Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY INFORMATION

Crystal structure, hydrogen bonding, mechanical properties and Raman spectrum of the lead uranyl silicate monohydrate mineral kasolite

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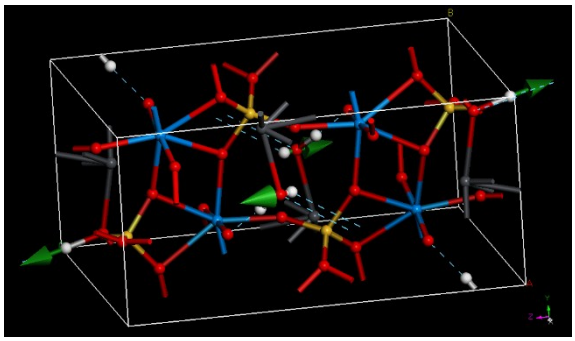
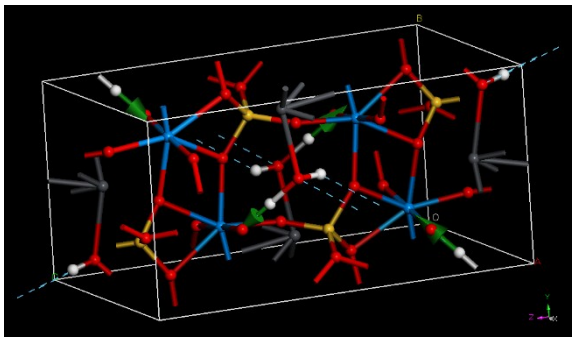
Figure S.1. The atomic motions associated to some Raman active vibrational normal modes of kasolite. Color code: U-blue; Si-brown; Pb-yellow; O-red.; H-white.

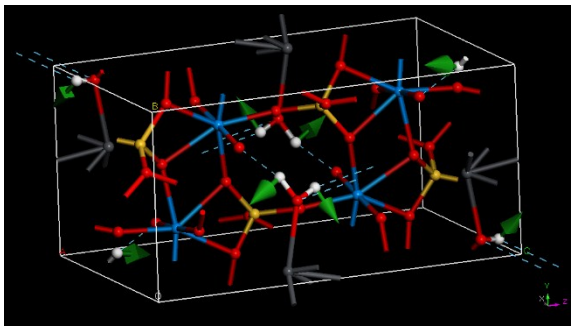
- Mode $\nu =$ 3540.5 cm^{-1} – $\nu(OH)$ – OH bond stretching.



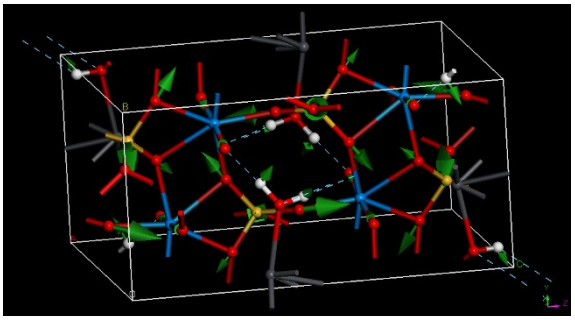
- Mode $\nu =$ 3173.7 cm^{-1} – $\nu(OH)$ – OH bond stretching.



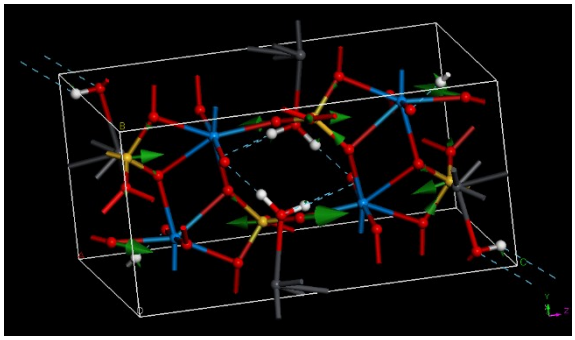
- Mode $\nu =$ 1578.3 cm^{-1} – $\delta(HOH)$ – Water HOH bending.



