | -4.99738000 | 3.26825300  |
| N                                                                                                       | 3.24112400  | -1.12434600 | -0.23266400 | H                                                                                                       | 0.38978800  | -4.97191300 | 4.26480600  |
| O                                                                                                       | 4.43507700  | -1.34788700 | -0.24283100 | H                                                                                                       | -0.76989000 | -4.17390400 | 3.19197400  |
| N                                                                                                       | 0.21676600  | 0.96481100  | 2.37538300  | H                                                                                                       | -0.60153600 | -5.93925900 | 3.16743300  |
| O                                                                                                       | 0.18153800  | 1.52401100  | 3.45275100  |                                                                                                         |             |             |             |
| H                                                                                                       | -2.81092800 | 0.56735900  | -1.22528800 | Am(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>2</sub> ) <sup>+</sup> |             |             |             |
| Am                                                                                                      | 0.33887900  | -0.46753900 | -0.25975900 | O                                                                                                       | 0.10815200  | -0.86550100 | 2.41124000  |
| O                                                                                                       | -0.39137500 | -2.54654500 | -1.70977500 | O                                                                                                       | 0.18290300  | 1.13548300  | 1.60473500  |
| N                                                                                                       | 0.51701000  | -4.93493100 | 0.83423200  | O                                                                                                       | 1.05800100  | 1.45613000  | -1.01423900 |
| C                                                                                                       | -0.32945100 | -3.88349600 | -1.22351600 | O                                                                                                       | 2.67168400  | -0.46183200 | 0.71800100  |

|   |             |             |             |                                                                                                         |             |             |             |
|---|-------------|-------------|-------------|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| O | 2.49623000  | -1.33233700 | -1.25452000 | H                                                                                                       | -3.47280600 | -1.03783800 | -5.85452500 |
| H | 1.03922400  | 2.23669500  | -0.44748600 | C                                                                                                       | 0.32172600  | 0.95201300  | -5.49660200 |
| H | 0.71640500  | 1.71475100  | -1.87862700 | H                                                                                                       | 0.26872900  | 2.01150600  | -5.75783700 |
| N | -2.48155600 | -0.04952600 | 0.21238700  | H                                                                                                       | 1.13277500  | 0.81519600  | -4.77886000 |
| C | -3.49882200 | -0.83752300 | 0.53437700  | H                                                                                                       | 0.56305600  | 0.39263400  | -6.40345900 |
| C | -2.76473700 | 1.24518100  | -0.03840100 | C                                                                                                       | 2.03758800  | -7.17874100 | -0.44075700 |
| C | -4.82269700 | -0.42069900 | 0.62987300  | H                                                                                                       | 1.84271400  | -8.18759000 | -0.81136300 |
| C | -4.04735700 | 1.76672600  | 0.02508200  | H                                                                                                       | 2.34574100  | -6.55839100 | -1.28524000 |
| C | -5.09570800 | 0.91545900  | 0.36665100  | H                                                                                                       | 2.86829500  | -7.23352800 | 0.26578900  |
| H | -5.60127900 | -1.12000800 | 0.89923300  | C                                                                                                       | 0.53403000  | -5.20715800 | 3.26767800  |
| H | -4.21601100 | 2.81369800  | -0.18828100 | H                                                                                                       | 1.03957800  | -5.19091600 | 4.23620600  |
| N | 3.26199800  | -0.91333900 | -0.32098400 | H                                                                                                       | -0.10531100 | -4.32516500 | 3.20083000  |
| O | 4.47146000  | -0.94250100 | -0.41573500 | H                                                                                                       | -0.09563500 | -6.09931600 | 3.23036000  |
| N | 0.09710300  | 0.39374300  | 2.63657500  | H                                                                                                       | -6.11267500 | 1.28282300  | 0.42805500  |
| O | 0.01158500  | 0.84660800  | 3.75934700  | Cl                                                                                                      | -3.13700700 | -2.52967100 | 0.86151200  |
| H | -1.92417400 | 1.87582600  | -0.29896000 | Am                                                                                                      | 0.30762100  | -0.80409400 | -0.10701600 |
| O | -0.19620700 | -2.89378000 | -1.63624800 |                                                                                                         |             |             |             |
| N | 0.96470500  | -5.28642800 | 0.80498300  | Am(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>3</sub> ) <sup>+</sup> |             |             |             |
| C | -0.00983400 | -4.23553700 | -1.19825400 | O                                                                                                       | 0.14620500  | -0.67713900 | 2.34540900  |
| H | 0.64716000  | -4.76802600 | -1.89244000 | O                                                                                                       | 0.38574000  | 1.29235100  | 1.48995800  |
| H | -0.97270500 | -4.75503800 | -1.15576700 | O                                                                                                       | 1.53012400  | 1.35028500  | -1.11721000 |
| O | 0.79999000  | -3.03688000 | 0.70770700  | O                                                                                                       | 2.80160800  | -0.56098400 | 0.80846500  |
| N | -1.02053800 | -0.93062200 | -4.55025000 | O                                                                                                       | 2.64582000  | -1.52145200 | -1.12379200 |
| C | 0.62058900  | -4.16159000 | 0.18571100  | H                                                                                                       | 1.52149700  | 2.16447400  | -0.59932600 |
| O | -0.25991800 | -0.47828100 | -2.46890100 | H                                                                                                       | 1.23570000  | 1.57507900  | -2.00887800 |
| C | 0.77519700  | -6.62999600 | 0.22487400  | N                                                                                                       | -2.23056200 | -0.03792000 | 0.17855900  |
| H | -0.05375400 | -6.60384900 | -0.48122100 | C                                                                                                       | -3.18288300 | -0.67612200 | 0.89234000  |
| C | 1.57530600  | -5.21053800 | 2.14946400  | C                                                                                                       | -2.56066000 | 1.11072000  | -0.44694200 |
| H | 2.18506400  | -4.30951900 | 2.18914100  | C                                                                                                       | -4.48183200 | -0.16023200 | 0.98091700  |
| C | -0.60698500 | -2.78925100 | -2.99376500 | C                                                                                                       | -3.82418500 | 1.67577300  | -0.40062200 |
| H | -1.59690600 | -3.23531700 | -3.12848500 | C                                                                                                       | -4.80951800 | 1.02084900  | 0.33319300  |
| H | 0.10590800  | -3.31317700 | -3.63931600 | H                                                                                                       | -5.22888300 | -0.68906400 | 1.55860100  |
| C | -0.62653400 | -1.30651000 | -3.33858500 | H                                                                                                       | -4.02352000 | 2.60158300  | -0.92428600 |
| C | -1.47846900 | -1.87495500 | -5.58925500 | N                                                                                                       | 3.39856500  | -1.11181200 | -0.17545600 |
| H | -1.01683200 | -2.84714400 | -5.42348800 | O                                                                                                       | 4.60583700  | -1.24035000 | -0.20997000 |
| H | -1.08631000 | -1.51063500 | -6.54035300 | N                                                                                                       | 0.18741800  | 0.58955800  | 2.53150200  |
| C | -1.01393500 | 0.50483200  | -4.90404800 | O                                                                                                       | 0.04179700  | 1.08002600  | 3.63303500  |
