**Supporting Information**

# Bonding trends across the series of tricarbonato-actinyl anions $[(AnO_2)(CO_3)_3]^{4-}$ (An = U–Cm): the plutonium turn

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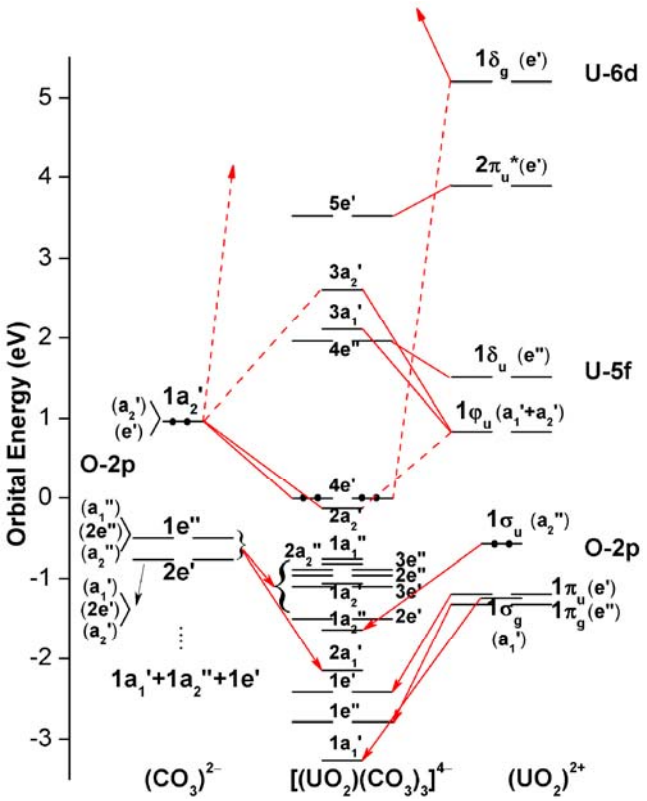


**Fig. S1.** Orbital energy level diagram (in eV) from scalar-relativistic Kohn-Sham (PBE, TZ2P basis) calculations. *Left*: $D_{3h}$-$(CO_3)^{2-}$ anion. *Right*: $D_{\infty h}$-$(UO_2)^{2+}$ cation. Middle: $D_{3h}$-$[(UO_2)(CO_3)_3]^{4-}$ complex with 4e′+2a$_2$′ as HOMOs. The local MO symmetry species of the fragments ($D_{3h}$ and $D_{\infty h}$) are given together with the induced group orbital symmetries in the complex ($D_{3h}$, in parentheses).

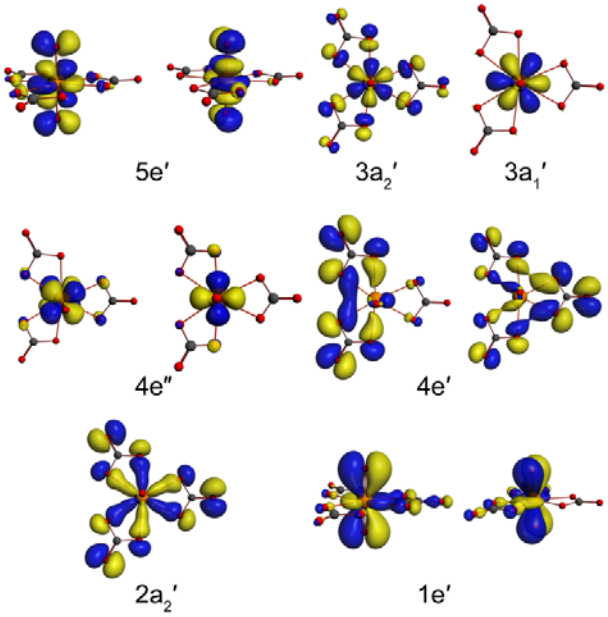


**Fig. S2.** Scalar-relativistic frontier molecular orbital (PBE-DF, TZ2P-basis) iso-contour surfaces of $[(UO_2)(CO_3)_3]^{4-}$ (cutoff = 0.03 a.u.). *Top*: virtual antibonding MOs 5e′ (U-5f$_\pi$ – O$_{ax}$-2p$_\pi$) and 3a$_2$′ (U-5f$_{\varphi 2}$ – $CO_3$-1a$_2$′) and nonbonding MO 3a$_1$′ (U-5f$_{\varphi 1}$). *Middle*: virtual nonbonding MO 4e″ (U-5f$_\delta$) and occupied bonding MO 4e′ ($CO_3$-1a$_2$′ + U-6d$_\delta$). *Bottom*: occupied bonding MOs 2a$_2$′ ($CO_3$-1a$_2$′ + U-5f$_{\varphi 2}$) and 1e′ (O$_{ax}$-2p$_\pi$ + U-5f$_\pi$).

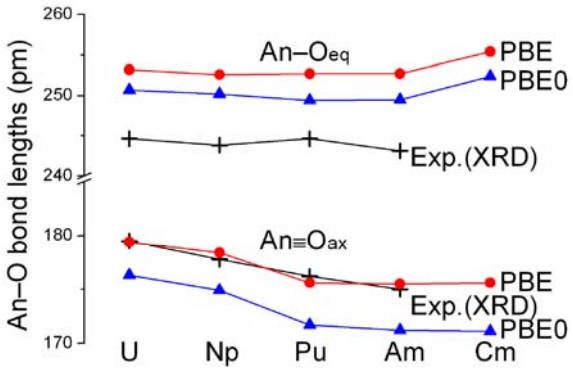


**Fig. S3.** Averaged An≡$O_{ax}$ and An–$O_{eq}$ bond lengths in $[(AnO_2)(CO_3)_3][C(NH_2)_3]_9^{5+}$.

**Table S1.** Calculated An–O bond lengths (in pm) in $[(UO_2)(CO_3)_3]^{4-}$ and $[(NpO_2)(CO_3)_3]^{4-}$ complexes at the PBE/TZ2P level by using SR-ZORA and SO-ZORA respectively

| | U≡$O_{ax}$ | U–$O_{eq}$ | Np≡$O_{ax}$ | Np–$O_{eq}$ |
|---|---|---|---|---|
| SR-ZORA | 184.7 | 254.2 | 183.7 | 253.8 |
| SO-ZORA | 184.7 | 253.9 | 182.5 | 255.2 |
| SO change | 0.0 | –0.3 | –1.2 | +1.4 |

**Table S2.** Relative energies (in kcal/mol) of different configurations of tricarbonato-actinyl(VI) ions for different DFs

| An | Config. | SVWN | PBE | PBE0 | BLYP | B3LYP | M06-L | M06 | M06-2X | TPSS | TPSSh |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Np | $(f_{\varphi 1u})^1$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| | $(f_\delta)^1$ | -2.27 | -0.79 | 23.4 | -0.64 | 18.9 | 4.42 | 28.98 | 42.65 | 0.99 | 10.62 |
| Pu | $(f_\delta)^2$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| | $(f_\delta)^1(f_{\varphi 1u})^1$ | 2.99 | 5.06 | 27.16 | 5.68 | 22.79 | 10.09 | 29.76 | 52.65 | – | – |

**Table S3.** Correlation of symmetry species of point groups $D_{3h}$, $C_{3v}$ and $C_{2v}$.[a]

| $D_{3h}$ | $C_{3v}$ | $C_{2v}$ |
|---|---|---|
| $A_1'$ | $A_1$ | $A_1$ |
| $A_2'$ | $A_2$ | $B_2$ |
| $E'$ | $E$ | $A_1+B_2$ |
| $A_1''$ | $A_2$ | $A_2$ |
| $A_2''$ | $A_1$ | $B_1$ |
| $E''$ | $E$ | $A_2+B_1$ |

[a] Since the CASSCF module of MOLPRO can only handle Abelian point-groups, the $C_{2v}$ symmetry was used.

**Table S4.** An≡$O_{ax}$ Bond Indices in $[(AnO_2)(CO_3)_3][C(NH_2)_3]_9^{5+}$ from DFT(PBE-DZP): $n$ = number of unpaired electrons on An; $R_{An\equiv Oax}$ = bond length (in pm), $k_{An\equiv Oax}$ = relaxed force constant (in N/cm); $BO_{NM2}$ = Nalewajski- Mrozek's valence index type 2; $BO_{FM}$, $BO_M$ = Mayer's fuzzy and conventional bond orders; $BO_L$ = Laplacian bond order.

| An | $n$ | $R_{An\equiv Oax}$ | $k_{An\equiv Oax}$ | $BO_{NM2}$ | $BO_{FM}$ | $BO_M$ | $BO_L$ |
|---|---|---|---|---|---|---|---|
| U | 0 | 179.4 | 6.31 | 2.80 | 2.89 | 1.94 | 1.27 |
| Np | 1 | 178.4 | 6.30 | 2.90 | 2.89 | 1.91 | 1.26 |
| Pu | 2 | 175.6 | 6.33 | 2.78 | 2.90 | 1.92 | 1.26 |
| Am | 3 | 175.5 | 5.95 | 2.48 | 2.88 | 1.89 | 1.19 |
| Cm | 4 | 175.6 | 5.32 | 2.43 | 2.80 | 1.81 | 0.96 |