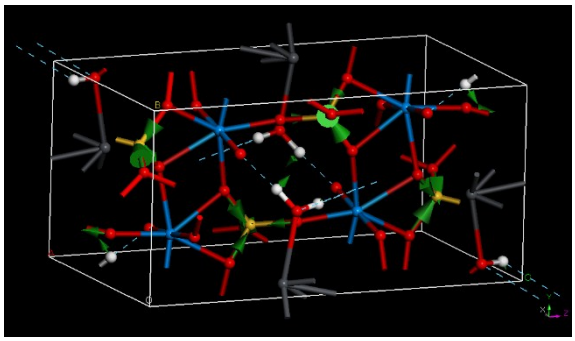
- Mode $\nu =$ 939.7 cm^{-1} – $\nu^{s}\left(SiO^{4-}_{4}\right) + \nu^{a}\left(UO^{2+}_{2}\right)$ – Symmetric silicate stretching and antisymmetric uranyl stretching.



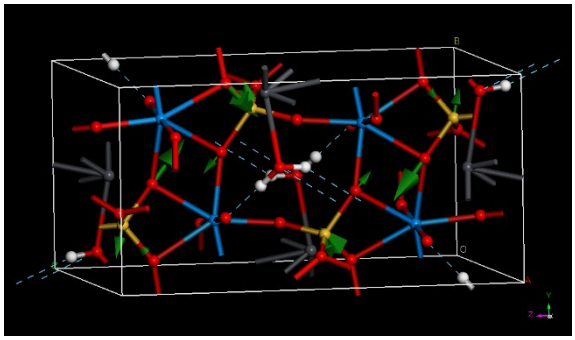
- Mode $\nu =$ 882.4 cm^{-1} – $\nu^{a}\left(SiO_{4}^{4-}\right)$ – Asymmetric silicate stretching.



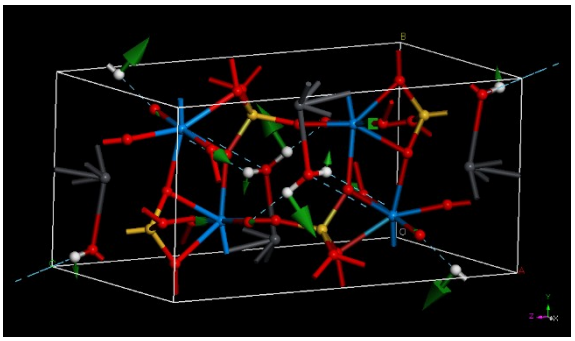
- Mode $\nu =$ 855.3 cm^{-1} – $\nu^{s}\left(SiO_{4}^{4-}\right) + l(H_2O)$ – Symmetric silicate stretching and water librations.



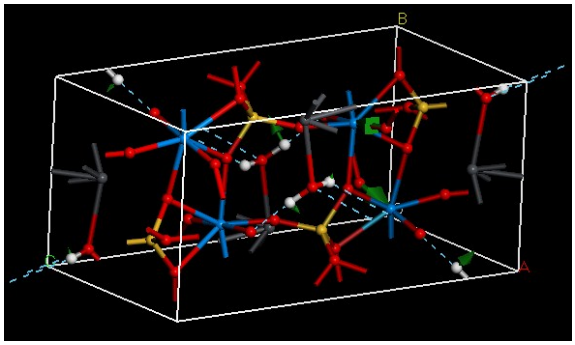
- Mode $\nu =$ 793.1 cm^{-1} – $\nu^{a}\left(SiO_{4}^{4-}\right)$ – Asymmetric silicate stretching.