| H | -1.25010600 | 1.07255600  | -4.00592000 | H                                                                                                       | -1.77662600 | 1.60577600  | -1.00908600 |
| H | -1.82403700 | 0.66002000  | -5.61738400 | O                                                                                                       | -0.09229500 | -2.81752600 | -1.65345800 |
| H | 0.45923700  | -7.28279900 | 1.04061000  | N                                                                                                       | 1.03884300  | -5.21282200 | 0.79334900  |
| H | 2.24095500  | -6.06911000 | 2.24369800  | C                                                                                                       | 0.09563100  | -4.16009000 | -1.21950000 |
| C | -3.00100500 | -2.00120800 | -5.65091300 | H                                                                                                       | 0.79042700  | -4.67371400 | -1.88985800 |
| H | -3.27502200 | -2.68763100 | -6.45510200 | H                                                                                                       | -0.85951200 | -4.69624100 | -1.22317000 |
| H | -3.40769200 | -2.39087900 | -4.71526600 | O                                                                                                       | 0.73619200  | -2.97301600 | 0.75702200  |

|   |             |             |             |                                                                                                         |             |             |             |
|---|-------------|-------------|-------------|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| N | -0.98808200 | -0.84838100 | -4.53968800 | H                                                                                                       | -4.11131900 | -1.71933600 | 3.36185300  |
| C | 0.65578300  | -4.09063100 | 0.19371100  | H                                                                                                       | -2.73691400 | -2.80207100 | 3.60056700  |
| O | -0.00149500 | -0.42772200 | -2.54742900 | Am                                                                                                      | 0.45036800  | -0.73151700 | -0.14443900 |
| C | 0.94928500  | -6.54494300 | 0.16291100  |                                                                                                         |             |             |             |
| H | 0.14706300  | -6.54159800 | -0.57380700 | Am(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>4</sub> ) <sup>+</sup> |             |             |             |
| C | 1.58330200  | -5.15136600 | 2.16636600  | O                                                                                                       | 0.21298800  | -0.34049600 | 2.34646800  |
| H | 2.10731700  | -4.20362400 | 2.27467600  | O                                                                                                       | 0.70493600  | 1.48465700  | 1.30367700  |
| C | -0.53433300 | -2.71491700 | -3.00250700 | O                                                                                                       | 1.78694400  | 1.34449700  | -1.25340400 |
| H | -1.54231600 | -3.12688700 | -3.10286000 | O                                                                                                       | 2.86691700  | -0.75912100 | 0.77055200  |
| H | 0.14103000  | -3.27180200 | -3.66148900 | O                                                                                                       | 2.55698300  | -1.68806300 | -1.16258800 |
| C | -0.50099300 | -1.23729000 | -3.36726600 | H                                                                                                       | 1.89427900  | 2.16578600  | -0.75781500 |
| C | -1.59481100 | -1.77429100 | -5.51742900 | H                                                                                                       | 1.46083400  | 1.58115900  | -2.13063700 |
| H | -1.16223900 | -2.76590100 | -5.39290700 | N                                                                                                       | -2.13164100 | -0.53602000 | 0.20902500  |
| H | -1.28791800 | -1.43144000 | -6.50687000 | C                                                                                                       | -2.69738100 | -1.28618800 | 1.16892500  |
| C | -0.93992700 | 0.58197000  | -4.91055000 | C                                                                                                       | -2.94965400 | 0.20804000  | -0.55759900 |
| H | -1.03151800 | 1.16771500  | -3.99802700 | C                                                                                                       | -4.06731200 | -1.32390900 | 1.38866600  |
| H | -1.81980800 | 0.78054200  | -5.52354700 | C                                                                                                       | -4.32682300 | 0.22713800  | -0.40007100 |
| H | 0.64020900  | -7.24186700 | 0.94390000  | C                                                                                                       | -4.92409400 | -0.55706100 | 0.59463300  |
| H | 2.31837700  | -5.95255200 | 2.25179400  | H                                                                                                       | -4.46154600 | -1.95219000 | 2.17848200  |
| C | -3.11963700 | -1.82787900 | -5.41842900 | H                                                                                                       | -4.92092400 | 0.85200400  | -1.05528300 |
| H | -3.50958800 | -2.50150900 | -6.18464100 | H                                                                                                       | -2.02124800 | -1.87331500 | 1.77809700  |
| H | -3.44390900 | -2.19564300 | -4.44247300 | N                                                                                                       | 3.36611900  | -1.38898900 | -0.22007900 |
| H | -3.56358000 | -0.84304600 | -5.57756400 | O                                                                                                       | 4.54391800  | -1.68955800 | -0.26530800 |
| C | 0.33840600  | 0.94601500  | -5.66468900 | N                                                                                                       | 0.45845200  | 0.90740100  | 2.42186600  |
| H | 0.31122700  | 2.00322600  | -5.93886700 | O                                                                                                       | 0.46231900  | 1.51106900  | 3.47232100  |
| H | 1.21993800  | 0.77489600  | -5.04380300 | H                                                                                                       | -2.47633000 | 0.80839700  | -1.32663400 |
| H | 0.44038000  | 0.36214100  | -6.58243100 | O                                                                                                       | -0.28812500 | -2.55797200 | -1.64109900 |
| C | 2.26537600  | -7.00078300 | -0.46785200 | N                                                                                                       | 0.53533700  | -5.00039700 | 0.88477200  |
| H | 2.13996000  | -8.00435700 | -0.88049800 | C                                                                                                       | -0.20610600 | -3.90781800 | -1.19078500 |
| H | 2.57429400  | -6.33536000 | -1.27694200 | H                                                                                                       | 0.50072800  | -4.46427600 | -1.81214600 |
| H | 3.06894400  | -7.03785100 | 0.27043500  | H                                                                                                       | -1.18924800 | -4.38625000 | -1.25743800 |
| C | 0.49941000  | -5.29538900 | 3.23383600  | O                                                                                                       | 0.37102800  | -2.74647200 | 0.81709800  |
| H | 0.95975800  | -5.27884000 | 4.22454900  | N                                                                                                       | -0.90019500 | -0.59345600 | -4.60687500 |
| H | -0.21613200 | -4.47327000 | 3.17484200  | C                                                                                                       | 0.26127200  | -3.86334000 | 0.25591300  |
| H | -0.04214500 | -6.23850800 | 3.12947900  | O                                                                                                       | -0.08904100 | -0.17467200 | -2.53398400 |
| H | -5.81284200 | 1.42475600  | 0.39958000  | C                                                                                                       | 0.42355100  | -6.32932100 | 0.25069800  |
| C | -2.83092800 | -1.97375100 | 1.59800300  | H                                                                                                       | -0.33457700 | -6.29387100 | -0.53059300 |
| C | -3.59611400 | -3.16312900 | 0.98810800  | C                                                                                                       | 0.99719100  | -4.96098200 | 2.28874300  |
| C | -3.05696800 | -1.87493800 | 3.11789400  | H                                                                                                       | 1.53435800  | -4.02599300 | 2.43483900  |
| H | -1.76611100 | -2.15175100 | 1.44906800  | C                                                                                                       | -0.63236800 | -2.45092900 | -3.01880300 |
| H | -3.40372300 | -3.24890000 | -0.08441700 | H                                                                                                       | -1.64311800 | -2.83380900 | -3.18339700 |
| H | -3.28147400 | -4.09450300 | 1.46590600  | H                                                                                                       | 0.06882900  | -3.03454800 | -3.62516600 |
| H | -4.67530800 | -3.06108200 | 1.13225100  | C                                                                                                       | -0.53144200 | -0.97951200 | -3.39113300 |
