Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information:

Extension of the D3 an D4 London Dispersion Corrections to the full Actinide Series

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A Definition of Statistical Measures

The error e for a given interaction i is given by the difference between the actual method and a reference.

$$e_i = \text{method}_i - \text{reference}_i \tag{1}$$

Mean Error (ME): Mean of the signed error, n corresponds to the number of data points of the respective set.

$$\text{ME} = \frac{1}{n}\sum_{i=1}^{n} e_i \equiv \bar{e} \tag{2}$$

Mean Absolute Error (MAE):

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n} |e_i| \tag{3}$$

Root Mean Square Error (RMSE):

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (e_i)^2} \tag{4}$$

Standard Deviation (SD): The standard deviation is defined using Bessel's correction.

$$\text{SD} = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n} (e_i - \bar{e})^2} \tag{5}$$

Largest Absolute Error (EMAX): Largest and smallest (absolute) error of all n interactions i of a given set.

$$\text{EMAX} = \max\left(|\{e_i\}|\right) \quad i = \{1, 2, \ldots, n\} \tag{6}$$

B DFT-D3

B.1 C_6 Coefficients

The pair-wise C_6^{AB} coefficients can be obtained with the data from Sec. C.4 using the following modified Casimir-Polder expression.

$$C_{6,\mathrm{ref}}^{\mathrm{AB}}\left(\mathrm{CN}^{\mathrm{A}},\mathrm{CN}^{\mathrm{B}}\right)=\frac{3}{\pi}\int_0^\infty\frac{1}{m}\left[\alpha^{\mathrm{A}_m\mathrm{H}_n}(i\omega^{\mathrm{I}})-\frac{n}{2}\alpha^{\mathrm{H}_2}(i\omega^{\mathrm{I}})\right]\times\frac{1}{k}\left[\alpha^{\mathrm{B}_k\mathrm{H}_l}(i\omega^{\mathrm{I}})-\frac{l}{2}\alpha^{\mathrm{H}_2}(i\omega^{\mathrm{I}})\right]\mathrm{d}\omega \tag{7}$$

B.2 $\frac{\langle r_{\mathrm{A}}^4\rangle}{\langle r_{\mathrm{A}}^2\rangle}$ Expectation Values

$\langle r_{\mathrm{A}}^4\rangle$ and $\langle r_{\mathrm{A}}^2\rangle$ are multipole-type expectation values derived from atomic densities.

$$\frac{\langle r_{\mathrm{Ac..Lr}}^4\rangle}{\langle r_{\mathrm{Ac..Lr}}^2\rangle}=\{19.1885,15.8542,16.1305,15.6161,15.1226,16.1576,14.6510,14.7178,13.9108,13.5623,13.2326,12.9189,12.6133,12.3142,14.8326\}$$

B.3 Covalent Radii

The following covalent radii are given in Bohr.

$$r_{\mathrm{cov}}^{\mathrm{Ac..Lr}}=\{1.67,1.58,1.52,1.53,1.54,1.55,1.49,1.49,1.51,1.51,1.48,1.50,1.56,1.58,1.45\}$$

B.4 Van-der-Waals Radii

The following pair-wise van-der-Waals radii are given in Bohr.

B.4.1 Actinium

$$r_{\text{vdw}}^{\text{Ac}-\{\text{H..He}\}} = \{2.8428, 3.0429\}$$

$$r_{\text{vdw}}^{\text{Ac}-\{\text{Li..Ne}\}} = \{4.1000, 3.7286, 3.4857, 3.4572, 3.4000, 3.2857, 3.3000, 3.3429\}$$

$$r_{\text{vdw}}^{\text{Ac}-\{\text{Na..Ar}\}} = \{4.3857, 4.1715, 4.0000, 3.8714, 3.9571, 3.8428, 3.8000, 3.7572\}$$

$$r_{\text{vdw}}^{\text{Ac}-\{\text{K..Kr}\}} = \{4.9000, 4.5857, 4.2857, 4.1286, 4.1143, 3.9571, 3.9143, 3.8714, 3.8143, 3.8000, 3.8286, 3.9428, 3.9857, 3.9428, 4.0286, 3.9571, 4.0143, 4.0571\}$$

$$r_{\text{vdw}}^{\text{Ac}-\{\text{Rb..Xe}\}} = \{5.0857, 4.7714, 4.4857, 4.3714, 4.2714, 4.1572, 4.0286, 4.0000, 4.0000, 3.9286, 4.0286, 4.1429, 4.2143, 4.1857, 4.1857, 4.1429, 4.2714, 4.2571\}$$

$$r_{\text{vdw}}^{\text{Ac}-\{\text{Cs..Rn}\}} = \{5.3714, 4.9000, 4.7000, 4.4857, 4.6428, 4.6286, 4.6143, 4.6000, 4.5429, 4.5572, 4.5429, 4.5286, 4.5143, 4.5143, 4.5000, 4.5714, 4.4714, 4.3429, 4.2571, 4.1429, 4.0714, 4.0429, 3.9714, 3.9857, 4.0000, 4.2714, 4.2428, 4.2428, 4.3286, 4.2571, 4.3571, 4.4143\}$$

$$r_{\text{vdw}}^{\text{Ac}-\{\text{Fr..Rn}\}} = \{5.2572, 4.9714, 4.7714, 4.6428, 4.5572, 4.5714, 4.5857, 4.6000, 4.5143, 4.5143, 4.5429, 4.5429, 4.5000, 4.5286, 4.6143, 4.6428, 4.4572\}$$

B.4.2 Thorium

$$r_{\text{vdw}}^{\text{Th}-\{\text{H..He}\}} = \{2.7143, 2.9143\}$$

$$r_{\text{vdw}}^{\text{Th}-\{\text{Li..Ne}\}} = \{3.9714, 3.6000, 3.3572, 3.3286, 3.2714, 3.1571, 3.1714, 3.2143\}$$

$$r_{\text{vdw}}^{\text{Th}-\{\text{Na..Ar}\}} = \{4.2571, 4.0429, 3.8714, 3.7429, 3.8286, 3.7143, 3.6714, 3.6286\}$$

$$r_{\text{vdw}}^{\text{Th}-\{\text{K..Kr}\}} = \{4.7714, 4.4572, 4.1572, 4.0000, 3.9857, 3.8286, 3.7857, 3.7429, 3.6857, 3.6714, 3.7000, 3.8143, 3.8571, 3.8143, 3.9000, 3.8286, 3.8857, 3.9286\}$$

$$r_{\text{vdw}}^{\text{Th}-\{\text{Rb..Xe}\}} = \{4.9571, 4.6428, 4.3571, 4.2428, 4.1429, 4.0286, 3.9000, 3.8714, 3.8714, 3.8000, 3.9000, 4.0143, 4.0857, 4.0571, 4.0571, 4.0143, 4.1429, 4.1286\}$$

$$r_{\text{vdw}}^{\text{Th}-\{\text{Cs..Rn}\}} = \{5.2429, 4.7714, 4.5714, 4.3571, 4.5143, 4.5000, 4.4857, 4.4714, 4.4143, 4.4286, 4.4143, 4.4000, 4.3857, 4.3857, 4.3714, 4.4429, 4.3429, 4.2143, 4.1286, 4.0143, 3.9428, 3.9143, 3.8428, 3.8571, 3.8714, 4.1429, 4.1143, 4.1143, 4.2000, 4.1286, 4.2285, 4.2857\}$$

$$r_{\text{vdw}}^{\text{Th}-\{\text{Fr..Rn}\}} = \{5.1286, 4.8429, 4.6428, 4.5143, 4.4286, 4.4429, 4.4572, 4.4714, 4.3857, 4.3857, 4.4143, 4.4143, 4.3714, 4.4000, 4.4857, 4.5143, 4.3286\}$$

B.4.3 Protactinium

$$r_{\text{vdw}}^{\text{Pa}-\{\text{H..He}\}} = \{2.6286, 2.8286\}$$

$$r_{\text{vdw}}^{\text{Pa}-\{\text{Li..Ne}\}} = \{3.8857, 3.5143, 3.2714, 3.2429, 3.1857, 3.0715, 3.0857, 3.1285\}$$

$$r_{\text{vdw}}^{\text{Pa}-\{\text{Na..Ar}\}} = \{4.1715, 3.9571, 3.7857, 3.6571, 3.7429, 3.6286, 3.5857, 3.5428\}$$

$$r_{\text{vdw}}^{\text{Pa}-\{\text{K..Kr}\}} = \{4.6857, 4.3714, 4.0714, 3.9143, 3.9000, 3.7429, 3.7000, 3.6571, 3.6000, 3.5857, 3.6143, 3.7286, 3.7714, 3.7286, 3.8143, 3.7429, 3.8000, 3.8428\}$$

$$r_{\text{vdw}}^{\text{Pa}-\{\text{Rb..Xe}\}} = \{4.8714, 4.5572, 4.2714, 4.1572, 4.0571, 3.9428, 3.8143, 3.7857, 3.7857, 3.7143, 3.8143, 3.9286, 4.0000, 3.9714, 3.9714, 3.9286, 4.0571, 4.0429\}$$

$$r_{\text{vdw}}^{\text{Pa}-\{\text{Cs..Rn}\}} = \{5.1571, 4.6857, 4.4857, 4.2714, 4.4286, 4.4143, 4.4000, 4.3857, 4.3286, 4.3429, 4.3286, 4.3143, 4.3000, 4.3000, 4.2857, 4.3571, 4.2571, 4.1286, 4.0429, 3.9286, 3.8571, 3.8286, 3.7572, 3.7714, 3.7857, 4.0571, 4.0286, 4.0286, 4.1143, 4.0429, 4.1429, 4.2000\}$$

$$r_{\text{vdw}}^{\text{Pa}-\{\text{Fr..Rn}\}} = \{5.0428, 4.7571, 4.5572, 4.4286, 4.3429, 4.3571, 4.3714, 4.3857, 4.3000, 4.3000, 4.3286, 4.3286, 4.2857, 4.3143, 4.4000, 4.4286, 4.2428\}$$

B.4.4 Uranium

$$r_{\text{vdw}}^{\text{U}-\{\text{H..He}\}} = \{2.6429, 2.8428\}$$

$$r_{\text{vdw}}^{\text{U}-\{\text{Li..Ne}\}} = \{3.9000, 3.5286, 3.2857, 3.2571, 3.2000, 3.0857, 3.1000, 3.1428\}$$

$$r_{\text{vdw}}^{\text{U}-\{\text{Na..Ar}\}} = \{4.1857, 3.9714, 3.8000, 3.6714, 3.7572, 3.6429, 3.6000, 3.5571\}$$

$$r_{\text{vdw}}^{\text{U}-\{\text{K..Kr}\}} = \{4.7000, 4.3857, 4.0857, 3.9286, 3.9143, 3.7572, 3.7143, 3.6714, 3.6143, 3.6000, 3.6286, 3.7429, 3.7857, 3.7429, 3.8286, 3.7572, 3.8143, 3.8571\}$$

$$r_{\text{vdw}}^{\text{U}-\{\text{Rb..Xe}\}} = \{4.8857, 4.5714, 4.2857, 4.1715, 4.0714, 3.9571, 3.8286, 3.8000, 3.8000, 3.7286, 3.8286, 3.9428, 4.0143, 3.9857, 3.9857, 3.9428, 4.0714, 4.0571\}$$

$$r_{\text{vdw}}^{\text{U}-\{\text{Cs..Rn}\}} = \{5.1714, 4.7000, 4.5000, 4.2857, 4.4429, 4.4286, 4.4143, 4.4000, 4.3429, 4.3571, 4.3429, 4.3286, 4.3143, 4.3143, 4.3000, 4.3714, 4.2714, 4.1429, 4.0571, 3.9428, 3.8714, 3.8428, 3.7714, 3.7857, 3.8000, 4.0714, 4.0429, 4.0429, 4.1286, 4.0571, 4.1572, 4.2143\}$$

$$r_{\text{vdw}}^{\text{U}-\{\text{Fr..Rn}\}} = \{5.0571, 4.7714, 4.5714, 4.4429, 4.3571, 4.3714, 4.3857, 4.4000, 4.3143, 4.3143, 4.3429, 4.3429, 4.3000, 4.3286, 4.4143, 4.4429, 4.2571\}$$