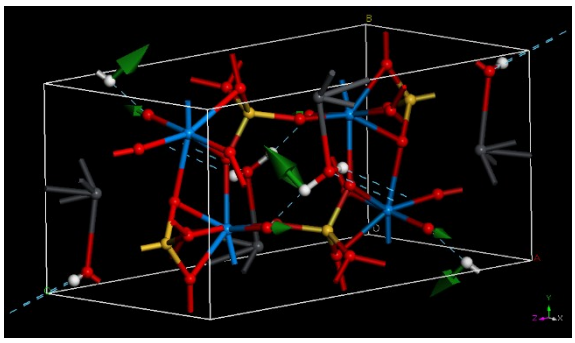
- Mode $\nu =$ 762.8 cm^{-1} – $\nu\left(UO_{2}^{2+}\right) + l(H_2O)$ – Uranyl UO bond stretching and water librations.



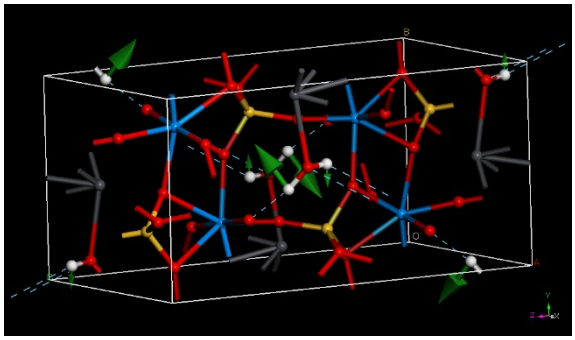
- Mode $\nu =$ 750.4 cm^{-1} – $\nu\left(UO_2^{2+}\right) + l(H_2O)$ – Uranyl UO bond stretching and water librations.



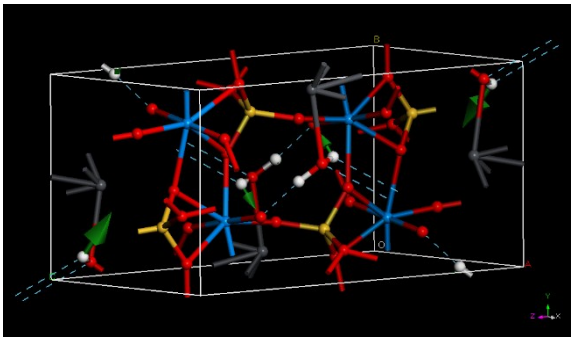
- Mode $\nu =$ 723.3 cm^{-1} – $\nu\left(UO_2^{2+}\right) + l(H_2O)$ – Uranyl UO bond stretching and water librations.



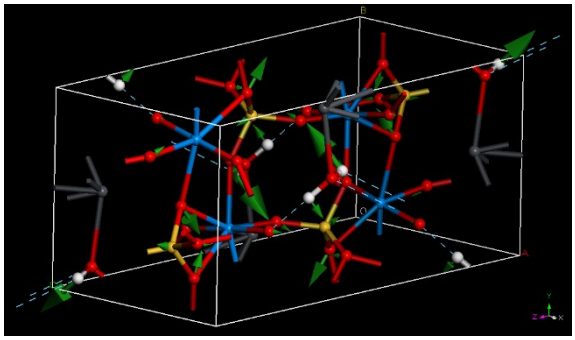
- Mode $\nu =$ 683.2 cm^{-1} – $l(H_2O)$ – Water librations.



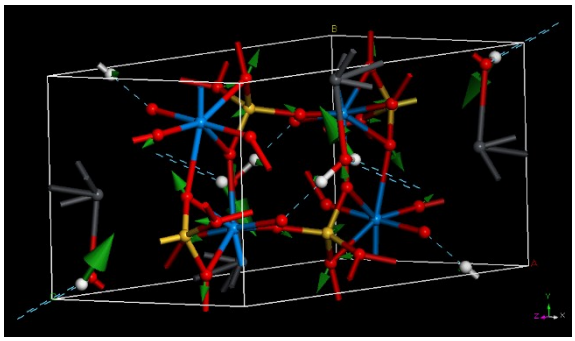
- Mode $\nu =$ 583.5 cm^{-1} – $l(H_2O)$ – Water librations.