| H | -2.47786900 | -1.05412200 | 3.54618800  | C                                                                                                       | -1.44377200 | -1.51795500 | -5.62308200 |

|                                                                                                         |             |             |             |   |             |             |             |
|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H                                                                                                       | -1.04725800 | -2.51753600 | -5.45122500 | C | -3.15651500 | -0.47089000 | 0.59337400  |
| H                                                                                                       | -1.04449300 | -1.19534300 | -6.58583400 | C | -2.30630900 | 1.58030100  | -0.02266600 |
| C                                                                                                       | -0.77715000 | 0.82800400  | -4.99416800 | C | -4.45452600 | 0.04745500  | 0.68065700  |
| H                                                                                                       | -0.87059600 | 1.42884900  | -4.09216300 | C | -3.55215000 | 2.18165800  | 0.03546900  |
| H                                                                                                       | -1.62736300 | 1.05808200  | -5.63769100 | C | -4.64312400 | 1.39147700  | 0.39486500  |
| H                                                                                                       | 0.04144700  | -7.00972200 | 1.01336700  | H | -5.28790500 | -0.57858000 | 0.96264500  |
| H                                                                                                       | 1.70817600  | -5.77910200 | 2.41174600  | H | -3.66146100 | 3.23306300  | -0.19277700 |
| C                                                                                                       | -2.97216900 | -1.53647800 | -5.65807500 | N | 3.31370400  | -1.25121400 | -0.25196200 |
| H                                                                                                       | -3.30713100 | -2.21073800 | -6.44935400 | O | 4.51391000  | -1.42070200 | -0.35505900 |
| H                                                                                                       | -3.39062300 | -1.88570400 | -4.71177700 | N | 0.46271800  | 0.74010500  | 2.52440500  |
| H                                                                                                       | -3.37770500 | -0.54445100 | -5.86649700 | O | 0.51740300  | 1.38302700  | 3.55257000  |
| C                                                                                                       | 0.53920900  | 1.12489400  | -5.71214600 | H | -1.42827100 | 2.15416900  | -0.29262100 |
| H                                                                                                       | 0.57071100  | 2.18066700  | -5.99106600 | O | -0.14496900 | -2.83891200 | -1.55229500 |
| H                                                                                                       | 1.39451700  | 0.91436200  | -5.06708800 | N | 1.00967600  | -5.24678300 | 0.89115500  |
| H                                                                                                       | 0.64052500  | 0.53298600  | -6.62459900 | C | 0.15469900  | -4.17398500 | -1.15046300 |
| C                                                                                                       | 1.75335700  | -6.84189600 | -0.30368100 | H | 0.93296600  | -4.59163500 | -1.79598000 |
| H                                                                                                       | 1.61130000  | -7.84315100 | -0.71639900 | H | -0.74313700 | -4.79458300 | -1.23468400 |
| H                                                                                                       | 2.13197900  | -6.19595900 | -1.09876000 | O | 0.64830700  | -3.01674000 | 0.88867400  |
| H                                                                                                       | 2.51290400  | -6.90394300 | 0.47817600  | N | -1.16480700 | -0.92265300 | -4.44170700 |
| C                                                                                                       | -0.15102600 | -5.08880600 | 3.28876700  | C | 0.62909600  | -4.11937500 | 0.29581900  |
| H                                                                                                       | 0.25056800  | -5.08707800 | 4.30483500  | O | -0.38628200 | -0.41800500 | -2.37571600 |
| H                                                                                                       | -0.84676000 | -4.25295700 | 3.19449600  | C | 1.02309200  | -6.56268100 | 0.22372700  |
| H                                                                                                       | -0.70435600 | -6.02007000 | 3.14709000  | H | 0.28170800  | -6.57086900 | -0.57392800 |
| C                                                                                                       | -6.42604000 | -0.58170700 | 0.80729100  | C | 1.46001700  | -5.20029100 | 2.29822800  |
| C                                                                                                       | -7.15986000 | -1.12958500 | -0.43082900 | H | 1.95941400  | -4.24627600 | 2.45770700  |
| C                                                                                                       | -6.96230700 | 0.80504700  | 1.2077070   | C | -0.52040300 | -2.74397500 | -2.92360100 |
| H                                                                                                       | -6.61861200 | -1.26656100 | 1.63898400  | H | -1.44524900 | -3.30094000 | -3.09605100 |
| H                                                                                                       | -6.79715700 | -2.12502500 | -0.69883600 | H | 0.26859300  | -3.16646700 | -3.55532000 |
| H                                                                                                       | -8.23168200 | -1.20126500 | -0.22876400 | C | -0.69846400 | -1.26668800 | -3.24538000 |
| H                                                                                                       | -7.02533100 | -0.47405200 | -1.29580600 | C | -1.53756700 | -1.90253200 | -5.48242400 |
| H                                                                                                       | -6.46321500 | 1.17933000  | 2.10485300  | H | -0.94284100 | -2.80626200 | -5.35710600 |
| H                                                                                                       | -6.81527300 | 1.53522700  | 0.40704500  | H | -1.23608200 | -1.47329000 | -6.43903400 |
| H                                                                                                       | -8.03406300 | 0.74552100  | 1.41389600  | C | -1.32669100 | 0.50731500  | -4.77859100 |
| Am                                                                                                      | 0.49220800  | -0.54163300 | -0.17415300 | H | -1.51254400 | 1.04690500  | -3.85226000 |
| Am(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>5</sub> ) <sup>+</sup> |             |             |             | H | -2.22096600 | 0.59048800  | -5.39798200 |
| O                                                                                                       | 0.27747200  | -0.51734300 | 2.51014500  | H | 0.68502800  | -7.29363400 | 0.96041500  |
| O                                                                                                       | 0.59048500  | 1.29204100  | 1.37500500  | H | 2.20108000  | -5.99088800 | 2.42094600  |
| O                                                                                                       | 1.53305200  | 1.19460700  | -1.22523700 | C | -3.03107000 | -2.22949300 | -5.49311800 |
| O                                                                                                       | 2.79441300  | -0.68118800 | 0.76262400  | H | -3.24169500 | -2.92938900 | -6.30483300 |
| O                                                                                                       | 2.49716200  | -1.63633400 | -1.15519800 | H | -3.34794200 | -2.69010700 | -4.55489800 |
| H                                                                                                       | 1.62235700  | 1.99881100  | -0.69852800 | H | -3.63342900 | -1.33350000 | -5.65606500 |
| H                                                                                                       | 1.09731700  | 1.44421500  | -2.04962200 | C | -0.11115300 | 1.08054500  | -5.50676500 |
| N                                                                                                       | -2.09989200 | 0.27805200  | 0.24682600  | H | -0.28758600 | 2.13433200  | -5.73471000 |
|                                                                                                         |             |             |             | H | 0.78683400  | 1.00869800  | -4.89003300 |

|                                                                                                         |             |             |             |                                                                                                         |             |             |             |
|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                                       | 0.07644400  | 0.56043300  | -6.44893500 | N                                                                                                       | -1.07322400 | -0.83663100 | -4.43341100 |
| C                                                                                                       | 2.40222200  | -6.94670400 | -0.31437500 | C                                                                                                       | 0.74371900  | -4.10336000 | 0.23495400  |
| H                                                                                                       | 2.35212000  | -7.94108100 | -0.76368900 | O                                                                                                       | -0.21026200 | -0.37898100 | -2.39204700 |