**Table S5.** An≡$O_{ax}$ bond lengths (in pm) in isolated $[(AnO_2)(CO_3)_3]^{4-}$ ions obtained with different DFs, and experimental values for condensed phases

| An | Density functional calculations of the isolated tricarbonato-uranyl anion | | | | | | | | | | | crystal | solution |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | El. Config. | M06 | M06-2X | PBE0 | M06-L | B3LYP | TPSSh | SVWN | PBE | TPSS | BLYP | XRD | EXAFS |
| $_{92}$U | $(f)^0$ | 179.4 | 179.5 | 180.8 | 182.3 | 183.0 | 182.9 | 183.4 | 184.7 | 184.9 | 186.8 | 179.5(±1.0) | 181 |
| $_{93}$Np | $(f_{\varphi 1})^1$ | 177.6 | 177.9 | 179.1 | 180.8 | 181.5 | 181.5 | 182.3 | 183.7 | 183.7 | 185.8 | 177.8(±1.5) | 179 |
| $_{94}$Pu | $(f_{\delta})^2$ | 175.9 | 174.4 | 176.1 | 179.1 | 179.0 | 179.0 | 178.7 | 180.7 | 181.0 | 183.2 | 176.2(±1.2) | 175 |
| $_{95}$Am | $(f_{\delta})^2(f_{\varphi 1})^1$ | 174.5 | 174.6 | 175.5 | 179.0 | 178.6 | 178.8 | 178.6 | 180.9 | 182.8 | 183.6 | 175.0±(1.2) | |
| $_{96}$Cm | $(f_{\delta})^2(f_{\varphi 1})^1(f_{\varphi 2})^1$ | 175.5 | 185.6 | 176.4 | 186.6 | 183.1 | 183.3 | 178.8 | 183.2 | 184.7 | 186.8 | | |

**Table S6.** An–$O_{eq}$ bond lengths (in pm) in isolated $[(AnO_2)(CO_3)_3]^{4-}$ ions obtained with different DFs, and experimental values for condensed phases

| An | Density Functional calculations of the isolated tricarbonato-uranyl anion | | | | | | | | | | | crystal | solution |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | El. Config. | SVWN | M06-2X | PBE0 | TPSSh | M06 | TPSS | B3LYP | PBE | M06L | BLYP | XRD | EXAFS |
| $_{92}$U | $(f)^0$ | 246.6 | 250.6 | 251.4 | 251.4 | 253.1 | 252.6 | 254.4 | 254.2 | 254.4 | 257.8 | 244.6(±0.6) | 244 |
| $_{93}$Np | $(f_{\varphi 1})^1$ | 245.7 | 250.3 | 251.0 | 250.8 | 252.9 | 251.9 | 254.1 | 253.8 | 254.1 | 257.5 | 243.8(±0.9) | 245 |
| $_{94}$Pu | $(f_{\delta})^2$ | 247.4 | 250.4 | 252.2 | 254.4 | 254.8 | 256.2 | 256.7 | 257.6 | 260.7 | 262.3 | 244.6(±1.0) | 246 |
| $_{95}$Am | $(f_{\delta})^2(f_{\varphi 1})^1$ | 247.2 | 250.6 | 252.2 | 253.1 | 252.8 | 255.4 | 256.3 | 258.0 | 257.1 | 262.5 | 243.1(±1.2) | |
| $_{96}$Cm | $(f_{\delta})^2(f_{\varphi 1})^1(f_{\varphi 2})^1$ | 252.0 | | 257.8 | 264.9 | 257.2 | 267.5 | 267.9 | 270.2 | 269.8 | 277.5 | | |

**Table S7.** Am≡$O_{ax}$ and Am–$O_{eq}$ bond lengths (in pm) in $[(AmO_2)(CO_3)_3]^{4-}$ depending on the percentage of Hartree-Fock exchange ($HF_x$) in the PBE0 density functional

| $D$ | XRD | $HF_x$ = 0 | 5 | 10 | 15 | 20 | 25 | 30 | 35 | 40 | 45 | 50 | $\Delta_{50-0}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Am≡$O_{ax}$ | 175.0 | 180.9 | 179.7 | 178.6 | 177.5 | 176.5 | 175.5 | 174.5 | 173.7 | 172.9 | 172.2 | 171.5 | -9.4pm |
| Am–$O_{eq}$ | 243.1 | 258.0 | 256.8 | 255.6 | 254.4 | 253.3 | 252.2 | 251.3 | 250.6 | 250.1 | 249.6 | 249.2 | -8.8pm |

**Table S8.** An≡$O_{ax}$ bond lengths (in pm) in isolated $[(AnO_2)(CO_3)_3]^{4-}$ ions obtained from a dispersion corrected functional (DFT-D3-BJ) of Grimme

| An | El. Config. | XRD/EXAFS | PBE | PBE-D3 | BLYP | BLYP –D3 | B3LYP | B3LYP-D3 |
|---|---|---|---|---|---|---|---|---|
| U | $(f)^0$ | 179.5/179.0 | 184.7 | 184.7 | 186.8 | 186.7 | 183.0 | 183.0 |
| Np | $(f_{\varphi 1})^1$ | 177.8/178.0 | 183.7 | 183.6 | 185.8 | 185.7 | 181.5 | 181.5 |
| Pu | $(f_{\delta})^2$ | 176.2/175.0 | 180.7 | 180.6 | 183.2 | 183.1 | 179.0 | 178.9 |

**Table S9.** An–$O_{eq}$ bond lengths (in pm) in isolated $[(AnO_2)(CO_3)_3]^{4-}$ ions obtained from a dispersion corrected functional (DFT-D3-BJ) of Grimme

| An | El. Config. | XRD/EXAFS | PBE | PBE-D3 | BLYP | BLYP –D3 | B3LYP | B3LYP-D3 |
|---|---|---|---|---|---|---|---|---|
| U | $(f)^0$ | 244.6/242.0 | 254.2 | 253.9 | 257.8 | 257.2 | 254.4 | 253.9 |
| Np | $(f_{\varphi 1})^1$ | 243.8/242.0 | 253.8 | 253.5 | 257.5 | 256.9 | 254.1 | 253.6 |
| Pu | $(f_{\delta})^2$ | 244.6/246.0 | 257.6 | 257.2 | 262.3 | 261.4 | 256.7 | 256.0 |

**Table S10.** Np–O bond lengths (in pm) in isolated $[(NpO_2)(CO_3)_3]^{4-}$ ions obtained for different DFs and two different electronic configurations

| | Config. | XRD/EXAFS | M06 | M06-2X | PBE0 | M06-L | B3LYP | TPSSh | SVWN | PBE | TPSS | BLYP |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Np=$O_{ax}$ | $(f_{\delta})^1$ | 177.8(±1.5)/178 | 177.0 | 176.5 | 178.0 | 180.0 | 180.5 | 180.4 | 180.8 | 182.4 | 182.5 | 184.7 |
| | $(f_{\varphi})^1$ | 177.8(±1.5)/178 | 177.6 | 177.9 | 179.1 | 180.8 | 181.5 | 181.5 | 182.3 | 183.7 | 183.7 | 185.8 |

| | Config. | XRD/EXAFS | SVWN | M06-2X | PBE0 | TPSSh | M06 | TPSS | B3LYP | PBE | M06-L | BLYP |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Np-$O_{eq}$ | $(f_{\delta})^1$ | 243.8(±0.9)/242 | 246.8 | 250.4 | 251.3 | 251.7 | 252.8 | 253.3 | 254.6 | 255.3 | 255.5 | 259.3 |
| | $(f_{\varphi})^1$ | 243.8(±0.9)/242 | 245.7 | 250.3 | 251.0 | 250.8 | 252.9 | 251.9 | 254.1 | 253.8 | 254.1 | 257.5 |

**Table S11.** Averaged An≡$O_{ax}$ and An–$O_{eq}$ bond lengths (in pm) in $[(AnO_2)(CO_3)_3][C(NH_2)_3]_9^{5+}$ (bond lengths of the complex in vacuum in parentheses)

| An | Config. | An≡$O_{ax}$ | | | | An–$O_{eq}$ | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | XRD | EXAFS | PBE | PBE0 | XRD | EXAFS | PBE | PBE0 |
| U | $(f)^0$ | 179.5(±1.0) | 179 | 179.4(184.7) | 176.3(180.8) | 244.6(±0.6) | 242 | 253.2(254.2) | 250.7(251.4) |
| Np | $(f_{\varphi 1})^1$ | 177.8(±1.5) | 178 | 178.4(183.7) | 174.9(179.1) | 243.8(±0.9) | 242 | 252.6(253.8) | 250.2(251.0) |
| Pu | $(f_{\delta})^2$ | 176.2(±1.2) | 175 | 175.6(180.7) | 171.7(176.1) | 244.6(±1.0) | 246 | 252.7(257.6) | 249.4(252.2) |
| Am | $(f_{\delta})^2(f_{\varphi 1})^1$ | 175.0±(1.2) | – | 175.5(180.9) | 171.2(175.5) | 243.1(±1.2) | – | 252.7(258.0) | 249.5(252.2) |
| Cm | $(f_{\delta})^2(f_{\varphi 1})^1(f_{\varphi 2})^1$ | – | – | 175.6(183.2) | 171.1(176.4) | – | – | 255.4(270.2) | 252.4(257.8) |