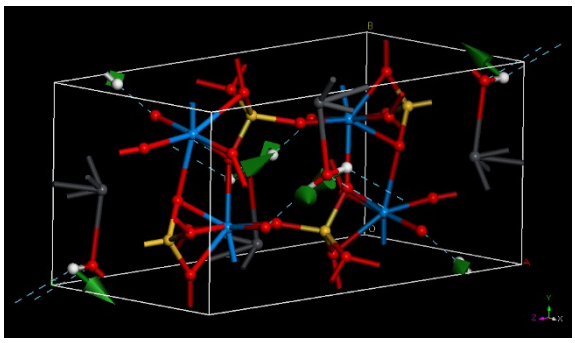
- Mode $\nu =$ 554.2 cm^{-1} – $\nu\left(UO_2^{2+}\right) + \nu(UO_{eq}) + \gamma\left(SiO_4^{4-}\right) + l(H_2O)$ – Uranyl and equatorial UO stretchings, silicate deformations and water librations.



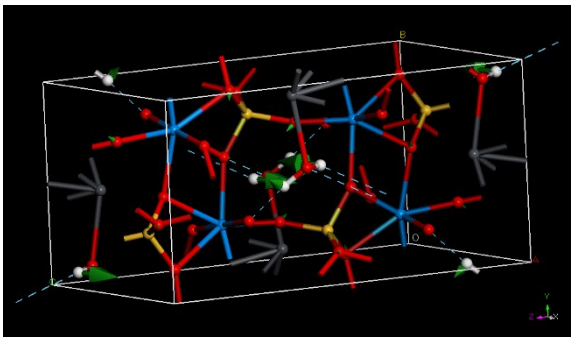
- Mode $\nu =$ 529.5 cm^{-1} – $\nu(UO_{eq}) + \gamma\left(SiO_4^{4-}\right) + l(H_2O)$ – Equatorial UO stretching, silicate deformations and water librations.



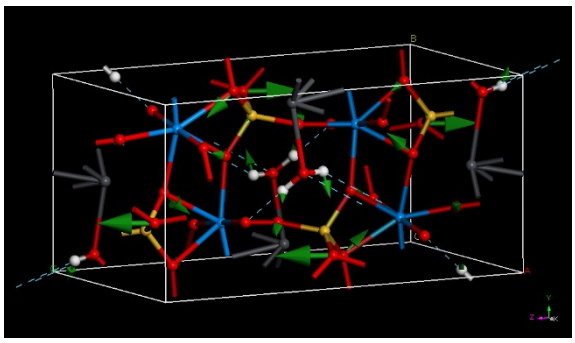
- Mode $\nu =$ 485.0 cm^{-1} – $l(H_2O)$ – Water librations.



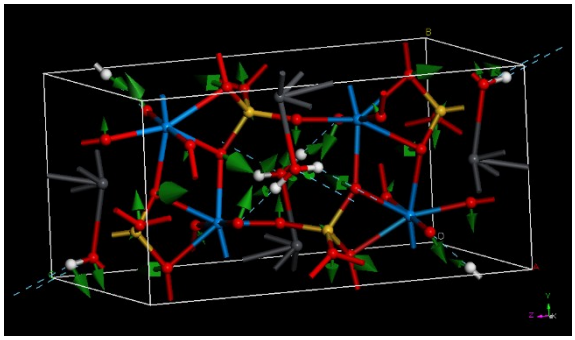
- Mode $\nu =$ 467.2 cm^{-1} – $l(H_2O)$ – Water librations.



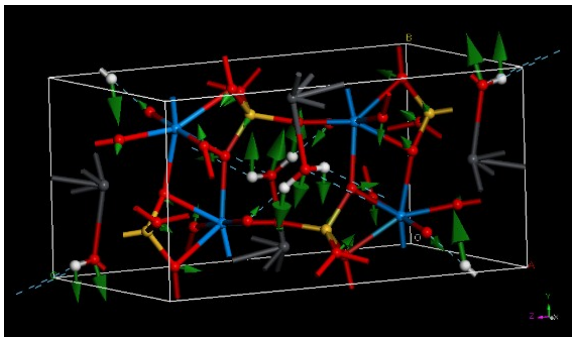
- Mode $\nu =$ 400.8 cm^{-1} – $\delta(OSiO) + l(H_2O)$ – Silicate OSiO bending and water librations.