B.4.5 Neptunium

$$r_{\text{vdw}}^{\text{Np}-\{\text{H..He}\}} = \{2.6572, 2.8571\}$$

$$r_{\text{vdw}}^{\text{Np}-\{\text{Li..Ne}\}} = \{3.9143, 3.5428, 3.3000, 3.2714, 3.2143, 3.1000, 3.1143, 3.1571\}$$

$$r_{\text{vdw}}^{\text{Np}-\{\text{Na..Ar}\}} = \{4.2000, 3.9857, 3.8143, 3.6857, 3.7714, 3.6571, 3.6143, 3.5714\}$$

$$r_{\text{vdw}}^{\text{Np}-\{\text{K..Kr}\}} = \{4.7143, 4.4000, 4.1000, 3.9428, 3.9286, 3.7714, 3.7286, 3.6857, 3.6286, 3.6143, 3.6429, 3.7572, 3.8000, 3.7572, 3.8428, 3.7714, 3.8286, 3.8714\}$$

$$r_{\text{vdw}}^{\text{Np}-\{\text{Rb..Xe}\}} = \{4.9000, 4.5857, 4.3000, 4.1857, 4.0857, 3.9714, 3.8428, 3.8143, 3.8143, 3.7429, 3.8428, 3.9571, 4.0286, 4.0000, 4.0000, 3.9571, 4.0857, 4.0714\}$$

$$r_{\text{vdw}}^{\text{Np}-\{\text{Cs..Rn}\}} = \{5.1857, 4.7143, 4.5143, 4.3000, 4.4572, 4.4429, 4.4286, 4.4143, 4.3571, 4.3714, 4.3571, 4.3429, 4.3286, 4.3286, 4.3143, 4.3857, 4.2857, 4.1572, 4.0714, 3.9571, 3.8857, 3.8571, 3.7857, 3.8000, 3.8143, 4.0857, 4.0571, 4.0571, 4.1429, 4.0714, 4.1715, 4.2285\}$$

$$r_{\text{vdw}}^{\text{Np}-\{\text{Fr..Rn}\}} = \{5.0714, 4.7857, 4.5857, 4.4572, 4.3714, 4.3857, 4.4000, 4.4143, 4.3286, 4.3286, 4.3571, 4.3571, 4.3143, 4.3429, 4.4286, 4.4572, 4.2714\}$$

B.4.6 Plutonium

$$r_{\text{vdw}}^{\text{Pu}-\{\text{H..He}\}} = \{2.6714, 2.8714\}$$

$$r_{\text{vdw}}^{\text{Pu}-\{\text{Li..Ne}\}} = \{3.9286, 3.5571, 3.3143, 3.2857, 3.2286, 3.1143, 3.1285, 3.1714\}$$

$$r_{\text{vdw}}^{\text{Pu}-\{\text{Na..Ar}\}} = \{4.2143, 4.0000, 3.8286, 3.7000, 3.7857, 3.6714, 3.6286, 3.5857\}$$

$$r_{\text{vdw}}^{\text{Pu}-\{\text{K..Kr}\}} = \{4.7286, 4.4143, 4.1143, 3.9571, 3.9428, 3.7857, 3.7429, 3.7000, 3.6429, 3.6286, 3.6571, 3.7714, 3.8143, 3.7714, 3.8571, 3.7857, 3.8428, 3.8857\}$$

$$r_{\text{vdw}}^{\text{Pu}-\{\text{Rb..Xe}\}} = \{4.9143, 4.6000, 4.3143, 4.2000, 4.1000, 3.9857, 3.8571, 3.8286, 3.8286, 3.7572, 3.8571, 3.9714, 4.0429, 4.0143, 4.0143, 3.9714, 4.1000, 4.0857\}$$

$$r_{\text{vdw}}^{\text{Pu}-\{\text{Cs..Rn}\}} = \{5.2000, 4.7286, 4.5286, 4.3143, 4.4714, 4.4572, 4.4429, 4.4286, 4.3714, 4.3857, 4.3714, 4.3571, 4.3429, 4.3429, 4.3286, 4.4000, 4.3000, 4.1715, 4.0857, 3.9714, 3.9000, 3.8714, 3.8000, 3.8143, 3.8286, 4.1000, 4.0714, 4.0714, 4.1572, 4.0857, 4.1857, 4.2428\}$$

$$r_{\text{vdw}}^{\text{Pu}-\{\text{Fr..Rn}\}} = \{5.0857, 4.8000, 4.6000, 4.4714, 4.3857, 4.4000, 4.4143, 4.4286, 4.3429, 4.3429, 4.3714, 4.3714, 4.3286, 4.3571, 4.4429, 4.4714, 4.2857\}$$

B.4.7 Americium

$$r_{\text{vdw}}^{\text{Am}-\{\text{H..He}\}} = \{2.5857, 2.7857\}$$

$$r_{\text{vdw}}^{\text{Am}-\{\text{Li..Ne}\}} = \{3.8428, 3.4714, 3.2286, 3.2000, 3.1428, 3.0286, 3.0429, 3.0857\}$$

$$r_{\text{vdw}}^{\text{Am}-\{\text{Na..Ar}\}} = \{4.1286, 3.9143, 3.7429, 3.6143, 3.7000, 3.5857, 3.5428, 3.5000\}$$

$$r_{\text{vdw}}^{\text{Am}-\{\text{K..Kr}\}} = \{4.6428, 4.3286, 4.0286, 3.8714, 3.8571, 3.7000, 3.6571, 3.6143, 3.5571, 3.5428, 3.5714, 3.6857, 3.7286, 3.6857, 3.7714, 3.7000, 3.7572, 3.8000\}$$

$$r_{\text{vdw}}^{\text{Am}-\{\text{Rb..Xe}\}} = \{4.8286, 4.5143, 4.2285, 4.1143, 4.0143, 3.9000, 3.7714, 3.7429, 3.7429, 3.6714, 3.7714, 3.8857, 3.9571, 3.9286, 3.9286, 3.8857, 4.0143, 4.0000\}$$

$$r_{\text{vdw}}^{\text{Am}-\{\text{Cs..Rn}\}} = \{5.1143, 4.6428, 4.4429, 4.2285, 4.3857, 4.3714, 4.3571, 4.3429, 4.2857, 4.3000, 4.2857, 4.2714, 4.2571, 4.2571, 4.2428, 4.3143, 4.2143, 4.0857, 4.0000, 3.8857, 3.8143, 3.7857, 3.7143, 3.7286, 3.7429, 4.0143, 3.9857, 3.9857, 4.0714, 4.0000, 4.1000, 4.1572\}$$

$$r_{\text{vdw}}^{\text{Am}-\{\text{Fr..Rn}\}} = \{5.0000, 4.7143, 4.5143, 4.3857, 4.3000, 4.3143, 4.3286, 4.3429, 4.2571, 4.2571, 4.2857, 4.2857, 4.2428, 4.2714, 4.3571, 4.3857, 4.2000\}$$

B.4.8 Curium

$$r_{\text{vdw}}^{\text{Cm}-\{\text{H..He}\}} = \{2.5857, 2.7857\}$$

$$r_{\text{vdw}}^{\text{Cm}-\{\text{Li..Ne}\}} = \{3.8428, 3.4714, 3.2286, 3.2000, 3.1428, 3.0286, 3.0429, 3.0857\}$$

$$r_{\text{vdw}}^{\text{Cm}-\{\text{Na..Ar}\}} = \{4.1286, 3.9143, 3.7429, 3.6143, 3.7000, 3.5857, 3.5428, 3.5000\}$$

$$r_{\text{vdw}}^{\text{Cm}-\{\text{K..Kr}\}} = \{4.6428, 4.3286, 4.0286, 3.8714, 3.8571, 3.7000, 3.6571, 3.6143, 3.5571, 3.5428, 3.5714, 3.6857, 3.7286, 3.6857, 3.7714, 3.7000, 3.7572, 3.8000\}$$

$$r_{\text{vdw}}^{\text{Cm}-\{\text{Rb..Xe}\}} = \{4.8286, 4.5143, 4.2285, 4.1143, 4.0143, 3.9000, 3.7714, 3.7429, 3.7429, 3.6714, 3.7714, 3.8857, 3.9571, 3.9286, 3.9286, 3.8857, 4.0143, 4.0000\}$$

$$r_{\text{vdw}}^{\text{Cm}-\{\text{Cs..Rn}\}} = \{5.1143, 4.6428, 4.4429, 4.2285, 4.3857, 4.3714, 4.3571, 4.3429, 4.2857, 4.3000, 4.2857, 4.2714, 4.2571, 4.2571, 4.2428, 4.3143, 4.2143, 4.0857, 4.0000, 3.8857, 3.8143, 3.7857, 3.7143, 3.7286, 3.7429, 4.0143, 3.9857, 3.9857, 4.0714, 4.0000, 4.1000, 4.1572\}$$

$$r_{\text{vdw}}^{\text{Cm}-\{\text{Fr..Rn}\}} = \{5.0000, 4.7143, 4.5143, 4.3857, 4.3000, 4.3143, 4.3286, 4.3429, 4.2571, 4.2571, 4.2857, 4.2857, 4.2428, 4.2714, 4.3571, 4.3857, 4.2000\}$$

B.4.9 Berkelium

$$r_{\text{vdw}}^{\text{Bk}-\{\text{H..He}\}} = \{2.6143, 2.8143\}$$

$$r_{\text{vdw}}^{\text{Bk}-\{\text{Li..Ne}\}} = \{3.8714, 3.5000, 3.2571, 3.2286, 3.1714, 3.0572, 3.0715, 3.1143\}$$

$$r_{\text{vdw}}^{\text{Bk}-\{\text{Na..Ar}\}} = \{4.1572, 3.9428, 3.7714, 3.6429, 3.7286, 3.6143, 3.5714, 3.5286\}$$

$$r_{\text{vdw}}^{\text{Bk}-\{\text{K..Kr}\}} = \{4.6714, 4.3571, 4.0571, 3.9000, 3.8857, 3.7286, 3.6857, 3.6429, 3.5857, 3.5714, 3.6000, 3.7143, 3.7572, 3.7143, 3.8000, 3.7286, 3.7857, 3.8286\}$$

$$r_{\text{vdw}}^{\text{Bk}-\{\text{Rb..Xe}\}} = \{4.8572, 4.5429, 4.2571, 4.1429, 4.0429, 3.9286, 3.8000, 3.7714, 3.7714, 3.7000, 3.8000, 3.9143, 3.9857, 3.9571, 3.9571, 3.9143, 4.0429, 4.0286\}$$

$$r_{\text{vdw}}^{\text{Bk}-\{\text{Cs..Rn}\}} = \{5.1429, 4.6714, 4.4714, 4.2571, 4.4143, 4.4000, 4.3857, 4.3714, 4.3143, 4.3286, 4.3143, 4.3000, 4.2857, 4.2857, 4.2714, 4.3429, 4.2428, 4.1143, 4.0286, 3.9143, 3.8428, 3.8143, 3.7429, 3.7572, 3.7714, 4.0429, 4.0143, 4.0143, 4.1000, 4.0286, 4.1286, 4.1857\}$$

$$r_{\text{vdw}}^{\text{Bk}-\{\text{Fr..Rn}\}} = \{5.0286, 4.7429, 4.5429, 4.4143, 4.3286, 4.3429, 4.3571, 4.3714, 4.2857, 4.2857, 4.3143, 4.3143, 4.2714, 4.3000, 4.3857, 4.4143, 4.2285\}$$

B.4.10 Californium

$$r_{\text{vdw}}^{\text{Cf}-\{\text{H..He}\}} = \{2.6143, 2.8143\}$$

$$r_{\text{vdw}}^{\text{Cf}-\{\text{Li..Ne}\}} = \{3.8714, 3.5000, 3.2571, 3.2286, 3.1714, 3.0572, 3.0715, 3.1143\}$$

$$r_{\text{vdw}}^{\text{Cf}-\{\text{Na..Ar}\}} = \{4.1572, 3.9428, 3.7714, 3.6429, 3.7286, 3.6143, 3.5714, 3.5286\}$$

$$r_{\text{vdw}}^{\text{Cf}-\{\text{K..Kr}\}} = \{4.6714, 4.3571, 4.0571, 3.9000, 3.8857, 3.7286, 3.6857, 3.6429, 3.5857, 3.5714, 3.6000, 3.7143, 3.7572, 3.7143, 3.8000, 3.7286, 3.7857, 3.8286\}$$

$$r_{\text{vdw}}^{\text{Cf}-\{\text{Rb..Xe}\}} = \{4.8572, 4.5429, 4.2571, 4.1429, 4.0429, 3.9286, 3.8000, 3.7714, 3.7714, 3.7000, 3.8000, 3.9143, 3.9857, 3.9571, 3.9571, 3.9143, 4.0429, 4.0286\}$$

$$r_{\text{vdw}}^{\text{Cf}-\{\text{Cs..Rn}\}} = \{5.1429, 4.6714, 4.4714, 4.2571, 4.4143, 4.4000, 4.3857, 4.3714, 4.3143, 4.3286, 4.3143, 4.3000, 4.2857, 4.2857, 4.2714, 4.3429, 4.2428, 4.1143, 4.0286, 3.9143, 3.8428, 3.8143, 3.7429, 3.7572, 3.7714, 4.0429, 4.0143, 4.0143, 4.1000, 4.0286, 4.1286, 4.1857\}$$

$$r_{\text{vdw}}^{\text{Cf}-\{\text{Fr..Rn}\}} = \{5.0286, 4.7429, 4.5429, 4.4143, 4.3286, 4.3429, 4.3571, 4.3714, 4.2857, 4.2857, 4.3143, 4.3143, 4.2714, 4.3000, 4.3857, 4.4143, 4.2285\}$$