**Table S12.** Full reference No. 17

Gaussian 09, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009

**Table S13.** Electron configurations of the (non-specified) S-L-J ground states of chemically unbound free atomic cations of charge q+ in physical vacuum from the first half-group of the lanthanide and actinide elements. [a]

| *q*+ | 1+ | 2+ | 3+ | 4+ | 5+ | 6+ | 7+ | 8+ |
|---|---|---|---|---|---|---|---|---|
| La | **$5d^2$** | **$5d^1$** | $4f^0$ | | | | | |
| Ce | **$4f^1 5d^2$** | $4f^2$ | $4f^1$ | $4f^0$ | | | | |
| Pr | **$4f^3 6s^1$** | $4f^3$ | $4f^2$ | $4f^1$ | $4f^0$ | **$4f^1 5p^{-2}$** | **$4f^1 5p^{-3}$** | **$4f^1 5p^{-4}$** |
| Nd | **$4f^4 6s^1$** | $4f^4$ | $4f^3$ | $4f^2$ | **$4f^2 5p^{-1}$** | **$4f^2 5p^{-2}$** | **$4f^2 5p^{-3}$** | **$4f^2 5p^{-4}$** |
| Pm | **$4f^5 6s^1$** | $4f^5$ | $4f^4$ | $4f^3$ | **$4f^3 5p^{-1}$** | **$4f^3 5p^{-2}$** | **$4f^3 5p^{-3}$** | **$4f^3 5p^{-4}$** |
| Sm | **$4f^6 6s^1$** | $4f^6$ | $4f^5$ | $4f^4$ | $4f^3$ | **$4f^4 5p^{-2}$** | **$4f^4 5p^{-3}$** | **$4f^4 5p^{-4}$** |
| Eu | **$4f^7 6s^1$** | $4f^7$ | $4f^6$ | $4f^5$ | **$4f^5 5p^{-1}$** | **$4f^5 5p^{-2}$** | **$4f^3 5p^{-1}$** | **$4f^3 5p^{-4}$** |
| Gd | **$4f^7 5d^1 6s^1$** | **$4f^7 5d^1$** | $4f^7$ | $4f^6$ | **$4f^6 5p^{-1}$** | **$4f^6 5p^{-2}$** | **$4f^6 5p^{-3}$** | **$4f^6 5p^{-4}$** |

| *q*+ | 1+ | 2+ | 3+ | 4+ | 5+ | 6+ | 7+ | 8+ |
|---|---|---|---|---|---|---|---|---|
| Ac | **$7s^2$** | **$7s^1$** | $5f^0$ | | | | | |
| Th | **$6d^1 7s^2$** | **$5f^1 6d^1$** | $5f^1$ | $5f^0$ | | | | |
| Pa | **$5f^2 7s^2$** | **$5f^2 6d^1$** | $5f^2$ | $5f^1$ | $5f^0$ | | | |
| U | **$5f^3 7s^2$** | $5f^4$ | $5f^3$ | $5f^2$ | $5f^1$ | $5f^0$ | | |
| Np | **$5f^4 6d^1 7s^1$** | $5f^5$ | $5f^4$ | $5f^3$ | $5f^2$ | $5f^1$ | **$5f^1 6p^{-1}$** | **$5f^1 6p^{-2}$** |
| Pu | **$5f^6 7s^1$** | $5f^6$ | $5f^5$ | $5f^4$ | $5f^3$ | **$5f^3 6p^{-1}$** | **$5f^3 6p^{-2}$** | **$5f^3 6p^{-3}$** |
| Am | **$5f^7 7s^1$** | $5f^7$ | $5f^6$ | $5f^5$ | $5f^4$ | $5f^3$ | **$5f^3 6p^{-1}$** | **$5f^3 6p^{-2}$** |
| Cm | **$5f^7 7s^2$** | $5f^8$ | $5f^7$ | $5f^6$ | $5f^5$ | $5f^4$ | **$5f^5 6p^{-2}$** | **$5f^5 6p^{-3}$** |

[a] **Bold face**: 'Nonsystematic' configurations of the ground states of the 4f- and 5f-elemental free atomic cations with, respectively, 5d6s- and 6d7s-valence occupations, or with 5p- and 6p-core holes. Empty entries have empty $f^0d^0s^0$ valence shells and the expected number of p core holes. The $(n\text{-}1)p^{-x}$ symbol means that ***x*** electron(s) are ionized from the $(n\text{-}1)p^6$ outer core shell.

**Table S14.** Atomic coordinates of the optimized $[(AnO_2)(CO_3)_3]^{4-}$ and $[(AnO_2)(CO_3)_3][C(NH_2)_3]_9^{5+}$ species using the PBE0 density functional.

**$UO_2(CO_3)_3^{4-}$**

| | | | |
|---|---|---|---|
| 1.U | 0.000000 | 0.000000 | 0.000000 |
| 2.O | 0.000000 | 0.000000 | 1.808061 |
| 3.O | 0.000000 | 0.000000 | -1.808061 |
| 4.O | -2.124960 | -3.680538 | 0.000000 |
| 5.O | -2.078811 | -1.413937 | 0.000000 |
| 6.O | -0.185100 | -2.507271 | 0.000000 |
| 7.O | 2.263911 | -1.093335 | 0.000000 |
| 8.O | 4.249919 | 0.000000 | 0.000000 |
| 9.O | -2.078811 | 1.413937 | 0.000000 |
| 10.O | -2.124960 | 3.680538 | 0.000000 |
| 11.O | -0.185100 | 2.507271 | 0.000000 |
| 12.O | 2.263911 | 1.093335 | 0.000000 |
| 13.C | -1.485113 | -2.572292 | 0.000000 |
| 14.C | 2.970227 | 0.000000 | 0.000000 |
| 15.C | -1.485113 | 2.572292 | 0.000000 |

**$NpO_2(CO_3)_3^{4-}$**

| | | | |
|---|---|---|---|
| 1.Np | 0.000000 | 0.000000 | 0.000000 |
| 2.O | 0.000000 | 0.000000 | 1.791489 |
| 3.O | 0.000000 | 0.000000 | -1.791489 |
| 4.O | -2.123145 | -3.677394 | 0.000000 |
| 5.O | -2.077064 | -1.410062 | 0.000000 |
| 6.O | -0.182617 | -2.503821 | 0.000000 |
| 7.O | 2.259681 | -1.093759 | 0.000000 |
| 8.O | 4.246289 | 0.000000 | 0.000000 |
| 9.O | -2.077064 | 1.410062 | 0.000000 |
| 10.O | -2.123145 | 3.677394 | 0.000000 |
| 11.O | -0.182617 | 2.503821 | 0.000000 |
| 12.O | 2.259681 | 1.093759 | 0.000000 |
| 13.C | -1.482404 | -2.567599 | 0.000000 |
| 14.C | 2.964808 | 0.000000 | 0.000000 |
| 15.C | -1.482404 | 2.567599 | 0.000000 |

**$PuO_2(CO_3)_3^{4-}$**

| | | | |
|---|---|---|---|
| 1.Pu | 0.000000 | 0.000000 | 0.000000 |
| 2.O | 0.000000 | 0.000000 | 1.760761 |
| 3.O | 0.000000 | 0.000000 | -1.760761 |
| 4.O | -2.128791 | -3.687175 | 0.000000 |
| 5.O | -2.082981 | -1.422530 | 0.000000 |
| 6.O | -0.190457 | -2.515179 | 0.000000 |
| 7.O | 2.273438 | -1.092649 | 0.000000 |
| 8.O | 4.257583 | 0.000000 | 0.000000 |
| 9.O | -2.082981 | 1.422530 | 0.000000 |
| 10.O | -2.128791 | 3.687175 | 0.000000 |
| 11.O | -0.190457 | 2.515179 | 0.000000 |
| 12.O | 2.273438 | 1.092649 | 0.000000 |
| 13.C | -1.487704 | -2.576779 | 0.000000 |
| 14.C | 2.975408 | 0.000000 | 0.000000 |
| 15.C | -1.487704 | 2.576779 | 0.000000 |

**$AmO_2(CO_3)_3^{4-}$**

| | | | |
|---|---|---|---|
| 1.Am | 0.000000 | 0.000000 | 0.000000 |
| 2.O | 0.000000 | 0.000000 | 1.754944 |
| 3.O | 0.000000 | 0.000000 | -1.754944 |
| 4.O | -2.128604 | -3.686851 | 0.000000 |
| 5.O | -2.083524 | -1.421578 | 0.000000 |
| 6.O | -0.189361 | -2.515174 | 0.000000 |
| 7.O | 2.272884 | -1.093596 | 0.000000 |
| 8.O | 4.257209 | 0.000000 | 0.000000 |
| 9.O | -2.083524 | 1.421578 | 0.000000 |
| 10.O | -2.128604 | 3.686851 | 0.000000 |
| 11.O | -0.189361 | 2.515174 | 0.000000 |
| 12.O | 2.272884 | 1.093596 | 0.000000 |
| 13.C | -1.486775 | -2.575169 | 0.000000 |
| 14.C | 2.973549 | 0.000000 | 0.000000 |
| 15.C | -1.486775 | 2.575169 | 0.000000 |