| H                                                                                                       | 2.74430700  | -6.24386700 | -1.07719900 | C                                                                                                       | 0.91327300  | -6.57294000 | 0.22215500  |
| H                                                                                                       | 3.14698000  | -6.97492700 | 0.48359700  | H                                                                                                       | 0.12193700  | -6.53670400 | -0.52537600 |
| C                                                                                                       | 0.30843400  | -5.37989000 | 3.28665500  | C                                                                                                       | 1.59547700  | -5.19939000 | 2.22152000  |
| H                                                                                                       | 0.69810500  | -5.36922100 | 4.30737300  | H                                                                                                       | 2.16356700  | -4.27750200 | 2.33005300  |
| H                                                                                                       | -0.41770200 | -4.57065800 | 3.18887600  | C                                                                                                       | -0.48942400 | -2.69504600 | -2.93477600 |
| H                                                                                                       | -0.20640600 | -6.33112400 | 3.13192300  | H                                                                                                       | -1.45883300 | -3.18905900 | -3.04712500 |
| H                                                                                                       | -5.63750100 | 1.81763500  | 0.45383300  | H                                                                                                       | 0.22858700  | -3.17024000 | -3.61193100 |
| O                                                                                                       | -2.83364200 | -1.75312300 | 0.84142100  | C                                                                                                       | -0.59327700 | -1.21019900 | -3.25295000 |
| C                                                                                                       | -3.86336500 | -2.67945100 | 1.21967000  | C                                                                                                       | -1.55445200 | -1.78784200 | -5.45623700 |
| H                                                                                                       | -4.61128100 | -2.77353000 | 0.42919000  | H                                                                                                       | -1.02835500 | -2.73508300 | -5.34642100 |
| H                                                                                                       | -3.35761300 | -3.63096600 | 1.36068500  | H                                                                                                       | -1.25482400 | -1.38455800 | -6.42472300 |
| H                                                                                                       | -4.33763000 | -2.37302200 | 2.15455100  | C                                                                                                       | -1.14760500 | 0.60122000  | -4.76918100 |
| Am                                                                                                      | 0.36143400  | -0.76687100 | -0.05957500 | H                                                                                                       | -1.29923600 | 1.15242700  | -3.84335500 |
| Am(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>6</sub> ) <sup>+</sup> |             |             |             | H                                                                                                       | -2.03528700 | 0.73836600  | -5.38773900 |
| O                                                                                                       | 0.57151100  | -0.58245400 | 2.44803900  | H                                                                                                       | 0.56177300  | -7.24846300 | 1.00407800  |
| O                                                                                                       | 0.51624400  | 1.31890100  | 1.42501400  | H                                                                                                       | 2.28980900  | -6.03468100 | 2.32008500  |
| O                                                                                                       | 1.59499200  | 1.28499500  | -1.18707300 | C                                                                                                       | -3.06848500 | -1.99697600 | -5.41104900 |
| O                                                                                                       | 2.94437100  | -0.62107200 | 0.61140000  | H                                                                                                       | -3.36380400 | -2.67499900 | -6.21479000 |
| O                                                                                                       | 2.62791100  | -1.50859700 | -1.33552700 | H                                                                                                       | -3.38411700 | -2.43495700 | -4.46168000 |
| H                                                                                                       | 1.61452500  | 2.09780200  | -0.66628800 | H                                                                                                       | -3.60427600 | -1.05575900 | -5.54953700 |
| H                                                                                                       | 1.18566500  | 1.50208700  | -2.03411400 | C                                                                                                       | 0.10120300  | 1.09454600  | -5.49962900 |
| N                                                                                                       | -2.22414400 | 0.01027700  | 0.24858500  | H                                                                                                       | -0.00881900 | 2.15619200  | -5.73263100 |
| C                                                                                                       | -3.25274200 | -0.65958500 | 0.80850200  | H                                                                                                       | 0.99275500  | 0.96942300  | -4.88199100 |
| C                                                                                                       | -2.48687700 | 1.20755800  | -0.30629400 | H                                                                                                       | 0.25534900  | 0.55828500  | -6.43890100 |
| C                                                                                                       | -4.55821900 | -0.15311900 | 0.81475200  | C                                                                                                       | 2.21273700  | -7.09649400 | -0.39057600 |
| C                                                                                                       | -3.74766800 | 1.78252200  | -0.34323100 | H                                                                                                       | 2.04521800  | -8.09800200 | -0.79320900 |
| C                                                                                                       | -4.80398000 | 1.08008900  | 0.22921100  | H                                                                                                       | 2.55807900  | -6.45494200 | -1.20419800 |
| H                                                                                                       | -5.36639600 | -0.70626000 | 1.26896500  | H                                                                                                       | 3.00695800  | -7.16167500 | 0.35589600  |
| H                                                                                                       | -3.88980500 | 2.74872800  | -0.80839000 | C                                                                                                       | 0.49424200  | -5.28367700 | 3.27800000  |
| N                                                                                                       | 3.45518100  | -1.12523100 | -0.44645700 | H                                                                                                       | 0.94327300  | -5.28161700 | 4.27407900  |
| O                                                                                                       | 4.65810700  | -1.23301300 | -0.58951800 | H                                                                                                       | -0.18140500 | -4.42930800 | 3.20531200  |
| N                                                                                                       | 0.55693200  | 0.69097500  | 2.53794100  | H                                                                                                       | -0.09058900 | -6.20072800 | 3.17401100  |
| O                                                                                                       | 0.58101200  | 1.26656500  | 3.60450100  | H                                                                                                       | -5.80858300 | 1.48601300  | 0.22466700  |
| H                                                                                                       | -1.65027700 | 1.73463800  | -0.74803200 | S                                                                                                       | -2.82212500 | -2.22123700 | 1.55047500  |