B.4.11 Einsteinium

$$r_{\text{vdw}}^{\text{Es}-\{\text{H..He}\}} = \{2.5714, 2.7714\}$$

$$r_{\text{vdw}}^{\text{Es}-\{\text{Li..Ne}\}} = \{3.8286, 3.4572, 3.2143, 3.1857, 3.1285, 3.0143, 3.0286, 3.0715\}$$

$$r_{\text{vdw}}^{\text{Es}-\{\text{Na..Ar}\}} = \{4.1143, 3.9000, 3.7286, 3.6000, 3.6857, 3.5714, 3.5286, 3.4857\}$$

$$r_{\text{vdw}}^{\text{Es}-\{\text{K..Kr}\}} = \{4.6286, 4.3143, 4.0143, 3.8571, 3.8428, 3.6857, 3.6429, 3.6000, 3.5428, 3.5286, 3.5571, 3.6714, 3.7143, 3.6714, 3.7572, 3.6857, 3.7429, 3.7857\}$$

$$r_{\text{vdw}}^{\text{Es}-\{\text{Rb..Xe}\}} = \{4.8143, 4.5000, 4.2143, 4.1000, 4.0000, 3.8857, 3.7572, 3.7286, 3.7286, 3.6571, 3.7572, 3.8714, 3.9428, 3.9143, 3.9143, 3.8714, 4.0000, 3.9857\}$$

$$r_{\text{vdw}}^{\text{Es}-\{\text{Cs..Rn}\}} = \{5.1000, 4.6286, 4.4286, 4.2143, 4.3714, 4.3571, 4.3429, 4.3286, 4.2714, 4.2857, 4.2714, 4.2571, 4.2428, 4.2428, 4.2285, 4.3000, 4.2000, 4.0714, 3.9857, 3.8714, 3.8000, 3.7714, 3.7000, 3.7143, 3.7286, 4.0000, 3.9714, 3.9714, 4.0571, 3.9857, 4.0857, 4.1429\}$$

$$r_{\text{vdw}}^{\text{Es}-\{\text{Fr..Rn}\}} = \{4.9857, 4.7000, 4.5000, 4.3714, 4.2857, 4.3000, 4.3143, 4.3286, 4.2428, 4.2428, 4.2714, 4.2714, 4.2285, 4.2571, 4.3429, 4.3714, 4.1857\}$$

B.4.12 Fermium

$$r_{\text{vdw}}^{\text{Fm}-\{\text{H..He}\}} = \{2.6000, 2.8000\}$$

$$r_{\text{vdw}}^{\text{Fm}-\{\text{Li..Ne}\}} = \{3.8571, 3.4857, 3.2429, 3.2143, 3.1571, 3.0429, 3.0572, 3.1000\}$$

$$r_{\text{vdw}}^{\text{Fm}-\{\text{Na..Ar}\}} = \{4.1429, 3.9286, 3.7572, 3.6286, 3.7143, 3.6000, 3.5571, 3.5143\}$$

$$r_{\text{vdw}}^{\text{Fm}-\{\text{K..Kr}\}} = \{4.6571, 4.3429, 4.0429, 3.8857, 3.8714, 3.7143, 3.6714, 3.6286, 3.5714, 3.5571, 3.5857, 3.7000, 3.7429, 3.7000, 3.7857, 3.7143, 3.7714, 3.8143\}$$

$$r_{\text{vdw}}^{\text{Fm}-\{\text{Rb..Xe}\}} = \{4.8429, 4.5286, 4.2428, 4.1286, 4.0286, 3.9143, 3.7857, 3.7572, 3.7572, 3.6857, 3.7857, 3.9000, 3.9714, 3.9428, 3.9428, 3.9000, 4.0286, 4.0143\}$$

$$r_{\text{vdw}}^{\text{Fm}-\{\text{Cs..Rn}\}} = \{5.1286, 4.6571, 4.4572, 4.2428, 4.4000, 4.3857, 4.3714, 4.3571, 4.3000, 4.3143, 4.3000, 4.2857, 4.2714, 4.2714, 4.2571, 4.3286, 4.2285, 4.1000, 4.0143, 3.9000, 3.8286, 3.8000, 3.7286, 3.7429, 3.7572, 4.0286, 4.0000, 4.0000, 4.0857, 4.0143, 4.1143, 4.1715\}$$

$$r_{\text{vdw}}^{\text{Fm}-\{\text{Fr..Rn}\}} = \{5.0143, 4.7286, 4.5286, 4.4000, 4.3143, 4.3286, 4.3429, 4.3571, 4.2714, 4.2714, 4.3000, 4.3000, 4.2571, 4.2857, 4.3714, 4.4000, 4.2143\}$$

B.4.13 Mendelevium

$$r_{\text{vdw}}^{\text{Md}-\{\text{H..He}\}} = \{2.6857, 2.8857\}$$

$$r_{\text{vdw}}^{\text{Md}-\{\text{Li..Ne}\}} = \{3.9428, 3.5714, 3.3286, 3.3000, 3.2429, 3.1285, 3.1428, 3.1857\}$$

$$r_{\text{vdw}}^{\text{Md}-\{\text{Na..Ar}\}} = \{4.2285, 4.0143, 3.8428, 3.7143, 3.8000, 3.6857, 3.6429, 3.6000\}$$

$$r_{\text{vdw}}^{\text{Md}-\{\text{K..Kr}\}} = \{4.7429, 4.4286, 4.1286, 3.9714, 3.9571, 3.8000, 3.7572, 3.7143, 3.6571, 3.6429, 3.6714, 3.7857, 3.8286, 3.7857, 3.8714, 3.8000, 3.8571, 3.9000\}$$

$$r_{\text{vdw}}^{\text{Md}-\{\text{Rb..Xe}\}} = \{4.9285, 4.6143, 4.3286, 4.2143, 4.1143, 4.0000, 3.8714, 3.8428, 3.8428, 3.7714, 3.8714, 3.9857, 4.0571, 4.0286, 4.0286, 3.9857, 4.1143, 4.1000\}$$

$$r_{\text{vdw}}^{\text{Md}-\{\text{Cs..Rn}\}} = \{5.2143, 4.7429, 4.5429, 4.3286, 4.4857, 4.4714, 4.4572, 4.4429, 4.3857, 4.4000, 4.3857, 4.3714, 4.3571, 4.3571, 4.3429, 4.4143, 4.3143, 4.1857, 4.1000, 3.9857, 3.9143, 3.8857, 3.8143, 3.8286, 3.8428, 4.1143, 4.0857, 4.0857, 4.1715, 4.1000, 4.2000, 4.2571\}$$

$$r_{\text{vdw}}^{\text{Md}-\{\text{Fr..Rn}\}} = \{5.1000, 4.8143, 4.6143, 4.4857, 4.4000, 4.4143, 4.4286, 4.4429, 4.3571, 4.3571, 4.3857, 4.3857, 4.3429, 4.3714, 4.4572, 4.4857, 4.3000\}$$

B.4.14 Nobelium

$$r_{\text{vdw}}^{\text{No}-\{\text{H..He}\}} = \{2.7143, 2.9143\}$$

$$r_{\text{vdw}}^{\text{No}-\{\text{Li..Ne}\}} = \{3.9714, 3.6000, 3.3572, 3.3286, 3.2714, 3.1571, 3.1714, 3.2143\}$$

$$r_{\text{vdw}}^{\text{No}-\{\text{Na..Ar}\}} = \{4.2571, 4.0429, 3.8714, 3.7429, 3.8286, 3.7143, 3.6714, 3.6286\}$$

$$r_{\text{vdw}}^{\text{No}-\{\text{K..Kr}\}} = \{4.7714, 4.4572, 4.1572, 4.0000, 3.9857, 3.8286, 3.7857, 3.7429, 3.6857, 3.6714, 3.7000, 3.8143, 3.8571, 3.8143, 3.9000, 3.8286, 3.8857, 3.9286\}$$

$$r_{\text{vdw}}^{\text{No}-\{\text{Rb..Xe}\}} = \{4.9571, 4.6428, 4.3571, 4.2428, 4.1429, 4.0286, 3.9000, 3.8714, 3.8714, 3.8000, 3.9000, 4.0143, 4.0857, 4.0571, 4.0571, 4.0143, 4.1429, 4.1286\}$$

$$r_{\text{vdw}}^{\text{No}-\{\text{Cs..Rn}\}} = \{5.2429, 4.7714, 4.5714, 4.3571, 4.5143, 4.5000, 4.4857, 4.4714, 4.4143, 4.4286, 4.4143, 4.4000, 4.3857, 4.3857, 4.3714, 4.4429, 4.3429, 4.2143, 4.1286, 4.0143, 3.9428, 3.9143, 3.8428, 3.8571, 3.8714, 4.1429, 4.1143, 4.1143, 4.2000, 4.1286, 4.2285, 4.2857\}$$

$$r_{\text{vdw}}^{\text{No}-\{\text{Fr..Rn}\}} = \{5.1286, 4.8429, 4.6428, 4.5143, 4.4286, 4.4429, 4.4572, 4.4714, 4.3857, 4.3857, 4.4143, 4.4143, 4.3714, 4.4000, 4.4857, 4.5143, 4.3286\}$$

B.4.15 Lawrencium

$$r_{\text{vdw}}^{\text{Lr}-\{\text{H..He}\}} = \{2.5286, 2.7286\}$$

$$r_{\text{vdw}}^{\text{Lr}-\{\text{Li..Ne}\}} = \{3.7857, 3.4143, 3.1714, 3.1428, 3.0857, 2.9714, 2.9857, 3.0286\}$$

$$r_{\text{vdw}}^{\text{Lr}-\{\text{Na..Ar}\}} = \{4.0714, 3.8571, 3.6857, 3.5571, 3.6429, 3.5286, 3.4857, 3.4429\}$$

$$r_{\text{vdw}}^{\text{Lr}-\{\text{K..Kr}\}} = \{4.5857, 4.2714, 3.9714, 3.8143, 3.8000, 3.6429, 3.6000, 3.5571, 3.5000, 3.4857, 3.5143, 3.6286, 3.6714, 3.6286, 3.7143, 3.6429, 3.7000, 3.7429\}$$

$$r_{\text{vdw}}^{\text{Lr}-\{\text{Rb..Xe}\}} = \{4.7714, 4.4572, 4.1715, 4.0571, 3.9571, 3.8428, 3.7143, 3.6857, 3.6857, 3.6143, 3.7143, 3.8286, 3.9000, 3.8714, 3.8714, 3.8286, 3.9571, 3.9428\}$$

$$r_{\text{vdw}}^{\text{Lr}-\{\text{Cs..Rn}\}} = \{5.0571, 4.5857, 4.3857, 4.1715, 4.3286, 4.3143, 4.3000, 4.2857, 4.2285, 4.2428, 4.2285, 4.2143, 4.2000, 4.2000, 4.1857, 4.2571, 4.1572, 4.0286, 3.9428, 3.8286, 3.7572, 3.7286, 3.6571, 3.6714, 3.6857, 3.9571, 3.9286, 3.9286, 4.0143, 3.9428, 4.0429, 4.1000\}$$

$$r_{\text{vdw}}^{\text{Lr}-\{\text{Fr..Rn}\}} = \{4.9428, 4.6571, 4.4572, 4.3286, 4.2428, 4.2571, 4.2714, 4.2857, 4.2000, 4.2000, 4.2285, 4.2285, 4.1857, 4.2143, 4.3000, 4.3286, 4.1429\}$$

C DFT-D4

C.1 Chemical Hardnesses

Element-specific chemical hardnesses for the charge scaling function used to extrapolate the C_6 coefficients in D4.

$$J_{\mathrm{Ac..Lr}} = \{0.09920295, 0.10418621, 0.14235633, 0.16394294, 0.18551941, 0.22370139, 0.25110000, 0.25030000, 0.28840000, 0.31000000, 0.33160000, 0.35320000, 0.36820000, 0.39630000, 0.40140000\}$$

C.2 Electronegativities

Pauling electronegativities are used for the covalent coordination number.

$$\mathrm{EN}_{\mathrm{Ac..Lr}} = \{1.10, 1.30, 1.50, 1.38, 1.36, 1.28, 1.30, 1.30, 1.30, 1.30, 1.30, 1.30, 1.30, 1.30, 1.30\}$$

C.3 Reference Systems

Table 1 List of used reference structures. '✓' indicates the use, '–' indicates no use.