**$[UO_2(CO_3)_3][C(NH_2)_3]_9^{5+}$**

| | | | |
|---|---|---|---|
| 1.U | 0.000000 | 0.000000 | 0.155164 |
| 2.O | 0.000000 | 0.000000 | 1.918051 |
| 3.O | 0.000000 | 0.000000 | -1.608101 |
| 4.O | -2.077302 | 1.401140 | 0.067488 |
| 5.O | -0.174772 | 2.499567 | 0.067488 |
| 6.O | -2.077298 | 3.597985 | -0.377781 |
| 7.C.tz2p | -1.464353 | 2.536333 | -0.087666 |
| 8.O | -0.174772 | -2.499567 | 0.067488 |
| 9.O | -2.077302 | -1.401140 | 0.067488 |
| 10.O | -2.077298 | -3.597985 | -0.377781 |
| 11.C.tz2p | -1.464353 | -2.536333 | -0.087666 |
| 12.O | 2.252074 | 1.098426 | 0.067488 |
| 13.O | 2.252074 | -1.098426 | 0.067488 |
| 14.O | 4.154596 | 0.000000 | -0.377781 |
| 15.C.tz2p | 2.928706 | 0.000000 | -0.087666 |
| 16.C.dzp | -0.231366 | 5.991089 | 1.373710 |
| 17.N | -0.912143 | 6.005892 | 0.237888 |
| 18.H | -1.158746 | 6.889887 | -0.192795 |
| 19.H | -1.355869 | 5.121709 | -0.084892 |
| 20.N | 0.231856 | 4.826542 | 1.830840 |
| 21.H | 0.141451 | 3.982334 | 1.255830 |
| 22.H | 0.439409 | 4.726513 | 2.816261 |
| 23.N | 0.010787 | 7.111308 | 2.046500 |
| 24.H | -0.467335 | 7.978216 | 1.822894 |
| 25.C.dzp | -0.231366 | -5.991089 | 1.373710 |
| 26.N | -0.912143 | -6.005892 | 0.237888 |
| 27.H | -1.355869 | -5.121709 | -0.084892 |
| 28.H | -1.158746 | -6.889887 | -0.192795 |
| 29.N | 0.010787 | -7.111308 | 2.046500 |
| 30.H | -0.467335 | -7.978216 | 1.822894 |
| 31.N | 0.231856 | -4.826542 | 1.830840 |
| 32.H | 0.141451 | -3.982334 | 1.255830 |
| 33.H | 0.439409 | -4.726513 | 2.816261 |
| 34.C.dzp | 5.304118 | 2.795176 | 1.373710 |
| 35.N | 5.657327 | 2.213007 | 0.237888 |
| 36.H | 5.113464 | 1.386637 | -0.084892 |
| 37.H | 6.546190 | 2.441440 | -0.192795 |
| 38.N | 6.153180 | 3.564996 | 2.046500 |

| | | | |
|---|---|---|---|
| 39.H | 7.143005 | 3.584384 | 1.822894 |
| 40.H | 5.835934 | 4.187932 | 2.780900 |
| 41.N | 4.063980 | 2.614065 | 1.830840 |
| 42.H | 3.378077 | 2.113667 | 1.255830 |
| 43.H | 3.873576 | 2.743795 | 2.816261 |
| 44.C.dzp | -5.072752 | -3.195913 | 1.373710 |
| 45.N | -4.745183 | -3.792885 | 0.237888 |
| 46.H | -5.387444 | -4.448447 | -0.192795 |
| 47.H | -3.757595 | -3.735072 | -0.084892 |
| 48.N | -4.295837 | -2.212478 | 1.830840 |
| 49.H | -3.519528 | -1.868667 | 1.255830 |
| 50.H | -4.312985 | -1.982717 | 2.816261 |
| 51.N | -6.163967 | -3.546312 | 2.046500 |
| 52.H | -6.544823 | -2.960101 | 2.780900 |
| 53.C.dzp | 5.304118 | -2.795176 | 1.373710 |
| 54.N | 5.657327 | -2.213007 | 0.237888 |
| 55.H | 6.546190 | -2.441440 | -0.192795 |
| 56.H | 5.113464 | -1.386637 | -0.084892 |
| 57.N | 4.063980 | -2.614065 | 1.830840 |
| 58.H | 3.378077 | -2.113667 | 1.255830 |
| 59.H | 3.873576 | -2.743795 | 2.816261 |
| 60.N | 6.153180 | -3.564996 | 2.046500 |
| 61.H | 7.143005 | -3.584384 | 1.822894 |
| 62.C.dzp | -5.072752 | 3.195913 | 1.373710 |
| 63.N | -4.745183 | 3.792885 | 0.237888 |
| 64.H | -3.757595 | 3.735072 | -0.084892 |
| 65.H | -5.387444 | 4.448447 | -0.192795 |
| 66.N | -6.163967 | 3.546312 | 2.046500 |
| 67.H | -6.675670 | 4.393832 | 1.822894 |
| 68.H | -6.544823 | 2.960101 | 2.780900 |
| 69.N | -4.295837 | 2.212478 | 1.830840 |
| 70.H | -3.519528 | 1.868667 | 1.255830 |
| 71.H | -4.312985 | 1.982717 | 2.816261 |
| 72.C.dzp | -4.104555 | 0.000000 | -2.763235 |
| 73.N | -4.826268 | 0.000000 | -3.881948 |
| 74.H | -5.148604 | 0.861544 | -4.307619 |
| 75.H | -5.148604 | -0.861544 | -4.307619 |
| 76.N | -3.745379 | -1.145416 | -2.199583 |
| 77.H | -3.989932 | -2.023168 | -2.637552 |
| 78.H | -3.151764 | -1.171294 | -1.358340 |
| 79.N | -3.745379 | 1.145416 | -2.199583 |
| 80.H | -3.989932 | 2.023168 | -2.637552 |
| 81.H | -3.151764 | 1.171294 | -1.358340 |
| 82.C.dzp | 2.052278 | -3.554649 | -2.763235 |
| 83.N | 2.413134 | -4.179671 | -3.881948 |
| 84.H | 1.828183 | -4.889594 | -4.307619 |
| 85.H | 3.320421 | -4.028050 | -4.307619 |
| 86.N | 2.864649 | -2.670886 | -2.199583 |
| 87.H | 3.747081 | -2.443798 | -2.637552 |
| 88.H | 2.590252 | -2.143860 | -1.358340 |
| 89.N | 0.880731 | -3.816302 | -2.199583 |
| 90.H | 0.242851 | -4.466966 | -2.637552 |
| 91.H | 0.561512 | -3.315154 | -1.358340 |
| 92.C.dzp | 2.052278 | 3.554649 | -2.763235 |
| 93.N | 2.413134 | 4.179671 | -3.881948 |
| 94.H | 3.320421 | 4.028050 | -4.307619 |

| | | | |
|---|---|---|---|
| 95.H | 1.828183 | 4.889594 | -4.307619 |
| 96.N | 0.880731 | 3.816302 | -2.199583 |
| 97.H | 0.242851 | 4.466966 | -2.637552 |
| 98.H | 0.561512 | 3.315154 | -1.358340 |
| 99.N | 2.864649 | 2.670886 | -2.199583 |
| 100.H | 3.747081 | 2.443798 | -2.637552 |
| 101.H | 2.590252 | 2.143860 | -1.358340 |
| 102.H | 5.835934 | -4.187932 | 2.780900 |
| 103.H | 0.708889 | -7.148033 | 2.780900 |
| 104.H | -6.675670 | -4.393832 | 1.822894 |
| 105.H | 0.708889 | 7.148033 | 2.780900 |

**$[NpO_2(CO_3)_3][C(NH_2)_3]_9^{5+}$**:

| | | | |
|---|---|---|---|
| 1.Np | 0.000000 | 0.000000 | 0.170049 |
| 2.O | 0.000000 | 0.000000 | 1.919513 |
| 3.O | 0.000000 | 0.000000 | -1.579298 |
| 4.O | -2.074612 | 1.396252 | 0.082940 |
| 5.O | -0.171884 | 2.494792 | 0.082940 |
| 6.O | -2.072383 | 3.589473 | -0.380003 |
| 7.C.tz2p | -1.460481 | 2.529627 | -0.077194 |
| 8.O | -0.171884 | -2.494792 | 0.082940 |
| 9.O | -2.074612 | -1.396252 | 0.082940 |
| 10.O | -2.072383 | -3.589473 | -0.380003 |
| 11.C.tz2p | -1.460481 | -2.529627 | -0.077194 |
| 12.O | 2.246495 | 1.098540 | 0.082940 |
| 13.O | 2.246495 | -1.098540 | 0.082940 |
| 14.O | 4.144766 | 0.000000 | -0.380003 |
| 15.C.tz2p | 2.920962 | 0.000000 | -0.077194 |
| 16.C.dzp | -0.212620 | 5.997253 | 1.337919 |
| 17.N | -0.902532 | 5.997828 | 0.207366 |
| 18.H | -1.159790 | 6.876937 | -0.226840 |
| 19.H | -1.354971 | 5.110251 | -0.093970 |
| 20.N | 0.253438 | 4.838238 | 1.805644 |
| 21.H | 0.150856 | 3.984805 | 1.245023 |
| 22.H | 0.472476 | 4.752613 | 2.790014 |
| 23.N | 0.035342 | 7.126022 | 1.994326 |
| 24.H | -0.442374 | 7.990483 | 1.762284 |
| 25.C.dzp | -0.212620 | -5.997253 | 1.337919 |
| 26.N | -0.902532 | -5.997828 | 0.207366 |
| 27.H | -1.354971 | -5.110251 | -0.093970 |
| 28.H | -1.159790 | -6.876937 | -0.226840 |
| 29.N | 0.035342 | -7.126022 | 1.994326 |
| 30.H | -0.442374 | -7.990483 | 1.762284 |
| 31.N | 0.253438 | -4.838238 | 1.805644 |
| 32.H | 0.150856 | -3.984805 | 1.245023 |
| 33.H | 0.472476 | -4.752613 | 2.790014 |
| 34.C.dzp | 5.300083 | 2.814493 | 1.337919 |
| 35.N | 5.645537 | 2.217299 | 0.207366 |
| 36.H | 5.103093 | 1.381687 | -0.093970 |
| 37.H | 6.535497 | 2.434061 | -0.226840 |
| 38.N | 6.153645 | 3.593618 | 1.994326 |
| 39.H | 7.141148 | 3.612134 | 1.762284 |
| 40.H | 5.842298 | 4.222261 | 2.725915 |
| 41.N | 4.063318 | 2.638603 | 1.805644 |
| 42.H | 3.375514 | 2.123048 | 1.245023 |
| 43.H | 3.879646 | 2.785483 | 2.790014 |