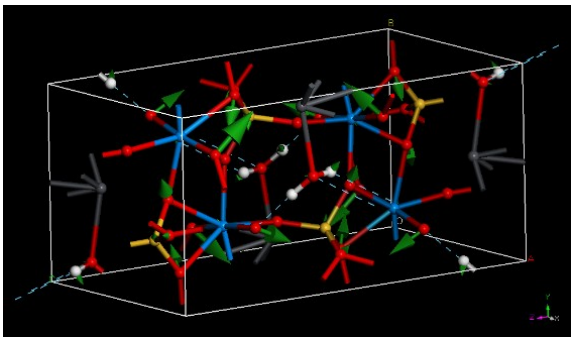
- Mode $\nu =$ 339.3 cm^{-1} – $\rho\left(UO_2^{2+}\right) + w(OUO_{eq}) + t(OUO_{eq}) + \gamma\left(SiO_4^{4-}\right) + l(H_2O)$ – Uranyl rotation, equatorial OUO wagging and twisting, silicate deformations and water librations.



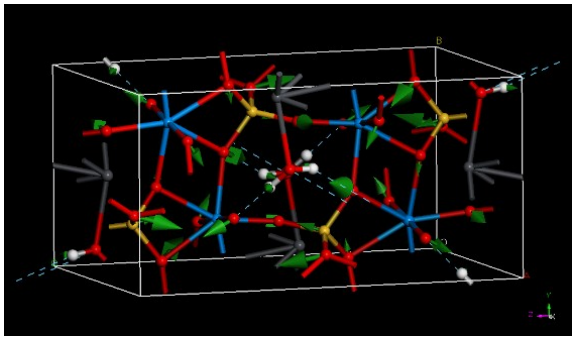
- Mode $\nu =$ 303.1 cm^{-1} – $\delta\left(UO_2^{2+}\right) + \delta^{op}(UO_{eq}) + \gamma\left(SiO_4^{4-}\right) + T(H_2O)$ – Uranyl and out of equatorial plane UO bending, silicate deformations and water translations.



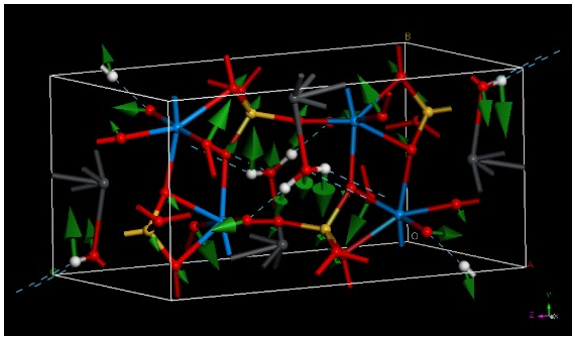
- Mode $\nu =$ 283.4 cm^{-1} – $\delta\left(UO_2^{2+}\right) + t(OUO_{eq}) + l(H_2O)$ – Uranyl bending, equatorial OUO twisting and water librations.



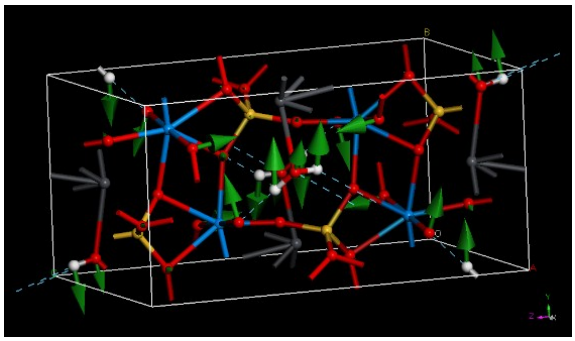
- Mode $\nu =$ 246.3 cm^{-1} – $\rho\left(UO_2^{2+}\right) + w(OUO_{eq}) + l(H_2O)$ – Uranyl rotation, equatorial OUO wagging and water librations.