A	AH_0	AH_1	AH_2	AH_3	AH_4	AH_5	AH_6
Fr	✓	✓	–	–	–	–	–
Ra	✓	✓	✓	–	–	–	–
Ac	✓	✓	✓	✓	✓	✓	✓
Th	✓	✓	✓	✓	✓	–	–
Pa	✓	✓	✓	✓	✓	✓	✓
U	✓	✓	–	✓	✓	✓	✓
Np	✓	✓	✓	✓	✓	✓	✓
Pu	✓	✓	✓	✓	✓	✓	✓
Am	✓	✓	✓	✓	–	✓	✓
Cm	✓	✓	✓	✓	✓	✓	✓
Bk	✓	✓	✓	✓	✓	–	–
Cf	✓	✓	✓	✓	✓	–	✓
Es	✓	✓	✓	✓	✓	✓	✓
Fm	✓	✓	✓	✓	✓	✓	✓
Md	✓	✓	✓	✓	✓	–	–
No	✓	✓	✓	✓	✓	✓	✓
Lr	✓	✓	✓	✓	✓	✓	✓

C.4 Reference Data

The EEQ reference charge and coordination number are always given for the central actinide. The dynamic purely-imaginary frequency polarizabilities are given each for all following imaginary frequencies:

$$
\begin{aligned}
i\omega^{\mathrm{I}} = \{&0.000001, 0.05, 0.10, 0.20, 0.30, 0.40,\\
&0.50, 0.60, 0.70, 0.80, 0.90, 1.00,\\
&1.20, 1.40, 1.60, 1.80, 2.00, 2.50,\\
&3.00, 4.00, 5.00, 7.50, 10.00\}
\end{aligned}
$$

C.4.1 Actinium

C.4.1.1 Ac

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Ac,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Ac}} = 0.0000$$

$$
\begin{aligned}
\alpha^{\mathrm{Ac}}(i\omega^{\mathrm{I}}) = \{&204.4018, 167.2136, 116.6977, 58.9802, 35.5482, 24.5444,\\
&18.4663, 14.6615, 12.0558, 10.1554, 8.7067, 7.5671,\\
&5.8965, 4.7423, 3.9076, 3.2826, 2.8016, 1.9881,\\
&1.4912, 0.9334, 0.6400, 0.3123, 0.1837\}
\end{aligned}
$$

C.4.1.2 AcH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Ac,ref}} = 0.1175\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Ac}} = 0.8122$$

$$
\begin{aligned}
\alpha^{\mathrm{Ac}}(i\omega^{\mathrm{I}}) = \{&183.4136, 151.7817, 106.8129, 57.3477, 36.6709, 26.2420,\\
&20.1263, 16.1394, 13.3399, 11.2679, 9.6751, 8.4158,\\
&6.5630, 5.2798, 4.3506, 3.6543, 3.1181, 2.2109,\\
&1.6568, 1.0354, 0.7092, 0.3456, 0.2031\}
\end{aligned}
$$

C.4.1.3 $\mathrm{AcH_2}$

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Ac,ref}} = 0.1897\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Ac}} = 1.6110$$

$$
\begin{aligned}
\alpha^{\mathrm{Ac}}(i\omega^{\mathrm{I}}) = \{&161.4080, 115.7143, 81.7712, 50.0678, 34.9562, 26.1999,\\
&20.5872, 16.7261, 13.9261, 11.8135, 10.1705, 8.8623,\\
&6.9259, 5.5789, 4.6011, 3.8673, 3.3014, 2.3426,\\
&1.7561, 1.0977, 0.7520, 0.3664, 0.2154\}
\end{aligned}
$$

C.4.1.4 AcH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Ac,ref}} = 0.2380\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Ac}} = 2.4082$$

$$\begin{aligned}\alpha^{\mathrm{Ac}}(i\omega^{\mathrm{I}}) = \{&67.3758, 65.1171, 59.4934, 45.8749, 34.8544, 27.0905,\\ &21.6504, 17.7357, 14.8287, 12.6069, 10.8667, 9.4755,\\ &7.4104, 5.9711, 4.9254, 4.1401, 3.5343, 2.5073,\\ &1.8789, 1.1737, 0.8036, 0.3913, 0.2299\}\end{aligned}$$

C.4.1.5 AcH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Ac,ref}} = 0.2714\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Ac}} = 3.1614$$

$$\begin{aligned}\alpha^{\mathrm{Ac}}(i\omega^{\mathrm{I}}) = \{&164.9995, 91.9493, 68.8421, 49.6465, 37.6576, 29.3282,\\ &23.4479, 19.1936, 16.0279, 13.6085, 11.7157, 10.2048,\\ &7.9669, 6.4111, 5.2827, 4.4365, 3.7843, 2.6802,\\ &2.0057, 1.2503, 0.8548, 0.4155, 0.2438\}\end{aligned}$$

C.4.1.6 AcH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Ac,ref}} = 0.2925\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Ac}} = 3.8682$$

$$\begin{aligned}\alpha^{\mathrm{Ac}}(i\omega^{\mathrm{I}}) = \{&171.2481, 134.6703, 94.9592, 58.8185, 42.2049, 32.1669,\\ &25.4549, 20.7157, 17.2343, 14.5948, 12.5410, 10.9080,\\ &8.4991, 6.8306, 5.6231, 4.7187, 4.0224, 2.8448,\\ &2.1262, 1.3227, 0.9030, 0.4379, 0.2567\}\end{aligned}$$

C.4.1.7 AcH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Ac,ref}} = 0.3094\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Ac}} = 4.6022$$

$$\begin{aligned}\alpha^{\mathrm{Ac}}(i\omega^{\mathrm{I}}) = \{&213.4703, 168.2418, 114.2009, 65.8444, 46.0049, 34.7218,\\ &27.3472, 22.1893, 18.4197, 15.5715, 13.3612, 11.6077,\\ &9.0275, 7.2449, 5.9573, 4.9943, 4.2536, 3.0025,\\ &2.2404, 1.3901, 0.9471, 0.4579, 0.2680\}\end{aligned}$$

C.4.2 Thorium

C.4.2.1 Th

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Th,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Th}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Th}}(i\omega^{\mathrm{I}}) = \{&151.3055, 132.0224, 100.3446, 57.1424, 36.8572, 26.3121,\\ &20.0922, 16.0586, 13.2527, 11.1957, 9.6267, 8.3935,\\ &6.5881, 5.3414, 4.4388, 3.7618, 3.2393, 2.3514,\\ &1.8034, 1.1756, 0.8333, 0.4292, 0.2597\}\end{aligned}$$

C.4.2.2 ThH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Th,ref}} = 0.0884\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Th}} = 0.8421$$

$$\begin{aligned}\alpha^{\mathrm{Th}}(i\omega^{\mathrm{I}}) = \{&142.0153, 121.7331, 91.8673, 54.6347, 36.9218, 27.1646,\\ &21.1161, 17.0504, 14.1521, 11.9929, 10.3287, 9.0119,\\ &7.0733, 5.7297, 4.7553, 4.0241, 3.4599, 2.5018,\\ &1.9119, 1.2389, 0.8745, 0.4477, 0.2701\}\end{aligned}$$

C.4.2.3 ThH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Th,ref}} = 0.1538\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Th}} = 1.6727$$

$$\begin{aligned}\alpha^{\mathrm{Th}}(i\omega^{\mathrm{I}}) = \{&117.3110, 99.2298, 76.8788, 50.3595, 36.4314, 27.8345,\\ &22.0825, 18.0277, 15.0511, 12.7932, 11.0337, 9.6319,\\ &7.5577, 6.1155, 5.0688, 4.2834, 3.6777, 2.6504,\\ &2.0194, 1.3024, 0.9162, 0.4667, 0.2809\}\end{aligned}$$

C.4.2.4 ThH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Th,ref}} = 0.2048\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Th}} = 2.5057$$

$$\begin{aligned}\alpha^{\mathrm{Th}}(i\omega^{\mathrm{I}}) = \{&94.3173, 83.8298, 69.2481, 49.5422, 37.3912, 29.1787,\\ &23.4000, 19.2060, 16.0744, 13.6753, 11.7953, 10.2930,\\ &8.0657, 6.5164, 5.3926, 4.5501, 3.9010, 2.8019,\\ &2.1286, 1.3664, 0.9580, 0.4858, 0.2917\}\end{aligned}$$

C.4.2.5 ThH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Th,ref}} = 0.2433\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Th}} = 3.3346$$

$$\begin{aligned}\alpha^{\mathrm{Th}}(i\omega^{\mathrm{I}}) = \{&63.9385, 62.4467, 58.5371, 47.9250, 38.0867, 30.4193,\\ &24.6745, 20.3674, 17.0925, 14.5574, 12.5588, 10.9565,\\ &8.5757, 6.9183, 5.7167, 4.8166, 4.1238, 2.9526,\\ &2.2370, 1.4299, 0.9995, 0.5046, 0.3024\}\end{aligned}$$

C.4.3 Protactinium

C.4.3.1 Pa

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pa,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pa}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Pa}}(i\omega^{\mathrm{I}}) = \{&166.6278, 141.2842, 102.4567, 54.4640, 34.1796, 24.3027,\\ &18.6668, 15.0571, 12.5482, 10.6994, 9.2777, 8.1496,\\ &6.4741, 5.2950, 4.4269, 3.7666, 3.2513, 2.3641,\\ &1.8105, 1.1737, 0.8277, 0.4230, 0.2550\}\end{aligned}$$

C.4.3.2 PaH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pa,ref}} = 0.1067\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pa}} = 0.8509$$

$$\begin{aligned}\alpha^{\mathrm{Pa}}(i\omega^{\mathrm{I}}) = \{&157.0761, 129.9417, 94.0821, 52.6867, 34.7765, 25.4912,\\ &19.9068, 16.1943, 13.5496, 11.5701, 10.0338, 8.8082,\\ &6.9822, 5.6965, 4.7513, 4.0337, 3.4750, 2.5159,\\ &1.9200, 1.2382, 0.8700, 0.4423, 0.2660\}\end{aligned}$$

C.4.3.3 PaH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pa,ref}} = 0.1829\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pa}} = 1.6824$$

$$\begin{aligned}\alpha^{\mathrm{Pa}}(i\omega^{\mathrm{I}}) = \{&125.3575, 97.8437, 72.3248, 46.3110, 33.6241, 25.9618,\\ &20.8400, 17.1994, 14.4963, 12.4215, 10.7866, 9.4709,\\ &7.4983, 6.1056, 5.0823, 4.3065, 3.7035, 2.6714,\\ &2.0326, 1.3050, 0.9143, 0.4630, 0.2779\}\end{aligned}$$

C.4.3.4 PaH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pa,ref}} = 0.2467\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pa}} = 2.5614$$

$$\begin{aligned}\alpha^{\mathrm{Pa}}(i\omega^{\mathrm{I}}) = \{&85.9686, 76.5628, 64.2652, 46.9224, 35.8901, 28.3127,\\ &22.9033, 18.9261, 15.9240, 13.6039, 11.7728, 10.3012,\\ &8.1048, 6.5655, 5.4425, 4.5965, 3.9422, 2.8299,\\ &2.1464, 1.3730, 0.9600, 0.4850, 0.2908\}\end{aligned}$$

C.4.3.5 PaH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pa,ref}} = 0.2930\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pa}} = 3.4147$$

$$\begin{aligned}\alpha^{\mathrm{Pa}}(i\omega^{\mathrm{I}}) = \{&68.2275, 65.6186, 60.0315, 47.6360, 37.5304, 29.9831,\\ &24.3945, 20.2072, 17.0134, 14.5306, 12.5653, 10.9836,\\ &8.6224, 6.9698, 5.7664, 4.8615, 4.1631, 2.9787,\\ &2.2534, 1.4359, 1.0013, 0.5039, 0.3016\}\end{aligned}$$

C.4.3.6 PaH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pa,ref}} = 0.3292\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pa}} = 4.3316$$

$$\begin{aligned}\alpha^{\mathrm{Pa}}(i\omega^{\mathrm{I}}) = \{&64.6792, 62.7769, 58.3982, 48.0808, 38.8770, 31.5484,\\ &25.8960, 21.5514, 18.1846, 15.5419, 13.4380, 11.7392,\\ &9.1986, 7.4202, 6.1268, 5.1560, 4.4081, 3.1435,\\ &2.3721, 1.5065, 1.0485, 0.5264, 0.3147\}\end{aligned}$$

C.4.4 Uranium

C.4.4.1 U

$$\zeta_{\mathrm{EEQ}}^{\mathrm{U,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{U}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{U}}(i\omega^{\mathrm{I}}) = \{&159.6502, 135.8961, 98.5087, 52.3885, 32.9240, 23.4921,\\ &18.1200, 14.6740, 12.2717, 10.4953, 9.1247, 8.0337,\\ &6.4061, 5.2540, 4.4012, 3.7494, 3.2387, 2.3549,\\ &1.8012, 1.1640, 0.8188, 0.4171, 0.2512\}\end{aligned}$$

C.4.4.2 UH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{U,ref}} = 0.0796\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{U}} = 0.8456$$

$$\begin{aligned}\alpha^{\mathrm{U}}(i\omega^{\mathrm{I}}) = \{&152.0261, 128.0014, 92.7351, 51.5592, 33.7877, 24.6849,\\ &19.2730, 15.7027, 13.1694, 11.2757, 9.8051, 8.6299,\\ &6.8722, 5.6267, 4.7053, 4.0017, 3.4512, 2.5004,\\ &1.9065, 1.2259, 0.8593, 0.4354, 0.2615\}\end{aligned}$$

C.4.4.3 UH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{U,ref}} = 0.1692\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{U}} = 2.5008$$

$$\begin{aligned}\alpha^{\mathrm{U}}(i\omega^{\mathrm{I}}) = \{&61.4628, 58.1569, 52.5979, 41.1736, 32.1633, 25.6872,\\ &21.0129, 17.5503, 14.9130, 12.8534, 11.2101, 9.8751,\\ &7.8534, 6.4113, 5.3438, 4.5301, 3.8949, 2.8030,\\ &2.1255, 1.3553, 0.9444, 0.4745, 0.2838\}\end{aligned}$$

C.4.4.4 UH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{U,ref}} = 0.2039\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{U}} = 3.3883$$

$$\begin{aligned}\alpha^{\mathrm{U}}(i\omega^{\mathrm{I}}) = \{&57.7404, 56.8542, 53.0160, 43.4071, 34.8272, 28.1717,\\ &23.1479, 19.3339, 16.3931, 14.0848, 12.2416, 10.7465,\\ &8.4924, 6.8967, 5.7239, 4.8357, 4.1463, 2.9696,\\ &2.2450, 1.4269, 0.9927, 0.4980, 0.2977\}\end{aligned}$$