| | | | |
|---|---|---|---|
| 44.C.dzp | -5.087464 | -3.182761 | 1.337919 |
| 45.N | -4.743006 | -3.780529 | 0.207366 |
| 46.H | -5.375707 | -4.442876 | -0.226840 |
| 47.H | -3.748122 | -3.728565 | -0.093970 |
| 48.N | -4.316756 | -2.199635 | 1.805644 |
| 49.H | -3.526371 | -1.861757 | 1.245023 |
| 50.H | -4.352122 | -1.967131 | 2.790014 |
| 51.N | -6.188987 | -3.532403 | 1.994326 |
| 52.H | -6.577734 | -2.948448 | 2.725915 |
| 53.C.dzp | 5.300083 | -2.814493 | 1.337919 |
| 54.N | 5.645537 | -2.217299 | 0.207366 |
| 55.H | 6.535497 | -2.434061 | -0.226840 |
| 56.H | 5.103093 | -1.381687 | -0.093970 |
| 57.N | 4.063318 | -2.638603 | 1.805644 |
| 58.H | 3.375514 | -2.123048 | 1.245023 |
| 59.H | 3.879646 | -2.785483 | 2.790014 |
| 60.N | 6.153645 | -3.593618 | 1.994326 |
| 61.H | 7.141148 | -3.612134 | 1.762284 |
| 62.C.dzp | -5.087464 | 3.182761 | 1.337919 |
| 63.N | -4.743006 | 3.780529 | 0.207366 |
| 64.H | -3.748122 | 3.728565 | -0.093970 |
| 65.H | -5.375707 | 4.442876 | -0.226840 |
| 66.N | -6.188987 | 3.532403 | 1.994326 |
| 67.H | -6.698774 | 4.378349 | 1.762284 |
| 68.H | -6.577734 | 2.948448 | 2.725915 |
| 69.N | -4.316756 | 2.199635 | 1.805644 |
| 70.H | -3.526371 | 1.861757 | 1.245023 |
| 71.H | -4.352122 | 1.967131 | 2.790014 |
| 72.C.dzp | -4.152076 | 0.000000 | -2.701934 |
| 73.N | -4.892548 | 0.000000 | -3.808618 |
| 74.H | -5.232440 | 0.861367 | -4.220885 |
| 75.H | -5.232440 | -0.861367 | -4.220885 |
| 76.N | -3.781973 | -1.145142 | -2.144809 |
| 77.H | -4.033082 | -2.022893 | -2.579016 |
| 78.H | -3.173870 | -1.170347 | -1.313350 |
| 79.N | -3.781973 | 1.145142 | -2.144809 |
| 80.H | -4.033082 | 2.022893 | -2.579016 |
| 81.H | -3.173870 | 1.170347 | -1.313350 |
| 82.C.dzp | 2.076038 | -3.595804 | -2.701934 |
| 83.N | 2.446274 | -4.237070 | -3.808618 |
| 84.H | 1.870255 | -4.962110 | -4.220885 |
| 85.H | 3.362186 | -4.100743 | -4.220885 |
| 86.N | 2.882709 | -2.702714 | -2.144809 |
| 87.H | 3.768418 | -2.481305 | -2.579016 |
| 88.H | 2.600485 | -2.163478 | -1.313350 |
| 89.N | 0.899265 | -3.847856 | -2.144809 |
| 90.H | 0.264664 | -4.504198 | -2.579016 |
| 91.H | 0.573384 | -3.333825 | -1.313350 |
| 92.C.dzp | 2.076038 | 3.595804 | -2.701934 |
| 93.N | 2.446274 | 4.237070 | -3.808618 |
| 94.H | 3.362186 | 4.100743 | -4.220885 |
| 95.H | 1.870255 | 4.962110 | -4.220885 |
| 96.N | 0.899265 | 3.847856 | -2.144809 |
| 97.H | 0.264664 | 4.504198 | -2.579016 |
| 98.H | 0.573384 | 3.333825 | -1.313350 |
| 99.N | 2.882709 | 2.702714 | -2.144809 |

| | | | |
|---|---|---|---|
| 100.H | 3.768418 | 2.481305 | -2.579016 |
| 101.H | 2.600485 | 2.163478 | -1.313350 |
| 102.H | 5.842298 | -4.222261 | 2.725915 |
| 103.H | 0.735436 | -7.170709 | 2.725915 |
| 104.H | -6.698774 | -4.378349 | 1.762284 |
| 105.H | 0.735436 | 7.170709 | 2.725915 |

**$[PuO_2(CO_3)_3][C(NH_2)_3]_9^{5+}$**

| | | | |
|---|---|---|---|
| 1.Pu | 0.000000 | 0.000000 | 0.166609 |
| 2.O | 0.000000 | 0.000000 | 1.883476 |
| 3.O | 0.000000 | 0.000000 | -1.551077 |
| 4.O | -2.069489 | 1.390075 | 0.084963 |
| 5.O | -0.169096 | 2.487267 | 0.084963 |
| 6.O | -2.068594 | 3.582909 | -0.375026 |
| 7.C.tz2p | -1.456196 | 2.522205 | -0.074502 |
| 8.O | -0.169096 | -2.487267 | 0.084963 |
| 9.O | -2.069489 | -1.390075 | 0.084963 |
| 10.O | -2.068594 | -3.582909 | -0.375026 |
| 11.C.tz2p | -1.456196 | -2.522205 | -0.074502 |
| 12.O | 2.238585 | 1.097192 | 0.084963 |
| 13.O | 2.238585 | -1.097192 | 0.084963 |
| 14.O | 4.137187 | 0.000000 | -0.375026 |
| 15.C.tz2p | 2.912391 | 0.000000 | -0.074502 |
| 16.C.dzp | -0.209059 | 5.987693 | 1.353337 |
| 17.N | -0.897820 | 5.993044 | 0.222104 |
| 18.H | -1.148073 | 6.873692 | -0.213194 |
| 19.H | -1.345525 | 5.106843 | -0.089947 |
| 20.N | 0.255923 | 4.826859 | 1.819199 |
| 21.H | 0.156512 | 3.975278 | 1.255400 |
| 22.H | 0.468575 | 4.738486 | 2.804939 |
| 23.N | 0.040239 | 7.114329 | 2.013359 |
| 24.H | -0.436240 | 7.980676 | 1.783453 |
| 25.C.dzp | -0.209059 | -5.987693 | 1.353337 |
| 26.N | -0.897820 | -5.993044 | 0.222104 |
| 27.H | -1.345525 | -5.106843 | -0.089947 |
| 28.H | -1.148073 | -6.873692 | -0.213194 |
| 29.N | 0.040239 | -7.114329 | 2.013359 |
| 30.H | -0.436240 | -7.980676 | 1.783453 |
| 31.N | 0.255923 | -4.826859 | 1.819199 |
| 32.H | 0.156512 | -3.975278 | 1.255400 |
| 33.H | 0.468575 | -4.738486 | 2.804939 |
| 34.C.dzp | 5.290023 | 2.812796 | 1.353337 |
| 35.N | 5.639039 | 2.218987 | 0.222104 |
| 36.H | 5.095418 | 1.388163 | -0.089947 |
| 37.H | 6.526828 | 2.442586 | -0.213194 |
| 38.N | 6.141070 | 3.592013 | 2.013359 |
| 39.H | 7.129588 | 3.612543 | 1.783453 |
| 40.H | 5.825919 | 4.222875 | 2.742000 |
| 41.N | 4.052221 | 2.635065 | 1.819199 |
| 42.H | 3.364435 | 2.123183 | 1.255400 |
| 43.H | 3.869362 | 2.775041 | 2.804939 |
| 44.C.dzp | -5.080965 | -3.174896 | 1.353337 |
| 45.N | -4.741218 | -3.774057 | 0.222104 |
| 46.H | -5.378755 | -4.431106 | -0.213194 |
| 47.H | -3.749893 | -3.718680 | -0.089947 |
| 48.N | -4.308144 | -2.191793 | 1.819199 |