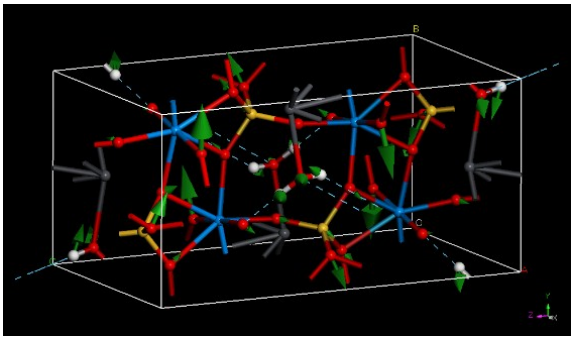
- Mode $\nu =$ 232.9 cm^{-1} – $\gamma\left(UO_2^{2+}\right) + T\left(SiO_4^{4-}\right) + T(H_2O)$ – Uranyl deformation and silicate and water translations.



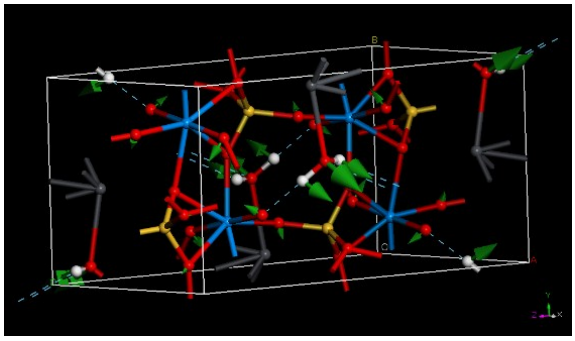
- Mode $\nu =$ 221.3 cm^{-1} – $\gamma\left(UO_2^{2+}\right) + T(H_2O)$ – Uranyl deformation and water translations.



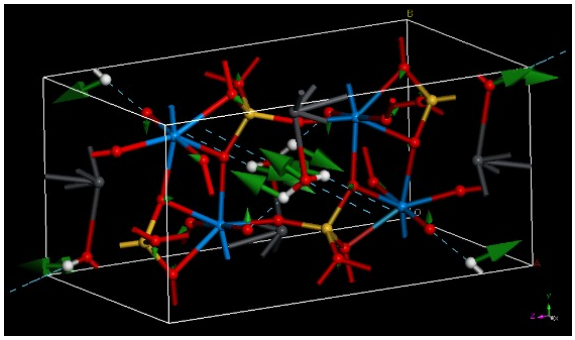
- Mode $\nu =$ 221.0 cm^{-1} – $\gamma\left(UO_2^{2+}\right) + \gamma\left(SiO_4^{4-}\right) + T(H_2O)$ – Uranyl and silicate deformations and water translations.



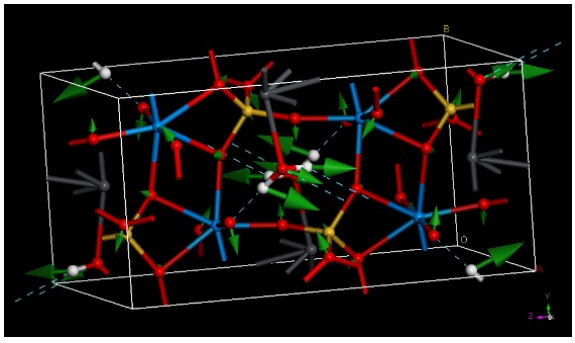
- Mode $\nu =$ 197.9 cm^{-1} – $\rho\left(UO^{2+}_{2}\right) + \delta(UOSi) + T(H_2O)$ – Uranyl rotation, USiO bending and water translations.