C.4.4.5 UH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{U,ref}} = 0.1949\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{U}} = 3.5705$$

$$\begin{aligned}\alpha^{\mathrm{U}}(i\omega^{\mathrm{I}}) = \{&79.4644, 66.1196, 58.3425, 45.8165, 36.2236, 29.1720,\\ &23.9622, 20.0392, 17.0204, 14.6497, 12.7535, 11.2118,\\ &8.8797, 7.2209, 5.9979, 5.0687, 4.3459, 3.1092,\\ &2.3465, 1.4858, 1.0304, 0.5142, 0.3066\}\end{aligned}$$

C.4.4.6 UH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{U,ref}} = 0.2456\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{U}} = 5.1256$$

$$\begin{aligned}\alpha^{\mathrm{U}}(i\omega^{\mathrm{I}}) = \{&70.4499, 68.4799, 63.4736, 50.8489, 40.1019, 32.1246,\\ &26.2551, 21.8601, 18.4967, 15.8684, 13.7751, 12.0799,\\ &9.5275, 7.7225, 6.3969, 5.3938, 4.6159, 3.2908,\\ &2.4779, 1.5649, 1.0839, 0.5404, 0.3221\}\end{aligned}$$

C.4.5 Neptunium

C.4.5.1 Np

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Np,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Np}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Np}}(i\omega^{\mathrm{I}}) = \{&152.1284, 112.6033, 75.4650, 40.7349, 27.3561, 20.6810,\\ &16.6271, 13.8530, 11.8127, 10.2409, 8.9907, 7.9726,\\ &6.4187, 5.2954, 4.4526, 3.8023, 3.2893, 2.3948,\\ &1.8309, 1.1805, 0.8288, 0.4212, 0.2535\}\end{aligned}$$

C.4.5.2 NpH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Np,ref}} = 0.0766\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Np}} = 0.8493$$

$$\begin{aligned}\alpha^{\mathrm{Np}}(i\omega^{\mathrm{I}}) = \{&134.2374, 104.3914, 73.7095, 42.8462, 29.7210, 22.6357,\\ &18.1747, 15.0874, 12.8156, 11.0712, 9.6899, 8.5700,\\ &6.8704, 5.6495, 4.7380, 4.0373, 3.4862, 2.5288,\\ &1.9277, 1.2375, 0.8661, 0.4381, 0.2630\}\end{aligned}$$

C.4.5.3 NpH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Np,ref}} = 0.1332\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Np}} = 1.6831$$

$$\begin{aligned}\alpha^{\mathrm{Np}}(i\omega^{\mathrm{I}}) = \{&114.7257, 89.7632, 66.6972, 42.9194, 31.1632, 24.1344,\\ &19.4813, 16.1874, 13.7402, 11.8547, 10.3605, 9.1500,\\ &7.3160, 6.0025, 5.0243, 4.2741, 3.6852, 2.6647,\\ &2.0261, 1.2953, 0.9038, 0.4550, 0.2725\}\end{aligned}$$

C.4.5.4 NpH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Np,ref}} = 0.1755\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Np}} = 2.5168$$

$$\begin{aligned}\alpha^{\mathrm{Np}}(i\omega^{\mathrm{I}}) = \{&60.0193, 57.7069, 52.4810, 40.8286, 31.7259, 25.2754,\\ &20.6624, 17.2654, 14.6872, 12.6774, 11.0747, 9.7721,\\ &7.7962, 6.3820, 5.3310, 4.5267, 3.8967, 2.8084,\\ &2.1298, 1.3566, 0.9441, 0.4735, 0.2831\}\end{aligned}$$

C.4.5.5 NpH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Np,ref}} = 0.2187\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Np}} = 3.3977$$

$$\begin{aligned}\alpha^{\mathrm{Np}}(i\omega^{\mathrm{I}}) = \{&57.6363, 55.7487, 51.6348, 42.1037, 33.8112, 27.4067,\\ &22.5760, 18.9076, 16.0757, 13.8491, 12.0672, 10.6182,\\ &8.4250, 6.8637, 5.7105, 4.8331, 4.1493, 2.9761,\\ &2.2502, 1.4285, 0.9925, 0.4970, 0.2969\}\end{aligned}$$

C.4.5.6 NpH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Np,ref}} = 0.2424\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Np}} = 4.2360$$

$$\begin{aligned}\alpha^{\mathrm{Np}}(i\omega^{\mathrm{I}}) = \{&79.8320, 75.1735, 66.0772, 49.2763, 37.7996, 29.9550,\\ &24.3771, 20.2708, 17.1576, 14.7371, 12.8142, 11.2583,\\ &8.9140, 7.2512, 6.0255, 5.0940, 4.3688, 3.1261,\\ &2.3586, 1.4919, 1.0338, 0.5156, 0.3074\}\end{aligned}$$

C.4.5.7 NpH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Np,ref}} = 0.2666\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Np}} = 5.0938$$

$$\begin{aligned}\alpha^{\mathrm{Np}}(i\omega^{\mathrm{I}}) = \{&90.8036, 85.6050, 74.5057, 54.1948, 40.9874, 32.2515,\\ &26.1389, 21.6751, 18.3065, 15.6954, 13.6262, 11.9552,\\ &9.4435, 7.6670, 6.3604, 5.3694, 4.5990, 3.2820,\\ &2.4709, 1.5580, 1.0773, 0.5356, 0.3189\}\end{aligned}$$

C.4.6 Plutonium

C.4.6.1 Pu

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pu,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pu}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Pu}}(i\omega^{\mathrm{I}}) = \{&172.7407, 145.6048, 101.7601, 50.1348, 29.9893, 20.8783,\\ &15.9825, 12.9731, 10.9295, 9.4374, 8.2894, 7.3721,\\ &5.9863, 4.9831, 4.2229, 3.6292, 3.1552, 2.3147,\\ &1.7750, 1.1444, 0.8014, 0.4049, 0.2429\}\end{aligned}$$

C.4.6.2 PuH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pu,ref}} = 0.1495\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pu}} = 0.8125$$

$$\begin{aligned}\alpha^{\mathrm{Pu}}(i\omega^{\mathrm{I}}) = \{&140.6592, 109.3083, 72.9348, 39.9874, 27.0422, 20.3958,\\ &16.3706, 13.6553, 11.6836, 10.1759, 8.9797, 8.0043,\\ &6.5061, 5.4099, 4.5766, 3.9257, 3.4065, 2.4886,\\ &1.9019, 1.2200, 0.8514, 0.4280, 0.2562\}\end{aligned}$$

C.4.6.3 PuH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pu,ref}} = 0.2479\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pu}} = 1.6569$$

$$\begin{aligned}\alpha^{\mathrm{Pu}}(i\omega^{\mathrm{I}}) = \{&97.7402, 76.6674, 59.4822, 39.5057, 28.9200, 22.5125,\\ &18.2688, 15.2650, 13.0298, 11.3020, 9.9268, 8.8070,\\ &7.0972, 5.8593, 4.9281, 4.2076, 3.6375, 2.6400,\\ &2.0093, 1.2830, 0.8931, 0.4478, 0.2677\}\end{aligned}$$

C.4.6.4 PuH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pu,ref}} = 0.3181\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pu}} = 2.4997$$

$$\begin{aligned}\alpha^{\mathrm{Pu}}(i\omega^{\mathrm{I}}) = \{&55.3410, 53.3924, 49.1138, 38.9121, 30.5324, 24.4542,\\ &20.0614, 16.8099, 14.3348, 12.4010, 10.8559, 9.5976,\\ &7.6829, 6.3067, 5.2796, 4.4906, 3.8702, 2.7936,\\ &2.1188, 1.3476, 0.9362, 0.4682, 0.2796\}\end{aligned}$$

C.4.6.5 PuH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pu,ref}} = 0.3779\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pu}} = 3.3624$$

$$\begin{aligned}\alpha^{\mathrm{Pu}}(i\omega^{\mathrm{I}}) = \{&64.4205, 57.8759, 51.6984, 41.3225, 33.0420, 26.7590,\\ &22.0509, 18.4870, 15.7401, 13.5812, 11.8529, 10.4461,\\ &8.3125, 6.7886, 5.6589, 4.7964, 4.1220, 2.9602,\\ &2.2381, 1.4185, 0.9838, 0.4912, 0.2932\}\end{aligned}$$

C.4.6.6 PuH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pu,ref}} = 0.4092\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pu}} = 4.1937$$

$$\begin{aligned}\alpha^{\mathrm{Pu}}(i\omega^{\mathrm{I}}) = \{&84.8162, 79.2048, 68.1431, 49.2446, 37.2618, 29.3656,\\ &23.8516, 19.8305, 16.7968, 14.4437, 12.5760, 11.0646,\\ &8.7844, 7.1628, 5.9634, 5.0491, 4.3349, 3.1060,\\ &2.3435, 1.4802, 1.0238, 0.5091, 0.3032\}\end{aligned}$$

C.4.6.7 PuH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Pu,ref}} = 0.4364\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Pu}} = 5.0202$$

$$\begin{aligned}\alpha^{\mathrm{Pu}}(i\omega^{\mathrm{I}}) = \{&104.8008, 96.5146, 80.5042, 55.4091, 40.9972, 31.9653,\\ &25.8009, 21.3575, 18.0288, 15.4598, 13.4288, 11.7907,\\ &9.3295, 7.5871, 6.3030, 5.3270, 4.5664, 3.2619,\\ &2.4554, 1.5458, 1.0668, 0.5288, 0.3144\}\end{aligned}$$

C.4.7 Americium

C.4.7.1 Am

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Am,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Am}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Am}}(i\omega^{\mathrm{I}}) = \{&165.6020, 140.4979, 99.0178, 49.3591, 29.6192, 20.6061,\\ &15.7483, 12.7644, 10.7433, 9.2722, 8.1437, 7.2442,\\ &5.8887, 4.9089, 4.1663, 3.5854, 3.1206, 2.2934,\\ &1.7596, 1.1336, 0.7927, 0.3995, 0.2395\}\end{aligned}$$

C.4.7.2 AmH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Am,ref}} = 0.1510\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Am}} = 0.7827$$

$$\begin{aligned}\alpha^{\mathrm{Am}}(i\omega^{\mathrm{I}}) = \{&133.0355, 104.9202, 71.4376, 39.7060, 26.7872, 20.1191,\\ &16.0991, 13.4054, 11.4613, 9.9818, 8.8117, 7.8596,\\ &6.3993, 5.3309, 4.5175, 3.8808, 3.3718, 2.4680,\\ &1.8874, 1.2101, 0.8434, 0.4231, 0.2530\}\end{aligned}$$

C.4.7.3 AmH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Am,ref}} = 0.2410\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Am}} = 1.5858$$

$$\begin{aligned}\alpha^{\mathrm{Am}}(i\omega^{\mathrm{I}}) = \{&60.0172, 56.0455, 48.5551, 35.1427, 26.4217, 20.8390,\\ &17.0639, 14.3637, 12.3397, 10.7653, 9.5045, 8.4717,\\ &6.8811, 5.7168, 4.8322, 4.1417, 3.5913, 2.6183,\\ &1.9964, 1.2748, 0.8861, 0.4428, 0.2643\}\end{aligned}$$

C.4.7.4 AmH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Am,ref}} = 0.3068\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Am}} = 2.4639$$

$$\begin{aligned}\alpha^{\mathrm{Am}}(i\omega^{\mathrm{I}}) = \{&54.6144, 51.1619, 47.1128, 37.5252, 29.5312, 23.6871,\\ &19.4572, 16.3295, 13.9514, 12.0946, 10.6105, 9.4006,\\ &7.5549, 6.2225, 5.2236, 4.4527, 3.8441, 2.7818,\\ &2.1119, 1.3428, 0.9318, 0.4650, 0.2775\}\end{aligned}$$

C.4.7.5 AmH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Am,ref}} = 0.3801\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Am}} = 4.1035$$

$$\begin{aligned}\alpha^{\mathrm{Am}}(i\omega^{\mathrm{I}}) = \{&98.4838, 88.6035, 72.3489, 49.5094, 36.7446, 28.7273,\\ &23.2552, 19.3162, 16.3679, 14.0917, 12.2893, 10.8319,\\ &8.6315, 7.0620, 5.8964, 5.0040, 4.3040, 3.0923,\\ &2.3355, 1.4743, 1.0183, 0.5049, 0.3003\}\end{aligned}$$

C.4.7.6 AmH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Am,ref}} = 0.4055\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Am}} = 4.9407$$

$$\begin{aligned}\alpha^{\mathrm{Am}}(i\omega^{\mathrm{I}}) = \{&113.3351, 102.5161, 83.0136, 55.2298, 40.3635, 31.3182,\\ &25.2332, 20.8827, 17.6396, 15.1435, 13.1728, 11.5836,\\ &9.1935, 7.4970, 6.2427, 5.2859, 4.5380, 3.2490,\\ &2.4479, 1.5406, 1.0620, 0.5253, 0.3121\}\end{aligned}$$

C.4.8 Curium

C.4.8.1 Cm

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cm,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cm}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Cm}}(i\omega^{\mathrm{I}}) = \{&134.3979, 116.1743, 86.3865, 47.1493, 29.7740, 21.2860,\\ &16.4818, 13.4222, 11.2973, 9.7266, 8.5121, 7.5415,\\ &6.0822, 5.0365, 4.2522, 3.6447, 3.1628, 2.3136,\\ &1.7710, 1.1385, 0.7954, 0.4006, 0.2401\}\end{aligned}$$