| O                                                                                                       | -0.03473800 | -2.80638000 | -1.59090400 | C                                                                                                       | -4.42422800 | -2.91515400 | 2.07389800  |
| N                                                                                                       | 1.06112900  | -5.24261200 | 0.84385500  | H                                                                                                       | -5.09289900 | -3.05138100 | 1.22488500  |
| C                                                                                                       | 0.17776200  | -4.15288900 | -1.17790300 | H                                                                                                       | -4.17907200 | -3.88997600 | 2.49483200  |
| H                                                                                                       | 0.87944700  | -4.64650600 | -1.85703400 | H                                                                                                       | -4.89029900 | -2.30366800 | 2.84527700  |
| H                                                                                                       | -0.77054600 | -4.69976000 | -1.19117300 | Am                                                                                                      | 0.51473400  | -0.74014800 | -0.08301800 |
| O                                                                                                       | 0.89453300  | -2.98991200 | 0.78827700  | Cm(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>1</sub> ) <sup>+</sup> |             |             |             |

|   |             |             |             |                                                                                                         |             |             |             |
|---|-------------|-------------|-------------|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| O | 0.10076600  | -0.26753000 | 2.29046100  | H                                                                                                       | -1.89285500 | 1.00540500  | -5.59893100 |
| O | 0.65517200  | 1.53816100  | 1.23805600  | H                                                                                                       | 0.11099400  | -7.04567000 | 0.92700800  |
| O | 1.94181600  | 1.17040800  | -1.37674100 | H                                                                                                       | 1.60535000  | -5.78146100 | 2.46817700  |
| O | 2.78454200  | -0.64076100 | 0.91688000  | C                                                                                                       | -2.98517000 | -1.71407900 | -5.68771900 |
| O | 2.63773000  | -1.91583800 | -0.82507100 | H                                                                                                       | -3.25445000 | -2.39292000 | -6.49989600 |
| H | 2.26780800  | 1.91795000  | -0.86056500 | H                                                                                                       | -3.36289200 | -2.13336400 | -4.75276000 |
| H | 1.54841200  | 1.53527900  | -2.17907100 | H                                                                                                       | -3.48840700 | -0.76119500 | -5.86348100 |
| N | -2.09960100 | -0.57505000 | 0.14691000  | C                                                                                                       | 0.25887800  | 1.27193400  | -5.66516600 |
| C | -2.65919500 | -1.34133200 | 1.09971800  | H                                                                                                       | 0.19563200  | 2.33430300  | -5.91194000 |
| C | -2.90613300 | 0.21247500  | -0.58642000 | H                                                                                                       | 1.12994900  | 1.11999600  | -5.02463900 |
| C | -4.02564500 | -1.35330800 | 1.34798100  | H                                                                                                       | 0.41514900  | 0.72008800  | -6.59499700 |
| C | -4.28166600 | 0.26425800  | -0.40041400 | C                                                                                                       | 1.92263700  | -6.79542300 | -0.23561600 |
| C | -4.85379300 | -0.53518700 | 0.58470000  | H                                                                                                       | 1.85521400  | -7.78958500 | -0.68292100 |
| H | -4.42558800 | -1.99152600 | 2.12522800  | H                                                                                                       | 2.34833000  | -6.11485200 | -0.97617100 |
| H | -4.88428300 | 0.91756800  | -1.01794700 | H                                                                                                       | 2.60975500  | -6.85240600 | 0.61100800  |
| H | -5.92366900 | -0.52057200 | 0.75475200  | C                                                                                                       | -0.32917800 | -5.13229000 | 3.20180800  |
| H | -1.98081300 | -1.95789600 | 1.67509600  | H                                                                                                       | -0.00795800 | -5.12540900 | 4.24609200  |
| N | 3.35528400  | -1.47199400 | 0.13118800  | H                                                                                                       | -1.03260500 | -4.31064700 | 3.05508800  |
| O | 4.50882800  | -1.81844400 | 0.28942500  | H                                                                                                       | -0.85061200 | -6.07425400 | 3.01615600  |
| N | 0.35888100  | 0.97914500  | 2.34964900  | Cm                                                                                                      | 0.51592800  | -0.57150700 | -0.21225200 |
| O | 0.32825000  | 1.59906200  | 3.39379900  |                                                                                                         |             |             |             |
| H | -2.42487000 | 0.81538600  | -1.34697200 | Cm(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>2</sub> ) <sup>+</sup> |             |             |             |
| O | -0.20627500 | -2.58628800 | -1.70388400 | O                                                                                                       | -0.04928000 | -0.70687700 | 2.45672700  |
| N | 0.53856500  | -5.01734800 | 0.85849500  | O                                                                                                       | 0.21472700  | 1.21279100  | 1.49962100  |
| C | -0.09761500 | -3.93473600 | -1.25761800 | O                                                                                                       | 1.31182100  | 1.30463700  | -1.08347400 |
| H | 0.66556600  | -4.46191200 | -1.83683100 | O                                                                                                       | 2.61053600  | -0.60027100 | 0.79716700  |
| H | -1.05620500 | -4.44945900 | -1.38508800 | O                                                                                                       | 2.46187500  | -1.43513800 | -1.19261900 |
| O | 0.29948200  | -2.76987200 | 0.79635300  | H                                                                                                       | 1.28766100  | 2.10473000  | -0.54379300 |
| N | -1.01665200 | -0.59937900 | -4.60896500 | H                                                                                                       | 0.94103300  | 1.53337100  | -1.94503100 |
| C | 0.27135800  | -3.88365300 | 0.21993900  | N                                                                                                       | -2.46136900 | -0.03820800 | 0.23742900  |
| O | -0.28829200 | -0.15765800 | -2.51046200 | C                                                                                                       | -3.49192700 | -0.81696600 | 0.54157000  |
| C | 0.53068000  | -6.34186600 | 0.20643300  | C                                                                                                       | -2.71956900 | 1.26536100  | 0.00786800  |
| H | -0.15770100 | -6.32581000 | -0.63724600 | C                                                                                                       | -4.80898800 | -0.37934300 | 0.63368800  |
| C | 0.88993500  | -4.97674600 | 2.29404200  | C                                                                                                       | -3.99411500 | 1.80614600  | 0.07135200  |
| H | 1.39569400  | -4.03241000 | 2.48592600  | C                                                                                                       | -5.05810100 | 0.96539200  | 0.38986000  |
| C | -0.57399500 | -2.46775000 | -3.07383500 | H                                                                                                       | -5.60094500 | -1.06962200 | 0.88681900  |
| H | -1.54649200 | -2.93878800 | -3.24313400 | H                                                                                                       | -4.14481800 | 2.85932600  | -0.12385200 |
| H | 0.17147600  | -2.96057100 | -3.70725000 | N                                                                                                       | 3.21329900  | -1.06773200 | -0.22933700 |
| C | -0.62613600 | -0.97958500 | -3.39685700 | O                                                                                                       | 4.42305600  | -1.15574600 | -0.28065500 |
| C | -1.46599300 | -1.54323600 | -5.65255900 | N                                                                                                       | 0.03112000  | 0.55793700  | 2.58317600  |
| H | -0.97028800 | -2.50270600 | -5.51164700 | O                                                                                                       | -0.05951100 | 1.11101800  | 3.66057400  |