| | | | |
|---|---|---|---|
| 49.H | -3.520948 | -1.852095 | 1.255400 |
| 50.H | -4.337937 | -1.963445 | 2.804939 |
| 51.N | -6.181310 | -3.522316 | 2.013359 |
| 52.H | -6.570077 | -2.933956 | 2.742000 |
| 53.C.dzp | 5.290023 | -2.812796 | 1.353337 |
| 54.N | 5.639039 | -2.218987 | 0.222104 |
| 55.H | 6.526828 | -2.442586 | -0.213194 |
| 56.H | 5.095418 | -1.388163 | -0.089947 |
| 57.N | 4.052221 | -2.635065 | 1.819199 |
| 58.H | 3.364435 | -2.123183 | 1.255400 |
| 59.H | 3.869362 | -2.775041 | 2.804939 |
| 60.N | 6.141070 | -3.592013 | 2.013359 |
| 61.H | 7.129588 | -3.612543 | 1.783453 |
| 62.C.dzp | -5.080965 | 3.174896 | 1.353337 |
| 63.N | -4.741218 | 3.774057 | 0.222104 |
| 64.H | -3.749893 | 3.718680 | -0.089947 |
| 65.H | -5.378755 | 4.431106 | -0.213194 |
| 66.N | -6.181310 | 3.522316 | 2.013359 |
| 67.H | -6.693348 | 4.368133 | 1.783453 |
| 68.H | -6.570077 | 2.933956 | 2.742000 |
| 69.N | -4.308144 | 2.191793 | 1.819199 |
| 70.H | -3.520948 | 1.852095 | 1.255400 |
| 71.H | -4.337937 | 1.963445 | 2.804939 |
| 72.C.dzp | -4.107261 | 0.000000 | -2.732755 |
| 73.N | -4.845398 | 0.000000 | -3.840811 |
| 74.H | -5.174793 | 0.861518 | -4.261098 |
| 75.H | -5.174793 | -0.861518 | -4.261098 |
| 76.N | -3.736953 | -1.144825 | -2.175474 |
| 77.H | -3.999265 | -2.023424 | -2.601345 |
| 78.H | -3.139548 | -1.169024 | -1.335582 |
| 79.N | -3.736953 | 1.144825 | -2.175474 |
| 80.H | -3.999265 | 2.023424 | -2.601345 |
| 81.H | -3.139548 | 1.169024 | -1.335582 |
| 82.C.dzp | 2.053630 | -3.556992 | -2.732755 |
| 83.N | 2.422699 | -4.196238 | -3.840811 |
| 84.H | 1.841300 | -4.912262 | -4.261098 |
| 85.H | 3.333494 | -4.050743 | -4.261098 |
| 86.N | 2.859924 | -2.663883 | -2.175474 |
| 87.H | 3.751969 | -2.451753 | -2.601345 |
| 88.H | 2.582179 | -2.134417 | -1.335582 |
| 89.N | 0.877029 | -3.808709 | -2.175474 |
| 90.H | 0.247296 | -4.475177 | -2.601345 |
| 91.H | 0.557370 | -3.303441 | -1.335582 |
| 92.C.dzp | 2.053630 | 3.556992 | -2.732755 |
| 93.N | 2.422699 | 4.196238 | -3.840811 |
| 94.H | 3.333494 | 4.050743 | -4.261098 |
| 95.H | 1.841300 | 4.912262 | -4.261098 |
| 96.N | 0.877029 | 3.808709 | -2.175474 |
| 97.H | 0.247296 | 4.475177 | -2.601345 |
| 98.H | 0.557370 | 3.303441 | -1.335582 |
| 99.N | 2.859924 | 2.663883 | -2.175474 |
| 100.H | 3.751969 | 2.451753 | -2.601345 |
| 101.H | 2.582179 | 2.134417 | -1.335582 |
| 102.H | 5.825919 | -4.222875 | 2.742000 |
| 103.H | 0.744158 | -7.156832 | 2.742000 |
| 104.H | -6.693348 | -4.368133 | 1.783453 |
| 105.H | 0.744158 | 7.156832 | 2.742000 |

**$[AmO_2(CO_3)_3][C(NH_2)_3]_9^{5+}$**

| | | | |
|---|---|---|---|
| 1.Am | 0.000000 | 0.000000 | 0.174552 |
| 2.O | 0.000000 | 0.000000 | 1.886374 |
| 3.O | 0.000000 | 0.000000 | -1.537654 |
| 4.O | -2.070232 | 1.390033 | 0.093118 |
| 5.O | -0.168688 | 2.487891 | 0.093118 |
| 6.O | -2.067124 | 3.580364 | -0.380815 |
| 7.C.tz2p | -1.455203 | 2.520486 | -0.070580 |
| 8.O | -0.168688 | -2.487891 | 0.093118 |
| 9.O | -2.070232 | -1.390033 | 0.093118 |
| 10.O | -2.067124 | -3.580364 | -0.380815 |
| 11.C.tz2p | -1.455203 | -2.520486 | -0.070580 |
| 12.O | 2.238920 | 1.097857 | 0.093118 |
| 13.O | 2.238920 | -1.097857 | 0.093118 |
| 14.O | 4.134248 | 0.000000 | -0.380815 |
| 15.C.tz2p | 2.910406 | 0.000000 | -0.070580 |
| 16.C.dzp | -0.218220 | 5.999438 | 1.328343 |
| 17.N | -0.913407 | 5.995729 | 0.201215 |
| 18.H | -1.175042 | 6.873190 | -0.233357 |
| 19.H | -1.358491 | 5.104608 | -0.102357 |
| 20.N | 0.253157 | 4.842973 | 1.797017 |
| 21.H | 0.154138 | 3.987405 | 1.237558 |
| 22.H | 0.477938 | 4.762026 | 2.780379 |
| 23.N | 0.030256 | 7.130460 | 1.981134 |
| 24.H | -0.449886 | 7.993880 | 1.748637 |
| 25.C.dzp | -0.218220 | -5.999438 | 1.328343 |
| 26.N | -0.913407 | -5.995729 | 0.201215 |
| 27.H | -1.358491 | -5.104608 | -0.102357 |
| 28.H | -1.175042 | -6.873190 | -0.233357 |
| 29.N | 0.030256 | -7.130460 | 1.981134 |
| 30.H | -0.449886 | -7.993880 | 1.748637 |
| 31.N | 0.253157 | -4.842973 | 1.797017 |
| 32.H | 0.154138 | -3.987405 | 1.237558 |
| 33.H | 0.477938 | -4.762026 | 2.780379 |
| 34.C.dzp | 5.304776 | 2.810735 | 1.328343 |
| 35.N | 5.649157 | 2.206831 | 0.201215 |
| 36.H | 5.099966 | 1.375816 | -0.102357 |
| 37.H | 6.539878 | 2.418979 | -0.233357 |
| 38.N | 6.160031 | 3.591432 | 1.981134 |
| 39.H | 7.147846 | 3.607327 | 1.748637 |
| 40.H | 5.849160 | 4.226696 | 2.707610 |
| 41.N | 4.067559 | 2.640727 | 1.797017 |
| 42.H | 3.376125 | 2.127190 | 1.237558 |
| 43.H | 3.885067 | 2.794920 | 2.780379 |
| 44.C.dzp | -5.086556 | -3.188703 | 1.328343 |
| 45.N | -4.735750 | -3.788898 | 0.201215 |
| 46.H | -5.364836 | -4.454211 | -0.233357 |
| 47.H | -3.741475 | -3.728792 | -0.102357 |
| 48.N | -4.320716 | -2.202246 | 1.797017 |
| 49.H | -3.530263 | -1.860216 | 1.237558 |
| 50.H | -4.363005 | -1.967107 | 2.780379 |
| 51.N | -6.190287 | -3.539028 | 1.981134 |
| 52.H | -6.585006 | -2.952174 | 2.707610 |
| 53.C.dzp | 5.304776 | -2.810735 | 1.328343 |
| 54.N | 5.649157 | -2.206831 | 0.201215 |
| 55.H | 6.539878 | -2.418979 | -0.233357 |