C.4.8.2 CmH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cm,ref}} = 0.0764\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cm}} = 0.8347$$

$$\begin{aligned}\alpha^{\mathrm{Cm}}(i\omega^{\mathrm{I}}) = \{&126.6120, 109.3213, 81.5724, 47.0010, 31.2024, 22.8861,\\ &17.8997, 14.6120, 12.2878, 10.5566, 9.2154, 8.1445,\\ &6.5400, 5.3965, 4.5431, 3.8848, 3.3643, 2.4515,\\ &1.8710, 1.1977, 0.8343, 0.4183, 0.2502\}\end{aligned}$$

C.4.8.3 CmH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cm,ref}} = 0.1338\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cm}} = 1.6490$$

$$\begin{aligned}\alpha^{\mathrm{Cm}}(i\omega^{\mathrm{I}}) = \{&99.2440, 79.0152, 60.3295, 40.0819, 29.3586, 22.7763,\\ &18.3964, 15.3029, 13.0129, 11.2537, 9.8618, 8.7346,\\ &7.0244, 5.7943, 4.8728, 4.1614, 3.5990, 2.6141,\\ &1.9897, 1.2687, 0.8813, 0.4401, 0.2627\}\end{aligned}$$

C.4.8.4 CmH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cm,ref}} = 0.1780\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cm}} = 2.4732$$

$$\begin{aligned}\alpha^{\mathrm{Cm}}(i\omega^{\mathrm{I}}) = \{&54.6754, 52.9826, 48.7627, 38.4660, 29.9916, 23.8922,\\ &19.5266, 16.3254, 13.9078, 12.0305, 10.5370, 9.3243,\\ &7.4828, 6.1595, 5.1700, 4.4077, 3.8062, 2.7562,\\ &2.0930, 1.3299, 0.9217, 0.4587, 0.2733\}\end{aligned}$$

C.4.8.5 CmH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cm,ref}} = 0.2112\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cm}} = 3.2623$$

$$\begin{aligned}\alpha^{\mathrm{Cm}}(i\omega^{\mathrm{I}}) = \{&84.5347, 75.7999, 62.7375, 44.4811, 33.5258, 26.3562,\\ &21.3871, 17.7920, 15.0970, 13.0154, 11.3666, 10.0329,\\ &8.0176, 6.5777, 5.5061, 4.6836, 4.0368, 2.9122,\\ &2.2055, 1.3962, 0.9652, 0.4787, 0.2847\}\end{aligned}$$

C.4.8.6 CmH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cm,ref}} = 0.2378\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cm}} = 4.0576$$

$$\begin{aligned}\alpha^{\mathrm{Cm}}(i\omega^{\mathrm{I}}) = \{&110.6679, 96.7153, 75.9750, 50.3031, 36.9564, 28.7507,\\ &23.1991, 19.2245, 16.2621, 13.9830, 12.1837, 10.7324,\\ &8.5474, 6.9930, 5.8404, 4.9585, 4.2667, 3.0681,\\ &2.3178, 1.4623, 1.0087, 0.4986, 0.2961\}\end{aligned}$$

C.4.8.7 CmH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cm,ref}} = 0.2595\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cm}} = 4.8597$$

$$\begin{aligned}\alpha^{\mathrm{Cm}}(i\omega^{\mathrm{I}}) = \{&133.9582, 116.0315, 88.6352, 56.0351, 40.3478, 31.1150,\\ &24.9872, 20.6390, 17.4139, 14.9409, 12.9936, 11.4265,\\ &9.0741, 7.4064, 6.1735, 5.2324, 4.4958, 3.2235,\\ &2.4299, 1.5282, 1.0519, 0.5185, 0.3074\}\end{aligned}$$

C.4.9 Berkelium

C.4.9.1 Bk

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Bk,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Bk}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Bk}}(i\omega^{\mathrm{I}}) = \{&150.0842, 129.4893, 93.3386, 47.5744, 28.7210, 19.9726,\\ &15.2302, 12.3184, 10.3534, 8.9302, 7.8439, 6.9817,\\ &5.6883, 4.7563, 4.0499, 3.4961, 3.0514, 2.2539,\\ &1.7337, 1.1173, 0.7796, 0.3907, 0.2336\}\end{aligned}$$

C.4.9.2 BkH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Bk,ref}} = 0.0221\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Bk}} = 0.8298$$

$$\begin{aligned}\alpha^{\mathrm{Bk}}(i\omega^{\mathrm{I}}) = \{&125.9274, 104.0728, 75.8864, 43.2370, 28.7503, 21.1786,\\ &16.6538, 13.6738, 11.5652, 9.9909, 8.7667, 7.7850,\\ &6.3038, 5.2375, 4.4339, 3.8085, 3.3100, 2.4257,\\ &1.8563, 1.1893, 0.8273, 0.4132, 0.2466\}\end{aligned}$$

C.4.9.3 $\mathrm{BkH_2}$

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Bk,ref}} = 0.0409\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Bk}} = 1.6684$$

$$\begin{aligned}\alpha^{\mathrm{Bk}}(i\omega^{\mathrm{I}}) = \{&94.2401, 77.5244, 58.9430, 39.0623, 28.6154, 22.2014,\\ &17.9362, 14.9285, 12.7061, 11.0009, 9.6529, 8.5611,\\ &6.9035, 5.7088, 4.8113, 4.1163, 3.5652, 2.5959,\\ &1.9780, 1.2611, 0.8750, 0.4358, 0.2598\}\end{aligned}$$

C.4.9.4 $\mathrm{BkH_3}$

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Bk,ref}} = 0.0562\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Bk}} = 2.5022$$

$$\begin{aligned}\alpha^{\mathrm{Bk}}(i\omega^{\mathrm{I}}) = \{&52.9670, 51.2081, 47.2097, 37.3875, 29.2191, 23.3037,\\ &19.0603, 15.9482, 13.5995, 11.7770, 10.3277, 9.1508,\\ &7.3623, 6.0746, 5.1094, 4.3635, 3.7735, 2.7388,\\ &2.0819, 1.3228, 0.9157, 0.4546, 0.2705\}\end{aligned}$$

C.4.9.5 BkH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Bk,ref}} = 0.0711\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Bk}} = 3.3645$$

$$\begin{aligned}\alpha^{\mathrm{Bk}}(i\omega^{\mathrm{I}}) = \{&64.0310, 57.6316, 50.4511, 39.9025, 31.7426, 25.6004,\\ &21.0403, 17.6214, 15.0076, 12.9657, 11.3372, 10.0143,\\ &8.0081, 6.5712, 5.5009, 4.6791, 4.0329, 2.9094,\\ &2.2032, 1.3943, 0.9636, 0.4776, 0.2840\}\end{aligned}$$

C.4.10 Californium

C.4.10.1 Cf

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cf,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cf}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Cf}}(i\omega^{\mathrm{I}}) = \{&148.0092, 127.6683, 91.8844, 46.6739, 28.1153, 19.5156,\\ &14.8547, 11.9926, 10.0613, 8.6633, 7.5975, 6.7529,\\ &5.4898, 4.5835, 3.8992, 3.3644, 2.9358, 2.1685,\\ &1.6685, 1.0759, 0.7512, 0.3775, 0.2265\}\end{aligned}$$

C.4.10.2 CfH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cf,ref}} = 0.1535\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cf}} = 0.8190$$

$$\begin{aligned}\alpha^{\mathrm{Cf}}(i\omega^{\mathrm{I}}) = \{&130.7987, 103.8692, 70.9979, 39.3131, 26.2475, 19.4914,\\ &15.4458, 12.7645, 10.8527, 9.4146, 8.2889, 7.3811,\\ &6.0027, 5.0037, 4.2470, 3.6557, 3.1827, 2.3393,\\ &1.7930, 1.1501, 0.8003, 0.4003, 0.2395\}\end{aligned}$$

C.4.10.3 CfH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cf,ref}} = 0.2539\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cf}} = 1.6345$$

$$\begin{aligned}\alpha^{\mathrm{Cf}}(i\omega^{\mathrm{I}}) = \{&53.3942, 50.4801, 44.7056, 33.0885, 24.9852, 19.6813,\\ &16.0762, 13.5014, 11.5795, 10.0918, 8.9061, 7.9390,\\ &6.4567, 5.3760, 4.5561, 3.9154, 3.4034, 2.4929,\\ &1.9055, 1.2173, 0.8448, 0.4208, 0.2512\}\end{aligned}$$

C.4.10.4 CfH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cf,ref}} = 0.3321\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cf}} = 2.5078$$

$$\begin{aligned}\alpha^{\mathrm{Cf}}(i\omega^{\mathrm{I}}) = \{&50.4030, 48.8895, 45.1750, 36.0185, 28.2961, 22.6345,\\ &18.5399, 15.5218, 13.2371, 11.4613, 10.0478, 8.8997,\\ &7.1552, 5.9002, 4.9604, 4.2349, 3.6615, 2.6568,\\ &2.0193, 1.2829, 0.8883, 0.4418, 0.2636\}\end{aligned}$$

C.4.10.5 CfH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cf,ref}} = 0.3868\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cf}} = 3.3439$$

$$\begin{aligned}\alpha^{\mathrm{Cf}}(i\omega^{\mathrm{I}}) = \{&81.5875, 68.6608, 56.5880, 41.3108, 31.7640, 25.2149,\\ &20.5502, 17.1270, 14.5428, 12.5405, 10.9528, 9.6682,\\ &7.7278, 6.3424, 5.3117, 4.5206, 3.8982, 2.8146,\\ &2.1321, 1.3490, 0.9318, 0.4619, 0.2752\}\end{aligned}$$

C.4.10.6 CfH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Cf,ref}} = 0.4500\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Cf}} = 4.9836$$

$$\begin{aligned}\alpha^{\mathrm{Cf}}(i\omega^{\mathrm{I}}) = \{&129.7015, 111.1969, 84.3720, 53.9448, 39.1948, 30.3205,\\ &24.3568, 20.1026, 16.9428, 14.5209, 12.6163, 11.0861,\\ &8.7940, 7.1734, 5.9775, 5.0658, 4.3527, 3.1210,\\ &2.3523, 1.4783, 1.0166, 0.5008, 0.2974\}\end{aligned}$$

C.4.11 Einsteinium

C.4.11.1 Es

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Es,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Es}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Es}}(i\omega^{\mathrm{I}}) = \{&141.2202, 122.5207, 89.0107, 45.7447, 27.7132, 19.2897,\\ &14.6963, 11.8616, 9.9415, 8.5483, 7.4848, 6.6421,\\ &5.3832, 4.4828, 3.8054, 3.2777, 2.8561, 2.1041,\\ &1.6159, 1.0394, 0.7247, 0.3640, 0.2187\}\end{aligned}$$

C.4.11.2 EsH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Es,ref}} = 0.1135\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Es}} = 0.7985$$

$$\begin{aligned}\alpha^{\mathrm{Es}}(i\omega^{\mathrm{I}}) = \{&127.1191, 101.1672, 69.0945, 38.4335, 25.7934, 19.2100,\\ &15.2410, 12.5963, 10.7034, 9.2761, 8.1578, 7.2557,\\ &5.8873, 4.8979, 4.1504, 3.5677, 3.1025, 2.2754,\\ &1.7412, 1.1143, 0.7743, 0.3869, 0.2318\}\end{aligned}$$

C.4.11.3 $\mathrm{EsH_2}$

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Es,ref}} = 0.1914\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Es}} = 1.6077$$

$$\begin{aligned}\alpha^{\mathrm{Es}}(i\omega^{\mathrm{I}}) = \{&51.5499, 49.1952, 43.8725, 32.7274, 24.7931, 19.5486,\\ &15.9633, 13.3936, 11.4717, 9.9828, 8.7965, 7.8296,\\ &6.3506, 5.2757, 4.4628, 3.8295, 3.3245, 2.4294,\\ &1.8537, 1.1814, 0.8187, 0.4075, 0.2435\}\end{aligned}$$

C.4.11.4 $\mathrm{EsH_3}$

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Es,ref}} = 0.2550\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Es}} = 2.4859$$

$$\begin{aligned}\alpha^{\mathrm{Es}}(i\omega^{\mathrm{I}}) = \{&48.7142, 47.1908, 43.6761, 35.1176, 27.7849, 22.3133,\\ &18.3100, 15.3383, 13.0793, 11.3191, 9.9161, 8.7758,\\ &7.0434, 5.7984, 4.8676, 4.1505, 3.5844, 2.5952,\\ &1.9692, 1.2483, 0.8632, 0.4290, 0.2563\}\end{aligned}$$

C.4.11.5 $\mathrm{EsH_4}$

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Es,ref}} = 0.2969\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Es}} = 3.3091$$

$$\begin{aligned}\alpha^{\mathrm{Es}}(i\omega^{\mathrm{I}}) = \{&85.3607, 70.4284, 56.8604, 40.9584, 31.3950, 24.9037,\\ &20.2901, 16.9043, 14.3470, 12.3647, 10.7924, 9.5203,\\ &7.5995, 6.2294, 5.2114, 4.4310, 3.8176, 2.7517,\\ &2.0815, 1.3142, 0.9065, 0.4489, 0.2677\}\end{aligned}$$