| H | -1.10542600 | -1.15277700 | -6.60522600 | H                                                                                                       | -1.86371800 | 1.88447500  | -0.23052600 |
| C | -1.02536200 | 0.83677800  | -4.95932100 | O                                                                                                       | -0.19188100 | -2.87557900 | -1.63603600 |
| H | -1.17203000 | 1.40306900  | -4.04225800 | N                                                                                                       | 0.96852800  | -5.27442000 | 0.80536400  |

|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C  | 0.04179100  | -4.21444200 | -1.21306900 | O | 0.12843800  | -0.61774700 | 2.38731700  |
| H  | 0.74705400  | -4.70326800 | -1.89194400 | O | 0.50050100  | 1.28756200  | 1.43605800  |
| H  | -0.89713700 | -4.77750100 | -1.21544900 | O | 1.66550200  | 1.22700800  | -1.20643500 |
| O  | 0.74603400  | -3.02734100 | 0.74446400  | O | 2.80722200  | -0.68696800 | 0.77221500  |
| N  | -1.05879000 | -0.92190700 | -4.54704700 | O | 2.61351900  | -1.61023300 | -1.17489100 |
| C  | 0.61763900  | -4.14544500 | 0.19542400  | H | 1.71482000  | 2.04425800  | -0.69503800 |
| O  | -0.31384100 | -0.45721400 | -2.46109400 | H | 1.28924100  | 1.45782200  | -2.06523900 |
| C  | 0.84619200  | -6.61010700 | 0.18978800  | N | -2.19482700 | -0.04227600 | 0.21486100  |
| H  | 0.04775400  | -6.59497000 | -0.55084500 | C | -3.15617200 | -0.64568500 | 0.94658500  |
| C  | 1.51407900  | -5.21319700 | 2.17786300  | C | -2.50839300 | 1.08945400  | -0.44828200 |
| H  | 2.06326500  | -4.27885900 | 2.27725000  | C | -4.44751200 | -0.10788200 | 1.01675500  |
| C  | -0.58528700 | -2.77364000 | -2.99927800 | C | -3.76265100 | 1.67538900  | -0.41969300 |
| H  | -1.55508800 | -3.25630300 | -3.15217400 | C | -4.75742500 | 1.05794300  | 0.33356700  |
| H  | 0.15636500  | -3.26482800 | -3.63836600 | H | -5.20395100 | -0.60924700 | 1.60649500  |
| C  | -0.65425600 | -1.28973500 | -3.33565300 | H | -3.94853200 | 2.58611800  | -0.97383600 |
| C  | -1.48318800 | -1.87734900 | -5.59014700 | N | 3.38340200  | -1.23695100 | -0.22810000 |
| H  | -0.97387300 | -2.82799500 | -5.43891900 | O | 4.58640700  | -1.39524100 | -0.27078800 |
| H  | -1.11901700 | -1.48621500 | -6.54149200 | N | 0.24419800  | 0.64759600  | 2.51048600  |
| C  | -1.10357600 | 0.51394200  | -4.89530600 | O | 0.11557000  | 1.20678200  | 3.58124700  |
| H  | -1.31880800 | 1.07135000  | -3.98569100 | H | -1.71802100 | 1.54465900  | -1.03360600 |
| H  | -1.94469000 | 0.65074600  | -5.57608700 | O | -0.05832700 | -2.80604500 | -1.67215400 |
| H  | 0.51688800  | -7.29063900 | 0.97705200  | N | 1.01712600  | -5.22985100 | 0.78024500  |
| H  | 2.22708200  | -6.03290300 | 2.27391600  | C | 0.16881500  | -4.15074400 | -1.26236100 |
| C  | -2.99876600 | -2.07415700 | -5.63948900 | H | 0.91668100  | -4.61831200 | -1.90929200 |
| H  | -3.24801500 | -2.76292900 | -6.44974500 | H | -0.76191400 | -4.72422200 | -1.32730000 |
| H  | -3.37834800 | -2.49388900 | -4.70546900 | O | 0.70333000  | -2.99303000 | 0.76623700  |
| H  | -3.51674400 | -1.13143000 | -5.82699800 | N | -1.04301900 | -0.82713100 | -4.52745800 |
| C  | 0.19516900  | 1.00049800  | -5.53771800 | C | 0.65723400  | -4.10099100 | 0.17954500  |
| H  | 0.10445800  | 2.06089800  | -5.78463800 | O | -0.22128300 | -0.37395000 | -2.46679900 |
| H  | 1.03978000  | 0.87770500  | -4.85703100 | C | 0.98226100  | -6.55209600 | 0.12475700  |
| H  | 0.41424600  | 0.45793900  | -6.46033100 | H | 0.22901300  | -6.54510000 | -0.66175500 |
| C  | 2.15243300  | -7.10623000 | -0.43149700 | C | 1.48717300  | -5.18492700 | 2.18155600  |
| H  | 2.00487700  | -8.11286500 | -0.82912800 | H | 2.00402200  | -4.23854400 | 2.32943300  |
| H  | 2.47736900  | -6.46034700 | -1.25012700 | C | -0.47668100 | -2.68912100 | -3.02723000 |
| H  | 2.95370100  | -7.15043900 | 0.30897800  | H | -1.43837200 | -3.19021500 | -3.16920500 |
| C  | 0.42452700  | -5.31570300 | 3.24469900  | H | 0.26351200  | -3.15316000 | -3.68803800 |
| H  | 0.88235800  | -5.29974100 | 4.23662700  | C | -0.58341700 | -1.20170700 | -3.33857200 |
| H  | -0.26926100 | -4.47587600 | 3.17439700  | C | -1.49798700 | -1.77830200 | -5.56227800 |
| H  | -0.14204000 | -6.24510300 | 3.14989300  | H | -0.96098200 | -2.71929500 | -5.45092700 |
| Cm | 0.27107300  | -0.78961100 | -0.09450100 | H | -1.19026300 | -1.36566000 | -6.52421200 |
| H  | -6.06957200 | 1.34785600  | 0.44962600  | C | -1.12135600 | 0.61116000  | -4.85939900 |
| Cl | -3.15512600 | -2.51653200 | 0.84963000  | H | -1.29039600 | 1.15793900  | -3.93405100 |
|    |             |             |             | H | -2.00021100 | 0.74521300  | -5.49125600 |
|    |             |             |             | H | 0.63306900  | -7.26505300 | 0.87369000  |

Cm(H<sub>2</sub>O)<sub>5</sub>(NO<sub>3</sub>)<sub>2</sub>(TEDGA)(L<sub>3</sub>)<sup>+</sup>

|                                                                                                         |             |             |             |   |             |             |             |
|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H                                                                                                       | 2.21701000  | -5.98703800 | 2.29648100  | H | -4.40547600 | -1.96939600 | 2.11747500  |
| C                                                                                                       | -3.00976200 | -2.00710800 | -5.53986700 | H | -4.84151300 | 0.92380900  | -1.03984800 |
| H                                                                                                       | -3.28522200 | -2.68436600 | -6.35129100 | H | -1.96894400 | -1.93431900 | 1.68841000  |
| H                                                                                                       | -3.33330900 | -2.45447000 | -4.59755000 | N | 3.37581600  | -1.47694300 | 0.12210100  |
| H                                                                                                       | -3.55556600 | -1.07198800 | -5.68067600 | O | 4.52979100  | -1.82426800 | 0.27731900  |
| C                                                                                                       | 0.13550800  | 1.11593600  | -5.56756600 | N | 0.39268800  | 0.98220100  | 2.35331900  |
| H                                                                                                       | 0.02146900  | 2.17748200  | -5.79916500 | O | 0.36692200  | 1.60364300  | 3.39686700  |
| H                                                                                                       | 1.01714200  | 0.99551100  | -4.93498100 | H | -2.40106600 | 0.82661100  | -1.34631900 |
| H                                                                                                       | 0.30949600  | 0.58392500  | -6.50580000 | O | -0.19744300 | -2.58130200 | -1.70095700 |
| C                                                                                                       | 2.34147300  | -6.98181700 | -0.42856600 | N | 0.53550000  | -5.01730900 | 0.86055100  |
| H                                                                                                       | 2.25528600  | -7.97942700 | -0.86493300 | C | -0.10012400 | -3.93001000 | -1.25317300 |
| H                                                                                                       | 2.69237300  | -6.29838900 | -1.20488200 | H | 0.65504200  | -4.46543900 | -1.83531700 |
| H                                                                                                       | 3.09701500  | -7.02267300 | 0.35856600  | H | -1.06442800 | -4.43539100 | -1.37512400 |
| C                                                                                                       | 0.34787500  | -5.34279800 | 3.18760800  | O | 0.31916500  | -2.76756600 | 0.79790400  |
| H                                                                                                       | 0.75494700  | -5.33924200 | 4.20152800  | N | -1.01265900 | -0.59138800 | -4.60307400 |
| H                                                                                                       | -0.36437600 | -4.52012500 | 3.10210400  | C | 0.27670700  | -3.88117800 | 0.22247300  |
| H                                                                                                       | -0.18675300 | -6.28446900 | 3.04224200  | O | -0.26780700 | -0.15276400 | -2.50995500 |
| Cm                                                                                                      | 0.45872900  | -0.75346900 | -0.13060000 | C | 0.50803600  | -6.34247100 | 0.21033300  |
| H                                                                                                       | -5.75525600 | 1.47729300  | 0.38553600  | H | -0.18745200 | -6.32023900 | -0.62738800 |
| C                                                                                                       | -2.82917200 | -1.93259400 | 1.68341700  | C | 0.89554400  | -4.97909700 | 2.29396000  |
| C                                                                                                       | -3.58940900 | -3.12479800 | 1.07183800  | H | 1.41229300  | -4.03995500 | 2.48196700  |
| C                                                                                                       | -3.09311600 | -1.80848500 | 3.19507500  | C | -0.57628000 | -2.46126300 | -3.06770200 |
| H                                                                                                       | -1.76256600 | -2.12212900 | 1.56551500  | H | -1.55467100 | -2.92333300 | -3.22763600 |
| H                                                                                                       | -3.37012200 | -3.22860500 | 0.00603800  | H | 0.15876900  | -2.96203900 | -3.70700200 |
| H                                                                                                       | -3.29590300 | -4.05157500 | 1.57160300  | C | -0.61779600 | -0.97319900 | -3.39273000 |