| | | | |
|---|---|---|---|
| 56.H | 5.099966 | -1.375816 | -0.102357 |
| 57.N | 4.067559 | -2.640727 | 1.797017 |
| 58.H | 3.376125 | -2.127190 | 1.237558 |
| 59.H | 3.885067 | -2.794920 | 2.780379 |
| 60.N | 6.160031 | -3.591432 | 1.981134 |
| 61.H | 7.147846 | -3.607327 | 1.748637 |
| 62.C.dzp | -5.086556 | 3.188703 | 1.328343 |
| 63.N | -4.735750 | 3.788898 | 0.201215 |
| 64.H | -3.741475 | 3.728792 | -0.102357 |
| 65.H | -5.364836 | 4.454211 | -0.233357 |
| 66.N | -6.190287 | 3.539028 | 1.981134 |
| 67.H | -6.697960 | 4.386552 | 1.748637 |
| 68.H | -6.585006 | 2.952174 | 2.707610 |
| 69.N | -4.320716 | 2.202246 | 1.797017 |
| 70.H | -3.530263 | 1.860216 | 1.237558 |
| 71.H | -4.363005 | 1.967107 | 2.780379 |
| 72.C.dzp | -4.143827 | 0.000000 | -2.686094 |
| 73.N | -4.900696 | 0.000000 | -3.781630 |
| 74.H | -5.233111 | 0.861655 | -4.199263 |
| 75.H | -5.233111 | -0.861655 | -4.199263 |
| 76.N | -3.763650 | -1.144856 | -2.135440 |
| 77.H | -4.033334 | -2.023248 | -2.556926 |
| 78.H | -3.156735 | -1.169806 | -1.301586 |
| 79.N | -3.763650 | 1.144856 | -2.135440 |
| 80.H | -4.033334 | 2.023248 | -2.556926 |
| 81.H | -3.156735 | 1.169806 | -1.301586 |
| 82.C.dzp | 2.071914 | -3.588660 | -2.686094 |
| 83.N | 2.450348 | -4.244127 | -3.781630 |
| 84.H | 1.870340 | -4.962834 | -4.199263 |
| 85.H | 3.362771 | -4.101179 | -4.199263 |
| 86.N | 2.873300 | -2.686988 | -2.135440 |
| 87.H | 3.768852 | -2.481346 | -2.556926 |
| 88.H | 2.591450 | -2.148910 | -1.301586 |
| 89.N | 0.890350 | -3.831845 | -2.135440 |
| 90.H | 0.264483 | -4.504594 | -2.556926 |
| 91.H | 0.565286 | -3.318716 | -1.301586 |
| 92.C.dzp | 2.071914 | 3.588660 | -2.686094 |
| 93.N | 2.450348 | 4.244127 | -3.781630 |
| 94.H | 3.362771 | 4.101179 | -4.199263 |
| 95.H | 1.870340 | 4.962834 | -4.199263 |
| 96.N | 0.890350 | 3.831845 | -2.135440 |
| 97.H | 0.264483 | 4.504594 | -2.556926 |
| 98.H | 0.565286 | 3.318716 | -1.301586 |
| 99.N | 2.873300 | 2.686988 | -2.135440 |
| 100.H | 3.768852 | 2.481346 | -2.556926 |
| 101.H | 2.591450 | 2.148910 | -1.301586 |
| 102.H | 5.849160 | -4.226696 | 2.707610 |
| 103.H | 0.735846 | -7.178869 | 2.707610 |
| 104.H | -6.697960 | -4.386552 | 1.748637 |
| 105.H | 0.735846 | 7.178869 | 2.707610 |

**$[CmO_2(CO_3)_3][C(NH_2)_3]_9^{5+}$**

| | | | |
|---|---|---|---|
| 1.Cm | 0.000000 | 0.000000 | 0.209598 |
| 2.O | 0.000000 | 0.000000 | 1.920497 |
| 3.O | 0.000000 | 0.000000 | -1.501050 |
| 4.O | -2.087987 | 1.415158 | 0.122268 |

| | | | |
|---|---|---|---|
| 5.O | -0.181569 | 2.515829 | 0.122268 |
| 6.O | -2.079616 | 3.602000 | -0.365971 |
| 7.C.tz2p | -1.467852 | 2.542394 | -0.045765 |
| 8.O | -0.181569 | -2.515829 | 0.122268 |
| 9.O | -2.087987 | -1.415158 | 0.122268 |
| 10.O | -2.079616 | -3.602000 | -0.365971 |
| 11.C.tz2p | -1.467852 | -2.542394 | -0.045765 |
| 12.O | 2.269556 | 1.100671 | 0.122268 |
| 13.O | 2.269556 | -1.100671 | 0.122268 |
| 14.O | 4.159232 | 0.000000 | -0.365971 |
| 15.C.tz2p | 2.935703 | 0.000000 | -0.045765 |
| 16.C.dzp | -0.227853 | 6.051865 | 1.280746 |
| 17.N | -0.940683 | 6.021814 | 0.164899 |
| 18.H | -1.219432 | 6.889653 | -0.278657 |
| 19.H | -1.381922 | 5.119946 | -0.116247 |
| 20.N | 0.256856 | 4.907364 | 1.765100 |
| 21.H | 0.144895 | 4.038501 | 1.228861 |
| 22.H | 0.502596 | 4.849304 | 2.745385 |
| 23.N | 0.025467 | 7.197047 | 1.906526 |
| 24.H | -0.460985 | 8.053747 | 1.662609 |
| 25.C.dzp | -0.227853 | -6.051865 | 1.280746 |
| 26.N | -0.940683 | -6.021814 | 0.164899 |
| 27.H | -1.381922 | -5.119946 | -0.116247 |
| 28.H | -1.219432 | -6.889653 | -0.278657 |
| 29.N | 0.025467 | -7.197047 | 1.906526 |
| 30.H | -0.460985 | -8.053747 | 1.662609 |
| 31.N | 0.256856 | -4.907364 | 1.765100 |
| 32.H | 0.144895 | -4.038501 | 1.228861 |
| 33.H | 0.502596 | -4.849304 | 2.745385 |
| 34.C.dzp | 5.354995 | 2.828606 | 1.280746 |
| 35.N | 5.685385 | 2.196252 | 0.164899 |
| 36.H | 5.124964 | 1.363193 | -0.116247 |
| 37.H | 6.576331 | 2.388767 | -0.278657 |
| 38.N | 6.220092 | 3.620578 | 1.906526 |
| 39.H | 7.205241 | 3.627649 | 1.662609 |
| 40.H | 5.920139 | 4.272336 | 2.623038 |
| 41.N | 4.121474 | 2.676125 | 1.765100 |
| 42.H | 3.424997 | 2.144733 | 1.228861 |
| 43.H | 3.948323 | 2.859913 | 2.745385 |
| 44.C.dzp | -5.127143 | -3.223259 | 1.280746 |
| 45.N | -4.744702 | -3.825562 | 0.164899 |
| 46.H | -5.356899 | -4.500886 | -0.278657 |
| 47.H | -3.743042 | -3.756753 | -0.116247 |
| 48.N | -4.378330 | -2.231238 | 1.765100 |
| 49.H | -3.569892 | -1.893768 | 1.228861 |
| 50.H | -4.450919 | -1.989392 | 2.745385 |
| 51.N | -6.245559 | -3.576468 | 1.906526 |
| 52.H | -6.660021 | -2.990823 | 2.623038 |
| 53.C.dzp | 5.354995 | -2.828606 | 1.280746 |
| 54.N | 5.685385 | -2.196252 | 0.164899 |
| 55.H | 6.576331 | -2.388767 | -0.278657 |
| 56.H | 5.124964 | -1.363193 | -0.116247 |
| 57.N | 4.121474 | -2.676125 | 1.765100 |
| 58.H | 3.424997 | -2.144733 | 1.228861 |
| 59.H | 3.948323 | -2.859913 | 2.745385 |
| 60.N | 6.220092 | -3.620578 | 1.906526 |

| | | | |
|---|---|---|---|
| 61.H | 7.205241 | -3.627649 | 1.662609 |
| 62.C.dzp | -5.127143 | 3.223259 | 1.280746 |
| 63.N | -4.744702 | 3.825562 | 0.164899 |
| 64.H | -3.743042 | 3.756753 | -0.116247 |
| 65.H | -5.356899 | 4.500886 | -0.278657 |
| 66.N | -6.245559 | 3.576468 | 1.906526 |
| 67.H | -6.744257 | 4.426098 | 1.662609 |
| 68.H | -6.660021 | 2.990823 | 2.623038 |
| 69.N | -4.378330 | 2.231238 | 1.765100 |
| 70.H | -3.569892 | 1.893768 | 1.228861 |
| 71.H | -4.450919 | 1.989392 | 2.745385 |
| 72.C.dzp | -4.204684 | 0.000000 | -2.605719 |
| 73.N | -4.982126 | 0.000000 | -3.687354 |
| 74.H | -5.321403 | 0.861624 | -4.099411 |
| 75.H | -5.321403 | -0.861624 | -4.099411 |
| 76.N | -3.813916 | -1.145541 | -2.064006 |
| 77.H | -4.096833 | -2.022665 | -2.479603 |
| 78.H | -3.190663 | -1.176677 | -1.240211 |
| 79.N | -3.813916 | 1.145541 | -2.064006 |
| 80.H | -4.096833 | 2.022665 | -2.479603 |
| 81.H | -3.190663 | 1.176677 | -1.240211 |
| 82.C.dzp | 2.102342 | -3.641363 | -2.605719 |
| 83.N | 2.491063 | -4.314648 | -3.687354 |
| 84.H | 1.914513 | -5.039283 | -4.099411 |
| 85.H | 3.406890 | -4.177658 | -4.099411 |
| 86.N | 2.899025 | -2.730177 | -2.064006 |
| 87.H | 3.800095 | -2.536629 | -2.479603 |
| 88.H | 2.614363 | -2.174856 | -1.240211 |
| 89.N | 0.914890 | -3.875718 | -2.064006 |
| 90.H | 0.296737 | -4.559293 | -2.479603 |
| 91.H | 0.576299 | -3.351533 | -1.240211 |
| 92.C.dzp | 2.102342 | 3.641363 | -2.605719 |
| 93.N | 2.491063 | 4.314648 | -3.687354 |
| 94.H | 3.406890 | 4.177658 | -4.099411 |
| 95.H | 1.914513 | 5.039283 | -4.099411 |
| 96.N | 0.914890 | 3.875718 | -2.064006 |
| 97.H | 0.296737 | 4.559293 | -2.479603 |
| 98.H | 0.576299 | 3.351533 | -1.240211 |
| 99.N | 2.899025 | 2.730177 | -2.064006 |
| 100.H | 3.800095 | 2.536629 | -2.479603 |
| 101.H | 2.614363 | 2.174856 | -1.240211 |
| 102.H | 5.920139 | -4.272336 | 2.623038 |
| 103.H | 0.739882 | -7.263159 | 2.623038 |
| 104.H | -6.744257 | -4.426098 | 1.662609 |
| 105.H | 0.739882 | 7.263159 | 2.623038 |