C.4.11.6 EsH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Es,ref}} = 0.3268\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Es}} = 4.1146$$

$$\begin{aligned}\alpha^{\mathrm{Es}}(i\omega^{\mathrm{I}}) = \{&117.4576, 94.0369, 70.6831, 47.1236, 35.1066, 27.5008,\\ &22.2442, 18.4361, 15.5817, 13.3811, 11.6436, 10.2434,\\ &8.1401, 6.6487, 5.5461, 4.7042, 4.0450, 2.9043,\\ &2.1910, 1.3783, 0.9486, 0.4682, 0.2787\}\end{aligned}$$

C.4.11.7 EsH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Es,ref}} = 0.3471\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Es}} = 4.8927$$

$$\begin{aligned}\alpha^{\mathrm{Es}}(i\omega^{\mathrm{I}}) = \{&150.7635, 117.5979, 85.0999, 53.7332, 38.9845, 30.1309,\\ &24.1805, 19.9357, 16.7838, 14.3694, 12.4720, 10.9488,\\ &8.6702, 7.0621, 5.8775, 4.9758, 4.2715, 3.0573,\\ &2.3010, 1.4429, 0.9909, 0.4876, 0.2897\}\end{aligned}$$

C.4.12 Fermium

C.4.12.1 Fm

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Fm,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Fm}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Fm}}(i\omega^{\mathrm{I}}) = \{&134.5132, 117.3651, 86.0922, 44.8044, 27.3253, 19.0895,\\ &14.5665, 11.7578, 9.8460, 8.4541, 7.3900, 6.5464,\\ &5.2878, 4.3906, 3.7182, 3.1965, 2.7809, 2.0431,\\ &1.5662, 1.0052, 0.7001, 0.3517, 0.2116\}\end{aligned}$$

C.4.12.2 FmH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Fm,ref}} = 0.0986\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Fm}} = 0.8119$$

$$\begin{aligned}\alpha^{\mathrm{Fm}}(i\omega^{\mathrm{I}}) = \{&123.4198, 98.0796, 67.3261, 37.7049, 25.4442, 19.0089,\\ &15.0993, 12.4780, 10.5937, 9.1694, 8.0521, 7.1509,\\ &5.7858, 4.8017, 4.0608, 3.4851, 3.0267, 2.2145,\\ &1.6918, 1.0804, 0.7499, 0.3747, 0.2248\}\end{aligned}$$

C.4.12.3 FmH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Fm,ref}} = 0.1669\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Fm}} = 1.6382$$

$$\begin{aligned}\alpha^{\mathrm{Fm}}(i\omega^{\mathrm{I}}) = \{&49.2490, 47.1165, 42.3468, 32.0195, 24.4466, 19.3483,\\ &15.8217, 13.2749, 11.3611, 9.8750, 8.6897, 7.7238,\\ &6.2483, 5.1792, 4.3731, 3.7470, 3.2490, 2.3689,\\ &1.8049, 1.1480, 0.7947, 0.3954, 0.2366\}\end{aligned}$$

C.4.12.4 FmH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Fm,ref}} = 0.2230\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Fm}} = 2.5122$$

$$\begin{aligned}\alpha^{\mathrm{Fm}}(i\omega^{\mathrm{I}}) = \{&48.8290, 46.7101, 42.7342, 34.2569, 27.1850, 21.8935,\\ &17.9996, 15.0946, 12.8774, 11.1448, 9.7612, 8.6353,\\ &6.9236, 5.6936, 4.7749, 4.0677, 3.5103, 2.5374,\\ &1.9230, 1.2169, 0.8407, 0.4177, 0.2498\}\end{aligned}$$

C.4.12.5 FmH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Fm,ref}} = 0.2583\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Fm}} = 3.3309$$

$$\begin{aligned}\alpha^{\mathrm{Fm}}(i\omega^{\mathrm{I}}) = \{&89.9278, 70.7327, 55.9993, 40.2168, 30.9059, 24.5634,\\ &20.0342, 16.6976, 14.1706, 12.2082, 10.6501, 9.3888,\\ &7.4844, 6.1272, 5.1200, 4.3490, 3.7438, 2.6938,\\ &2.0351, 1.2826, 0.8838, 0.4375, 0.2611\}\end{aligned}$$

C.4.12.6 FmH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Fm,ref}} = 0.2846\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Fm}} = 4.1502$$

$$\begin{aligned}\alpha^{\mathrm{Fm}}(i\omega^{\mathrm{I}}) = \{&116.8174, 93.2645, 70.0509, 46.6547, 34.7568, 27.2346,\\ &22.0313, 18.2566, 15.4237, 13.2378, 11.5112, 10.1197,\\ &8.0302, 6.5502, 5.4575, 4.6245, 3.9729, 2.8478,\\ &2.1456, 1.3474, 0.9263, 0.4571, 0.2723\}\end{aligned}$$

C.4.12.7 FmH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Fm,ref}} = 0.3046\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Fm}} = 4.9727$$

$$\begin{aligned}\alpha^{\mathrm{Fm}}(i\omega^{\mathrm{I}}) = \{&135.6122, 112.6928, 83.8706, 53.3717, 38.7176, 29.9159,\\ &24.0013, 19.7799, 16.6433, 14.2394, 12.3499, 10.8330,\\ &8.5652, 6.9665, 5.7906, 4.8969, 4.1998, 3.0005,\\ &2.2553, 1.4119, 0.9688, 0.4767, 0.2835\}\end{aligned}$$

C.4.13 Mendelevium

C.4.13.1 Md

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Md,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Md}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Md}}(i\omega^{\mathrm{I}}) = \{&130.2072, 114.1115, 84.3233, 44.1736, 26.9220, 18.7618,\\ &14.2891, 11.5253, 9.6545, 8.2988, 7.2654, 6.4473,\\ &5.2262, 4.3528, 3.6953, 3.1826, 2.7725, 2.0398,\\ &1.5632, 1.0002, 0.6938, 0.3454, 0.2067\}\end{aligned}$$

C.4.13.2 MdH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Md,ref}} = 0.0678\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Md}} = 0.8302$$

$$\begin{aligned}\alpha^{\mathrm{Md}}(i\omega^{\mathrm{I}}) = \{&122.3584, 96.7486, 66.8293, 37.3575, 25.1065, 18.6943,\\ &14.8200, 12.2393, 10.3950, 9.0070, 7.9210, 7.0460,\\ &5.7195, 4.7603, 4.0351, 3.4690, 3.0165, 2.2102,\\ &1.6882, 1.0751, 0.7434, 0.3684, 0.2199\}\end{aligned}$$

C.4.13.3 MdH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Md,ref}} = 0.1158\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Md}} = 1.6730$$

$$\begin{aligned}\alpha^{\mathrm{Md}}(i\omega^{\mathrm{I}}) = \{&50.5776, 48.2323, 43.1075, 32.1978, 24.3574, 19.1618,\\ &15.6147, 13.0800, 11.1906, 9.7313, 8.5713, 7.6275,\\ &6.1860, 5.1392, 4.3475, 3.7302, 3.2377, 2.3633,\\ &1.8001, 1.1419, 0.7877, 0.3889, 0.2316\}\end{aligned}$$

C.4.13.4 MdH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Md,ref}} = 0.1537\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Md}} = 2.5241$$

$$\begin{aligned}\alpha^{\mathrm{Md}}(i\omega^{\mathrm{I}}) = \{&71.2250, 59.4086, 48.9788, 35.5944, 27.1964, 21.5384,\\ &17.5690, 14.6827, 12.5134, 10.8341, 9.5007, 8.4192,\\ &6.7772, 5.5953, 4.7088, 4.0230, 3.4795, 2.5235,\\ &1.9142, 1.2089, 0.8320, 0.4098, 0.2437\}\end{aligned}$$

C.4.13.5 MdH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Md,ref}} = 0.1790\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Md}} = 3.3654$$

$$\begin{aligned}\alpha^{\mathrm{Md}}(i\omega^{\mathrm{I}}) = \{&100.3385, 84.3364, 64.3830, 42.1401, 30.8494, 23.9709,\\ &19.3556, 16.0718, 13.6333, 11.7604, 10.2817, 9.0876,\\ &7.2842, 5.9936, 5.0301, 4.2876, 3.7012, 2.6742,\\ &2.0231, 1.2732, 0.8742, 0.4292, 0.2548\}\end{aligned}$$

C.4.14 Nobelium

C.4.14.1 No

$$\zeta_{\mathrm{EEQ}}^{\mathrm{No,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{No}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{No}}(i\omega^{\mathrm{I}}) = \{&124.8053, 110.0045, 82.1184, 43.5324, 26.6191, 18.5568,\\ &14.1262, 11.3883, 9.5372, 8.1977, 7.1779, 6.3711,\\ &5.1672, 4.3056, 3.6562, 3.1492, 2.7430, 2.0162,\\ &1.5427, 0.9830, 0.6791, 0.3356, 0.2000\}\end{aligned}$$

C.4.14.2 NoH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{No,ref}} = 0.0480\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{No}} = 0.8313$$

$$\begin{aligned}\alpha^{\mathrm{No}}(i\omega^{\mathrm{I}}) = \{&116.7644, 95.7311, 67.1224, 37.6423, 25.1783, 18.6618,\\ &14.7430, 12.1468, 10.3011, 8.9178, 7.8389, 6.9716,\\ &5.6589, 4.7104, 3.9930, 3.4327, 2.9844, 2.1846,\\ &1.6662, 1.0571, 0.7282, 0.3583, 0.2130\}\end{aligned}$$

C.4.14.3 NoH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{No,ref}} = 0.0865\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{No}} = 1.6766$$

$$\begin{aligned}\alpha^{\mathrm{No}}(i\omega^{\mathrm{I}}) = \{&50.1539, 47.9468, 42.8473, 32.0060, 24.1920, 19.0044,\\ &15.4660, 12.9435, 11.0681, 9.6229, 8.4760, 7.5438,\\ &6.1208, 5.0872, 4.3047, 3.6940, 3.2061, 2.3386,\\ &1.7789, 1.1246, 0.7730, 0.3791, 0.2249\}\end{aligned}$$

C.4.14.4 NoH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{No,ref}} = 0.1174\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{No}} = 2.5187$$

$$\begin{aligned}\alpha^{\mathrm{No}}(i\omega^{\mathrm{I}}) = \{&91.3664, 69.0315, 53.6426, 36.5348, 27.1761, 21.2644,\\ &17.2505, 14.3838, 12.2513, 10.6103, 9.3115, 8.2595,\\ &6.6624, 5.5111, 4.6451, 3.9732, 3.4392, 2.4962,\\ &1.8924, 1.1916, 0.8171, 0.3995, 0.2367\}\end{aligned}$$

C.4.14.5 NoH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{No,ref}} = 0.1411\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{No}} = 3.3606$$

$$\begin{aligned}\alpha^{\mathrm{No}}(i\omega^{\mathrm{I}}) = \{&124.2502, 93.6045, 66.8688, 42.1118, 30.4955, 23.5931,\\ &19.0154, 15.7804, 13.3884, 11.5558, 10.1109, 8.9447,\\ &7.1826, 5.9194, 4.9742, 4.2439, 3.6657, 2.6499,\\ &2.0034, 1.2571, 0.8603, 0.4195, 0.2481\}\end{aligned}$$

C.4.14.6 NoH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{No,ref}} = 0.1577\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{No}} = 3.6258$$

$$\begin{aligned}\alpha^{\mathrm{No}}(i\omega^{\mathrm{I}}) = \{&129.4476, 97.8022, 70.5399, 44.9645, 32.7583, 25.4115,\\ &20.4945, 17.0008, 14.4106, 12.4243, 10.8583, 9.5952,\\ &7.6891, 6.3255, 5.3072, 4.5217, 3.9009, 2.8126,\\ &2.1222, 1.3278, 0.9069, 0.4408, 0.2602\}\end{aligned}$$

C.4.14.7 NoH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{No,ref}} = 0.1718\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{No}} = 3.8556$$

$$\begin{aligned}\alpha^{\mathrm{No}}(i\omega^{\mathrm{I}}) = \{&134.8207, 102.1887, 74.4006, 47.9165, 35.0576, 27.2358,\\ &21.9653, 18.2071, 15.4170, 13.2771, 11.5910, 10.2322,\\ &8.1849, 6.7231, 5.6333, 4.7940, 4.1314, 2.9723,\\ &2.2389, 1.3973, 0.9527, 0.4619, 0.2722\}\end{aligned}$$

C.4.15 Lawrencium

C.4.15.1 Lr

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Lr,ref}} = 0.0000\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Lr}} = 0.0000$$

$$\begin{aligned}\alpha^{\mathrm{Lr}}(i\omega^{\mathrm{I}}) = \{&206.6533, 83.6937, 64.8432, 38.7234, 25.1567, 18.0960,\\ &14.0318, 11.4483, 9.6674, 8.3601, 7.3535, 6.5499,\\ &5.3380, 4.4612, 3.7954, 3.2730, 2.8533, 2.1000,\\ &1.6079, 1.0247, 0.7070, 0.3475, 0.2059\}\end{aligned}$$

C.4.15.2 LrH

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Lr,ref}} = 0.0505\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Lr}} = 0.8179$$

$$\begin{aligned}\alpha^{\mathrm{Lr}}(i\omega^{\mathrm{I}}) = \{&92.3161, 82.9674, 65.8156, 40.9485, 27.9903, 20.6982,\\ &16.1942, 13.1960, 11.0780, 9.5086, 8.3004, 7.3410,\\ &5.9115, 4.8952, 4.1354, 3.5468, 3.0786, 2.2487,\\ &1.7134, 1.0857, 0.7467, 0.3654, 0.2160\}\end{aligned}$$