| H                                                                                                       | -4.67098400 | -3.01022800 | 1.18597600  | C | -1.47750200 | -1.53225500 | -5.64243000 |
| H                                                                                                       | -2.51901300 | -0.98456000 | 3.62426500  | H | -0.99220000 | -2.49707100 | -5.50185700 |
| H                                                                                                       | -4.15191400 | -1.64234700 | 3.41082000  | H | -1.11718400 | -1.14793500 | -6.59773000 |
| H                                                                                                       | -2.79189000 | -2.73016000 | 3.69970500  | C | -1.01035900 | 0.84431000  | -4.95536100 |
| Cm(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>4</sub> ) <sup>+</sup> |             |             |             | H | -1.14836700 | 1.41329200  | -4.03861700 |
| O                                                                                                       | 0.13575900  | -0.26456500 | 2.29711600  | H | -1.87882100 | 1.01957600  | -5.59184800 |
| O                                                                                                       | 0.68234400  | 1.54054000  | 1.23944900  | H | 0.08715300  | -7.04076400 | 0.93555400  |
| O                                                                                                       | 1.96037100  | 1.17140400  | -1.37829300 | H | 1.60348900  | -5.79112400 | 2.46479200  |
| O                                                                                                       | 2.80832800  | -0.64534700 | 0.90986500  | C | -2.99866800 | -1.68595000 | -5.66959700 |
| O                                                                                                       | 2.65569600  | -1.92012200 | -0.83208300 | H | -3.27995600 | -2.36245400 | -6.47964400 |
| H                                                                                                       | 2.28594200  | 1.92026000  | -0.86377600 | H | -3.37616900 | -2.09993900 | -4.73220300 |
| H                                                                                                       | 1.56563600  | 1.53429700  | -2.18088800 | H | -3.49199300 | -0.72757500 | -5.84363500 |
| N                                                                                                       | -2.06929600 | -0.55898100 | 0.15199800  | C | 0.27490300  | 1.26704200  | -5.66691000 |
| C                                                                                                       | -2.63955200 | -1.31919900 | 1.10201100  | H | 0.21951500  | 2.32916000  | -5.91664900 |
| C                                                                                                       | -2.88034900 | 0.22235600  | -0.58540400 | H | 1.14686200  | 1.10988800  | -5.02883300 |
| C                                                                                                       | -4.00705900 | -1.33109400 | 1.33791800  | H | 0.42320400  | 0.71100800  | -6.59554000 |
| C                                                                                                       | -4.25392800 | 0.26931600  | -0.40814900 | C | 1.89104400  | -6.81169600 | -0.24325800 |
| C                                                                                                       | -4.85621200 | -0.52500800 | 0.57504200  | H | 1.80943900  | -7.80687900 | -0.68592700 |
|                                                                                                         |             |             |             | H | 2.31606900  | -6.13838100 | -0.99074400 |

|                                                                                                         |             |             |             |                                                                                                         |             |             |             |
|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|---------------------------------------------------------------------------------------------------------|-------------|-------------|-------------|
| H                                                                                                       | 2.58572800  | -6.87208800 | 0.59691500  | N                                                                                                       | -1.21167300 | -0.92869400 | -4.34996400 |
| C                                                                                                       | -0.31981300 | -5.12097600 | 3.20902500  | C                                                                                                       | 0.76011400  | -4.11865300 | 0.31036200  |
| H                                                                                                       | 0.00749400  | -5.11619200 | 4.25143300  | O                                                                                                       | -0.24882700 | -0.43901700 | -2.35961100 |
| H                                                                                                       | -1.01557000 | -4.29231400 | 3.06525200  | C                                                                                                       | 1.03584800  | -6.57868800 | 0.29380800  |
| H                                                                                                       | -0.85189100 | -6.05776700 | 3.02748200  | H                                                                                                       | 0.24144900  | -6.57267600 | -0.45124800 |
| Cm                                                                                                      | 0.53444800  | -0.56849100 | -0.20993400 | C                                                                                                       | 1.67838600  | -5.17660000 | 2.28712500  |
| C                                                                                                       | -6.35559600 | -0.52062500 | 0.80504700  | H                                                                                                       | 2.21953300  | -4.23749000 | 2.38655900  |
| C                                                                                                       | -7.11190900 | -1.04348200 | -0.43059800 | C                                                                                                       | -0.56518100 | -2.76287400 | -2.84626800 |
| C                                                                                                       | -6.86024200 | 0.87311800  | 1.22176200  | H                                                                                                       | -1.53969900 | -3.25595800 | -2.90849900 |
| H                                                                                                       | -6.55346500 | -1.20854700 | 1.63294400  | H                                                                                                       | 0.12172500  | -3.25159400 | -3.54602600 |
| H                                                                                                       | -6.77291700 | -2.04435800 | -0.70923200 | C                                                                                                       | -0.67613200 | -1.28091400 | -3.18471000 |
| H                                                                                                       | -8.18329400 | -1.09353100 | -0.21981000 | C                                                                                                       | -1.74907000 | -1.89714100 | -5.32678800 |
| H                                                                                                       | -6.97010900 | -0.38434400 | -1.29171400 | H                                                                                                       | -1.22327200 | -2.84538500 | -5.22458200 |
| H                                                                                                       | -6.34424500 | 1.23041900  | 2.11626000  | H                                                                                                       | -1.49787200 | -1.51653400 | -6.31800500 |
| H                                                                                                       | -6.70795500 | 1.60688200  | 0.42539500  | C                                                                                                       | -1.29503200 | 0.50175900  | -4.71142700 |
| H                                                                                                       | -7.93064800 | 0.83266300  | 1.43914700  | H                                                                                                       | -1.38018400 | 1.07418300  | -3.79013600 |
| Cm(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>5</sub> ) <sup>+</sup> |             |             |             | H                                                                                                       | -2.21963600 | 0.63590300  | -5.27455400 |
| O                                                                                                       | 0.06468700  | -0.59690200 | 2.51304500  | H                                                                                                       | 0.71188200  | -7.26647700 | 1.07710500  |
| O                                                                                                       | 0.60641600  | 1.25431900  | 1.53596400  | H                                                                                                       | 2.39837900  | -5.98998900 | 2.38411700  |
| O                                                                                                       | 1.57651700  | 1.22454600  | -1.13777700 | C                                                                                                       | -3.26007500 | -2.09635900 | -5.20036400 |