**Table S15.** Standard oxidation energies of elements (in eV).[a]

| Group | Element | $M^{0\rightarrow}$ $M^{+}$ | $M^{0\rightarrow}$ $M^{2+}$ | $M^{+\rightarrow}$ $M^{2+}$ | $M^{2+\rightarrow}$ $M^{3+}$ | $M^{3+\rightarrow}$ $M^{4+}$ | $M^{4+\rightarrow}$ $M^{5+}$ | $M^{5+\rightarrow}$ $M^{6+}$ | $M^{6+\rightarrow}$ $M^{7+}$ | $M^{7+\rightarrow}$ $M^{8+}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| **1** | **Li** | 3.04 | | | | | | | | |
| | Na | 2.71 | | | | | | | | |
| | K | 2.93 | | | | | | | | |
| | Rb | 2.98 | | | | | | | | |
| | Cs | 3.03 | | | | | | | | |
| | Fr | 2.90 | | | | | | | | |
| **2** | **Be** | 2+δ | *3.69* | 1.69-δ | | | | | | |
| | Mg | 2.70 | *4.74* | 2.04 | | | | | | |
| | Ca | 3.80 | *5.74* | 1.94 | | | | | | |
| | Sr | 4.10 | *5.80* | 1.70 | | | | | | |
| | Ba | 4+δ | *5.82* | 1.82-δ | | | | | | |
| | Ra | 4+δ | *5.6* | 1.6-δ | | | | | | |
| **3** | **Sc** | 3+δ | | 2-δ+ε | 1.23-ε | | | | | |
| | Y | 3+δ | | 1.3-δ | 2.8 | | | | | |
| | La | 3+δ | *4.04* | 1.04-δ | 3.1 | | | | | |
| | Ac | 2+δ | *1.7* | -0.3-δ | 4.9 | | | | | |
| **4** | **Ti** | 2+δ | *3.25* | 1.25-δ | 0.85 | [-0.2] | | | | |
| | Zr | 2+δ | | 2-δ+ε | 1-ε+η | 0.80-η | | | | |
| | Hf | 2+δ | | 2-δ+ε | 1-ε+η | [1.2-η] | | | | |
| | Ce | 2+δ | *3.8* | 1.8-δ | 3.2 | -1.7 | | | | |
| | Th | 2+δ | *-0.9* | -2.9-δ | 4.8 | 3.6 | | | | |
| **5** | **V** | 2+δ | *2.26* | 0.26-δ | 0.26 | -0.34 | -0.99 | | | |
| | Nb | 2+δ | *1.5* | -0.5-δ | [1.8] | [-0.5] | [0.5] | | | |
| | Ta | 2+δ | | 0-δ+ε | -0.2-ε | 1+η | [0.95-η] | | | |
| | Pr | 2+δ | *4.0* | 2-δ | 2.8 | -3.0 | | | | |
| | Pa | 2+δ | | 0-δ+ε | 2.0 | 1.94 | | | | |
| **6** | **Cr** | 1+δ | *1.82* | 0.82-δ | 0.42 | ε | -1.34 | [-2.35-ε] | | |
| | Mo | 0+δ | | 0-δ+ε | 0.6-ε | [0] | [η] | [-0.2-η] | | |
| | W | 0+δ | | 0-δ+ε | -0.3-ε | [0.8] | [0.0] | [0.0] | | |
| | Nd | 3+δ | *4,25* | 1.25-δ | 2.7 | -4.5 | | | | |
| | U | 1+δ | *0.7* | -0.3-δ | 4.7 | 0.5 | [-0.15] | [-0.4] | | |
| **7** | **Mn** | 2+δ | *2.37* | 0.37-δ | -1.54 | [-0.91] | [-2+η] | [-2.6-η] | [-0.56] | |
| | Tc | -1+δ | | 0-δ+ε | -0.1-ε | [0.15] | [-1+η] | [-1-η+β] | [-0.35-β] | |
| | Re | -1+δ | | 0-δ+ε | 0.1-ε | [-0.1] | [η] | [-0.8-η] | [-0.77] | |
| | Pm | 2+δ | *4.4* | 2.4-δ | 2.6 | -4.7 | | | | |
| | Np | 1+δ | *0.9* | -0.1-δ | 4.7 | -0.15 | | | | |
| **8** | **Fe** | 1+δ | *0.9* | -0.1-δ | -0.78 | | | | | |
| | Ru | 0+δ | *-0.9* | -0.9-δ | -0.25 | [-2.0] | [-2+η] | [-1.55-η] | [-0.6] | [-1.0] |
| | Os | 0+δ | | 0-δ+ε | 0-ε+η | [0.73-η] | [-2+δ'] | [-1-δ'+ε'] | [-1-ε'+η'] | [-0.1-η'] |
| | Sm | 3+δ | *5,36* | 2.36-δ | 1.55 | -5.1 | | | | |
| | Pu | 1+δ | *2.6* | 1.6-δ | 3.5 | -1.0 | -1.1 | | | |

| Group | Element | $M^{0\rightarrow}$ $M^{+}$ | $M^{0\rightarrow}$ $M^{2+}$ | $M^{+\rightarrow}$ $M^{2+}$ | $M^{2+\rightarrow}$ $M^{3+}$ | $M^{3+\rightarrow}$ $M^{4+}$ | $M^{4+\rightarrow}$ $M^{5+}$ | $M^{5+\rightarrow}$ $M^{6+}$ | $M^{6+\rightarrow}$ $M^{7+}$ | $M^{7+\rightarrow}$ $M^{8+}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| **9** | **Co** | δ | *0.56* | 0.56-δ | -1.92 | | | | | |
| | Rh | -0.6 | | -1+δ | -1.67-δ | | | | | |
| | Ir | -1+δ | | -1-δ+ε | -1.47+δ-ε | | | | | |
| | Eu | 3+δ | *5.6* | 2.6-δ | 0.36 | -6.3 | | | | |
| | Am | 2+δ | *3.8* | 1.8-δ | 2.3 | -2.6 | | | | |
| **10** | **Ni** | δ | *0.5* | 0.5- δ | [-2+ε] | [-1.36-ε] | | | | |
| | Pd | -1+δ | *-1.9* | -0.9-δ | | | | | | |
| | Pt | -1+δ | *-2.36* | -1.36-δ | | | | | | |
| | Gd | 2+δ | *2.9* | 0.9-δ | 3.9 | -7.9 | | | | |
| | Cm | 1+δ | *1.7* | 0.7-δ | 4.4 | -3.5 | | | | |
| **11** | **Cu** | -0.50 | *-0.65* | -0.15 | -2.40 | | | | | |
| | Ag | -0.80 | *-1.98* | -1.18 | -1.80 | | | | | |
| | Au | -1.69 | *-3.49* | -1.80 | -1.00 | | | | | |
| | Tb | 2+δ | *3.15* | 1.15-δ | 3.7 | -3.1 | | | | |
| | Bk | -1+δ | *-0.8* | 0.2-δ | 2.8 | -1.67 | | | | |
| **12** | **Zn** | 1+δ | *1.52* | 0.52-δ | | | | | | |
| | Cd | 1+δ | *0.8* | -0.2-δ | | | | | | |
| | Hg | -0.8 | *-1.7* | -0.9 | | | | | | |
| | Dy | 2+δ | *4.35* | 2.35-δ | 2.6 | -5.0 | | | | |
| | Cf | 2+δ | *4.24* | 2.24-δ | 1.6 | -3.3 | | | | |

[a] Values after Lide[1] and Nugent et al.[2] Positive values mean strong tendency toward higher oxidation. Values in brackets [] refer to oxo-ions such as titantyl $[Ti^{4+}O^{2-}]^{2+}$. If only double or triple oxidation energies are available, unknown increments such as +δ and –δ are introduced for the individual oxidation steps, the δ, ε etc. being specific for each element row).

[1] D. R. Lide, Ed., CRC Handbook of Chemistry and Physics, CRC Press, Boca Raton FL, 2005. Internet Version http://www.hbcpnetbase.com.

[2] L. J. Nugent, R. D. Baybarz and J. L. Burnett, J. Inorg. Nucl. Chem., 1971, 33, 2503-2530. L. J. Nugent, R. D. Baybarz, J. L. Burnett and J. L. Ryan, J. Phys. Chem., 1973, 77, 1528-1539.