C.4.15.3 LrH_2

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Lr,ref}} = 0.0890\,\mathrm{e}^{-}$$

$$\mathrm{CN}^{\mathrm{Lr}} = 1.6426$$

$$\begin{aligned}\alpha^{\mathrm{Lr}}(i\omega^{\mathrm{I}}) = \{&84.5082, 70.8844, 54.6074, 36.7023, 26.9876, 20.8760,\\ &16.7762, 13.8910, 11.7750, 10.1664, 8.9060, 7.8928,\\ &6.3660, 5.2713, 4.4497, 3.8123, 3.3054, 2.4078,\\ &1.8307, 1.1565, 0.7938, 0.3873, 0.2286\}\end{aligned}$$

C.4.15.4 LrH_3

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Lr,ref}} = 0.1191\,\mathrm{e}^-$$

$$\mathrm{CN}^{\mathrm{Lr}} = 2.4757$$

$$\begin{aligned}\alpha^{\mathrm{Lr}}(i\omega^{\mathrm{I}}) = \{&47.5131, 46.1745, 42.8145, 34.3869, 27.1100, 21.6792,\\ &17.7219, 14.8051, 12.6061, 10.9063, 9.5606, 8.4723,\\ &6.8249, 5.6415, 4.7538, 4.0661, 3.5201, 2.5565,\\ &1.9394, 1.2216, 0.8370, 0.4074, 0.2401\}\end{aligned}$$

C.4.15.5 LrH_4

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Lr,ref}} = 0.1409\,\mathrm{e}^-$$

$$\mathrm{CN}^{\mathrm{Lr}} = 3.2166$$

$$\begin{aligned}\alpha^{\mathrm{Lr}}(i\omega^{\mathrm{I}}) = \{&242.4220, 51.7872, 46.2957, 36.7862, 29.2534, 23.5192,\\ &19.2598, 16.0852, 13.6785, 11.8139, 10.3373, 9.1439,\\ &7.3415, 6.0511, 5.0865, 4.3417, 3.7520, 2.7155,\\ &2.0549, 1.2901, 0.8821, 0.4281, 0.2519\}\end{aligned}$$

C.4.15.6 LrH_5

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Lr,ref}} = 0.1574\,\mathrm{e}^-$$

$$\mathrm{CN}^{\mathrm{Lr}} = 3.9996$$

$$\begin{aligned}\alpha^{\mathrm{Lr}}(i\omega^{\mathrm{I}}) = \{&143.6357, 96.0464, 68.6157, 45.5605, 33.9675, 26.5910,\\ &21.4849, 17.7938, 15.0382, 12.9231, 11.2596, 9.9227,\\ &7.9178, 6.4947, 5.4384, 4.6276, 3.9889, 2.8735,\\ &2.1677, 1.3559, 0.9251, 0.4478, 0.2631\}\end{aligned}$$

C.4.15.7 LrH_6

$$\zeta_{\mathrm{EEQ}}^{\mathrm{Lr,ref}} = 0.1708\,\mathrm{e}^-$$

$$\mathrm{CN}^{\mathrm{Lr}} = 4.7792$$

$$\begin{aligned}\alpha^{\mathrm{Lr}}(i\omega^{\mathrm{I}}) = \{&176.3109, 122.3955, 83.0181, 51.6133, 37.3991, 28.8828,\\ &23.1675, 19.1031, 16.0971, 13.8031, 12.0055, 10.5648,\\ &8.4103, 6.8854, 5.7561, 4.8910, 4.2107, 3.0257,\\ &2.2783, 1.4216, 0.9685, 0.4678, 0.2746\}\end{aligned}$$

D EEQ

D.1 AcQM

For the parameterization of the EEQ model, a set of actinide structures called AcQM was created. The set contains in total 2537 structures. The first part of 1283 structures contain realistic actinide complexes that were created using the Architector combined with our ArchitectorWrapper package, as described in our LnQM set. The structures were generated with only stable oxidation states of the central actinide with coordination numbers ranging from four to 10. The second part contains 1254 structures of smaller hydrides, fluorides, chlorides, oxides, and sulfides and various mindless structures with elements across the first five periods of the periodic table – all of those have coordination numbers ranging from one to 8. The AcQM set can be found on our GitHub (`https://github.com/grimme-lab/acqm`). For every structure, the system charge is given in the `.CHRG` file and the number of unpaired electrons in the `.UHF` file. The Hirshfeld population analysis partial charges are given in the `hirshfeld.apc` file.

D.2 Loss Function

$$f_{\text{err}} = \underbrace{\frac{5}{4}(1-|\rho_{\{q_{\text{EEQ}}\},\{q_{\text{ref}}\}}|)}_{\text{Pearson corr. coeff.}} + \underbrace{\frac{3}{5}\frac{1}{n}\sum_{i=1}^{n}|e_i|}_{\text{MAE}} + \underbrace{|\frac{1}{n}\sum_{i=1}^{n}e_i|}_{\text{ME}} \tag{8}$$

D.3 Parameters

Table 2 Parameters for the EEQ model. The four parameters per element A include the atomic electronegativity EN_A, atomic hardness terms J_{AA}, element-specific scaling parameter κ_A, and atomic van der Waals radii a_A.

Element A	EN_A	J_{AA}	κ_A	a_A
Ac	1.0458	-0.0007	0.0047	1.2226
Th	1.0989	-0.0017	0.0159	1.2874
Pa	1.0721	-0.0013	0.0037	1.4443
U	1.0982	-0.0010	0.0042	1.2903
Np	1.1090	-0.0009	0.0071	1.4101
Pu	1.0104	-0.0011	0.0049	1.2550
Am	1.0010	-0.0013	0.0051	1.1518
Cm	1.1100	-0.0010	0.0071	1.4201
Bk	1.1683	-0.0010	0.0046	1.4396
Cf	1.0089	-0.0010	0.0039	1.2857
Es	1.0593	-0.0011	0.0030	1.3502
Fm	1.0767	-0.0010	0.0040	1.3301
Md	1.1131	-0.0006	0.0055	1.3075
No	1.1434	-0.0001	0.0135	1.2653
Lr	1.1371	-0.0014	0.0068	1.3407

E Relativistic effects

The influence of the relativistic effects on geometries and dynamic purely-imaginary frequency polarizabilities of the reference structures was investigated and is shown in the following for the actinium hydrides.

E.1 Geometries

The geometries of $AcH_{1\text{-}6}$ were optimized using ZORA PBE0/ZORA-def2-TZVP (SARC-ZORA-TZVP for actinium) and PBE0/def2-TZVP and compared. The resulting geometries deviate only marginally from each other.
It should be noted that PaH_2, NpH_2, and CfH_4 were optimized with ZORA corrections since the non-corrected DFT calculations resulted in highly symmetric structures that possessed desymmetrizing imaginary frequencies.

Table 3 RMSD of $AcH_{1\text{-}6}$ geometries obtained with (ZORA, PBE0/ZORA-def2-TZVP) and without (PBE0/def2-TZVP) relativistic corrections.

Structure	RMSD
AcH	0.00032
AcH_2	0.00136
AcH_3	0.00099
AcH_4	0.00479
AcH_5	0.00502
AcH_6	0.00155

E.2 Dynamic Purely-Imaginary Frequency Polarizabilities

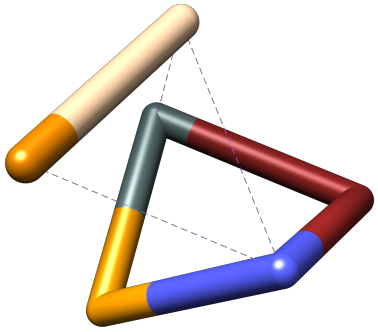
For the calculation of the dynamic purely-imaginary frequency polarizabilities, the same procedure is used as described in the main manuscript. However, for the relativistic approach, ZORA using ZORA-def2-TZVP (SARC-ZORA-TZVP for the actinide) is used. We find only small deviations upon using relativistic corrections, which are negligible for the use in the D3 and D4 schemes.

Table 4 Deviation of dynamic purely-imaginary frequency polarizabilities of $AcH_{1\text{-}6}$ obtained with (PBE0/ZORA-def2-TZVP) and without (PBE0/def2-TZVP) relativistic corrections.

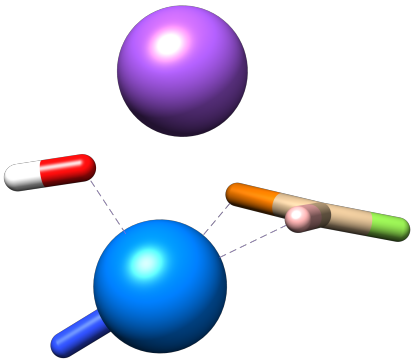
ω^{I}	AcH	AcH_2	AcH_3	AcH_4	AcH_5	AcH_6
0.000001	15.35	8.81	0.91	3.80	1.62	1.60
0.05	9.15	4.49	0.72	0.69	0.98	1.14
0.10	2.47	1.20	0.29	0.12	0.14	0.24
0.20	-1.03	-0.77	-0.56	-0.58	-0.81	-0.79
0.30	-1.31	-1.23	-0.99	-0.94	-1.17	-1.13
0.40	-1.17	-1.26	-1.11	-1.04	-1.24	-1.17
0.50	-0.99	-1.16	-1.07	-1.00	-1.16	-1.09
0.60	-0.83	-1.02	-0.97	-0.91	-1.04	-0.97
0.70	-0.71	-0.89	-0.86	-0.80	-0.91	-0.85
0.80	-0.61	-0.77	-0.75	-0.70	-0.79	-0.74
0.90	-0.54	-0.68	-0.67	-0.62	-0.69	-0.65
1.00	-0.48	-0.60	-0.59	-0.55	-0.61	-0.57
1.20	-0.41	-0.50	-0.48	-0.44	-0.48	-0.45
1.40	-0.36	-0.42	-0.41	-0.38	-0.40	-0.38
1.60	-0.33	-0.38	-0.35	-0.33	-0.34	-0.32
1.80	-0.30	-0.34	-0.32	-0.30	-0.30	-0.29
2.00	-0.29	-0.31	-0.29	-0.27	-0.27	-0.26
2.50	-0.26	-0.27	-0.25	-0.23	-0.23	-0.22
3.00	-0.23	-0.24	-0.22	-0.21	-0.20	-0.20
4.00	-0.19	-0.19	-0.17	-0.17	-0.16	-0.16
5.00	-0.16	-0.15	-0.14	-0.13	-0.13	-0.13
7.50	-0.10	-0.10	-0.09	-0.08	-0.08	-0.08
10.00	-0.07	-0.06	-0.06	-0.06	-0.06	-0.06
ME	0.72	0.14	-0.37	-0.22	-0.36	-0.33
MAE	1.62	1.12	0.53	0.62	0.60	0.59
MAX	15.35	8.81	1.11	3.80	1.62	1.60

F Mindless Structures in the AcQM

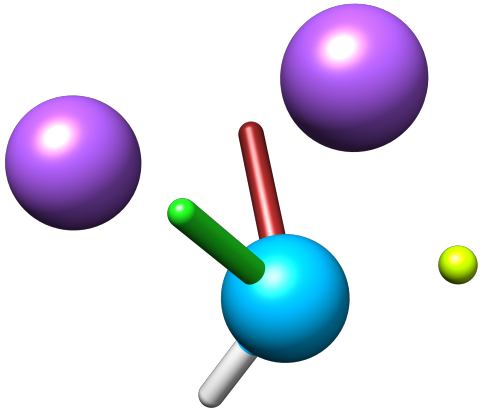
In the following, some examples of mindless structures in the AcQM are shown.



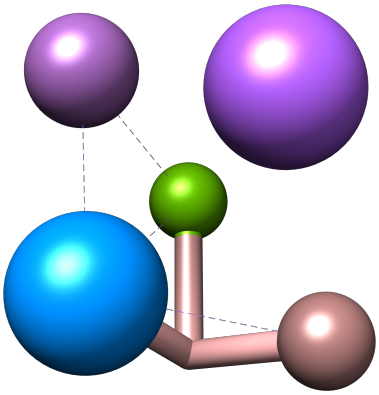
(a) $AmSiSnSeTeBr^{2+}$



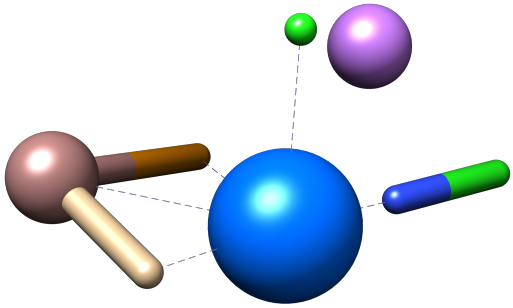
(b) $NpNaBNPHOFC^{-}$



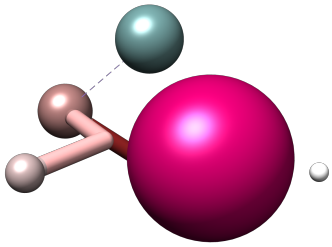
(c) $ThNaBeClBrHNa^{+}$



(d) UNaMgBInSb



(e) $PuInCNTeCl_2Li^{+}$



(f) $LrHBAlInGeBr^{2+}$

Fig. 1 Examples of mindless structures contained within the AcQM.