| O                                                                                                       | 2.81762800  | -0.65507700 | 0.82736500  | H                                                                                                       | -3.60043700 | -2.78815200 | -5.97409400 |
| O                                                                                                       | 2.60117100  | -1.56118500 | -1.12507200 | H                                                                                                       | -3.52864200 | -2.51353600 | -4.22741600 |
| H                                                                                                       | 1.64926100  | 2.05301000  | -0.64825700 | H                                                                                                       | -3.79723800 | -1.15457500 | -5.32955900 |
| H                                                                                                       | 1.17959600  | 1.43440600  | -1.99262600 | C                                                                                                       | -0.09111600 | 0.96716100  | -5.53051200 |
| N                                                                                                       | -2.09384900 | 0.28636100  | 0.16384300  | H                                                                                                       | -0.21049800 | 2.02244300  | -5.78696000 |
| C                                                                                                       | -3.18489800 | -0.47281200 | 0.33798600  | H                                                                                                       | 0.83535100  | 0.85426400  | -4.96396000 |
| C                                                                                                       | -2.26076400 | 1.61311900  | 0.01571000  | H                                                                                                       | 0.00268600  | 0.40344900  | -6.46163700 |
| C                                                                                                       | -4.47880600 | 0.06296800  | 0.37388100  | C                                                                                                       | 2.35262900  | -7.05392300 | -0.32141700 |
| C                                                                                                       | -3.49918800 | 2.23299500  | 0.03430300  | H                                                                                                       | 2.22129300  | -8.06037600 | -0.72516100 |
| C                                                                                                       | -4.62601200 | 1.43351800  | 0.21887500  | H                                                                                                       | 2.67433600  | -6.39915300 | -1.13423300 |
| H                                                                                                       | -5.34159500 | -0.57014200 | 0.51779700  | H                                                                                                       | 3.14961100  | -7.09139900 | 0.42403200  |
| H                                                                                                       | -3.57506300 | 3.30471200  | -0.08937800 | C                                                                                                       | 0.58922500  | -5.28780700 | 3.35342000  |
| N                                                                                                       | 3.38068900  | -1.19300800 | -0.18694000 | H                                                                                                       | 1.04615300  | -5.26463200 | 4.34563400  |
| O                                                                                                       | 4.58545800  | -1.34262600 | -0.24816000 | H                                                                                                       | -0.11287000 | -4.45513500 | 3.28041500  |
| N                                                                                                       | 0.29843400  | 0.65258300  | 2.62056100  | H                                                                                                       | 0.03242200  | -6.22324400 | 3.26028900  |
| O                                                                                                       | 0.23373200  | 1.23476200  | 3.68433100  | Cm                                                                                                      | 0.44227800  | -0.76667900 | -0.01049500 |
| H                                                                                                       | -1.35487200 | 2.19185200  | -0.11718900 | H                                                                                                       | -5.61638400 | 1.87230100  | 0.24239300  |
| O                                                                                                       | -0.05445700 | -2.85410200 | -1.52226000 | O                                                                                                       | -2.90633000 | -1.78379900 | 0.46988200  |
| N                                                                                                       | 1.13496700  | -5.24335000 | 0.91401000  | C                                                                                                       | -3.98050800 | -2.71168300 | 0.68342700  |
| C                                                                                                       | 0.18797600  | -4.19099800 | -1.09978600 | H                                                                                                       | -4.66958800 | -2.71210300 | -0.16412200 |
| H                                                                                                       | 0.89391500  | -4.67658500 | -1.78010400 | H                                                                                                       | -3.50723100 | -3.68612600 | 0.77089100  |
| H                                                                                                       | -0.74791500 | -4.75958900 | -1.09984000 | H                                                                                                       | -4.51714100 | -2.47995700 | 1.60613600  |
| O                                                                                                       | 0.86068600  | -3.00222500 | 0.86851300  | Cm(H <sub>2</sub> O) <sub>5</sub> (NO <sub>3</sub> ) <sub>2</sub> (TEDGA)(L <sub>6</sub> ) <sup>+</sup> |             |             |             |

|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| O | 0.16755400  | -0.68743600 | 2.51980500  | H  | -1.53216500 | -3.31297800 | -2.87841200 |
| O | 0.61131100  | 1.18680700  | 1.53666600  | H  | 0.11187900  | -3.27551500 | -3.55910100 |
| O | 1.62078700  | 1.17210500  | -1.11351600 | C  | -0.70602200 | -1.32161900 | -3.15352200 |
| O | 2.88169200  | -0.70843100 | 0.79457300  | C  | -1.79959600 | -1.92597100 | -5.28774100 |
| O | 2.63881600  | -1.60646500 | -1.15831300 | H  | -1.26217100 | -2.86916600 | -5.20074100 |
| H | 1.73076000  | 1.97937000  | -0.59610400 | H  | -1.56294400 | -1.53179400 | -6.27721500 |
| H | 1.23377800  | 1.42845700  | -1.95994400 | C  | -1.37151100 | 0.47162000  | -4.64777500 |
| N | -2.15142800 | 0.23281000  | 0.25451000  | H  | -1.45099900 | 1.03141000  | -3.71833900 |
| C | -3.30031700 | -0.40814200 | 0.55062300  | H  | -2.30567400 | 0.59984400  | -5.19616600 |
| C | -2.22764500 | 1.53889500  | -0.05866200 | H  | 0.93850600  | -7.34058700 | 0.96914700  |
| C | -4.54294800 | 0.23656600  | 0.52937800  | H  | 2.58889800  | -6.04527100 | 2.27990300  |
| C | -3.41429200 | 2.25404700  | -0.10600700 | C  | -3.30662600 | -2.14446000 | -5.14737700 |
| C | -4.59555400 | 1.58149200  | 0.19323900  | H  | -3.64635200 | -2.83414100 | -5.92325400 |
| H | -5.45002900 | -0.29637400 | 0.77238300  | H  | -3.55946900 | -2.57283500 | -4.17511100 |
| H | -3.40573900 | 3.30325800  | -0.36914900 | H  | -3.85681700 | -1.20852300 | -5.26340700 |
| N | 3.43292000  | -1.23520600 | -0.23210400 | C  | -0.18555600 | 0.96309800  | -5.47764800 |
| O | 4.63667500  | -1.37284800 | -0.31630300 | H  | -0.32289800 | 2.01961900  | -5.71953100 |
| N | 0.34664500  | 0.57115100  | 2.62546100  | H  | 0.74991800  | 0.85628000  | -4.92498900 |
| O | 0.27147200  | 1.14954600  | 3.69025800  | H  | -0.09685000 | 0.41199400  | -6.41678500 |
| H | -1.29012000 | 2.03298600  | -0.27997000 | C  | 2.54757200  | -7.04264300 | -0.45105500 |
| O | -0.01716000 | -2.90351300 | -1.52689500 | H  | 2.44414900  | -8.04334400 | -0.87656600 |
| N | 1.28982400  | -5.30109100 | 0.84028300  | H  | 2.83369100  | -6.35815800 | -1.25251400 |
| C | 0.27013300  | -4.24156000 | -1.13406400 | H  | 3.35719300  | -7.06986000 | 0.28113800  |
| H | 0.97456300  | -4.69440400 | -1.83794400 | C  | 0.78643000  | -5.38111500 | 3.28767500  |
| H | -0.65011700 | -4.83499300 | -1.12544700 | H  | 1.25952200  | -5.36270200 | 4.27238400  |
| O | 0.94378500  | -3.06989600 | 0.84333100  | H  | 0.07170300  | -4.55784200 | 3.23566400  |
| N | -1.26330400 | -0.96214500 | -4.30562700 | H  | 0.24200200  | -6.32357300 | 3.19214000  |
| C | 0.86817500  | -4.17869400 | 0.26531700  | Cm | 0.50304600  | -0.83552500 | -0.01406700 |
| O | -0.28049700 | -0.48413800 | -2.32228500 | H  | -5.54892600 | 2.09594200  | 0.17049700  |
| C | 1.22544600  | -6.62668300 | 0.19488800  | S  | -3.11051700 | -2.12542600 | 0.98386600  |
| H | 0.41920200  | -6.63292500 | -0.53722200 | C  | -4.82040000 | -2.72262800 | 1.18492200  |
| C | 1.85580500  | -5.24148300 | 2.20489000  | H  | -5.39101100 | -2.60700900 | 0.26436700  |
| H | 2.38511900  | -4.29572400 | 2.30639100  | H  | -4.71760900 | -3.78397100 | 1.40984400  |
| C | -0.56398300 | -2.80538000 | -2.83671600 | H  | -5.31858600 | -2.23027000 | 2.01884800  |