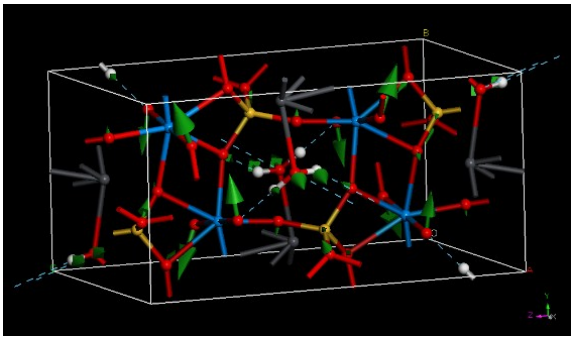
- Mode $\nu =$ 191.6 cm^{-1} – $\gamma\left(UO^{2+}_{2}\right) + \delta(UOSi) + T(H_2O)$ – Uranyl deformation, USiO bending and water translations.



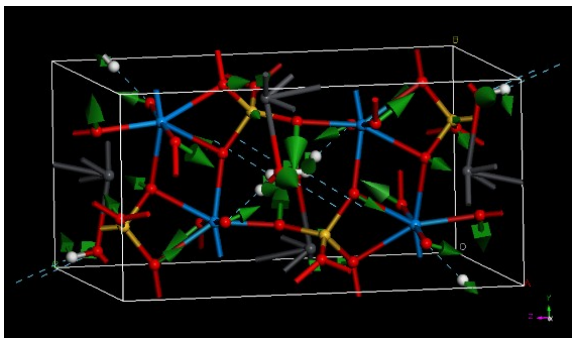
- Mode $\nu =$ 185.3 cm^{-1} – $\rho\left(UO^{2+}_{2}\right) + w(OUO_{eq}) + t(OUO_{eq}) + \gamma\left(SiO^{4-}_{4}\right) + T(H_2O)$ – Uranyl rotation, equatorial OUO wagging and twisting, silicate deformation and water translations.



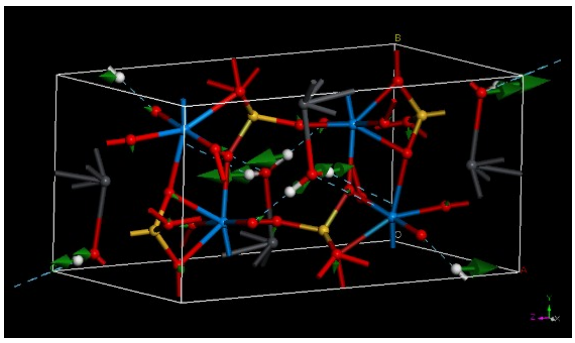
- Mode $\nu =$ 182.9 cm^{-1} – $\rho\left(UO^{2+}_{2}\right) + T(H_2O)$ – Uranyl rotation and water translations.



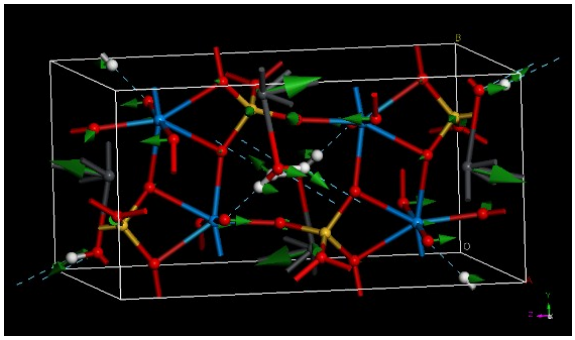
- Mode $\nu =$ 146.1 cm^{-1} – $\rho\left(UO_2^{2+}\right) + \delta^{op}\left(UO_{eq}\right) + T(H_2O)$ – Uranyl rotation, out of equatorial plane UO bending and water translations.



- Mode $\nu =$ 143.8 cm^{-1} – $T(H_2O)$ – Water translations.



- Mode $\nu =$ 90.6 cm^{-1} – $\nu(PbO) + T\left(UO_2^{2+}\right) + T(SiO) + T(H_2O)$ – PbO stretching and uranyl, SiO and water translations.



- Mode $\nu =$ 53.6 cm^{-1} – $\nu(PbO) + \gamma\left(UO_2^{2+}\right) + T(H_2O)$ – PbO stretching, uranyl deformation and water translations.

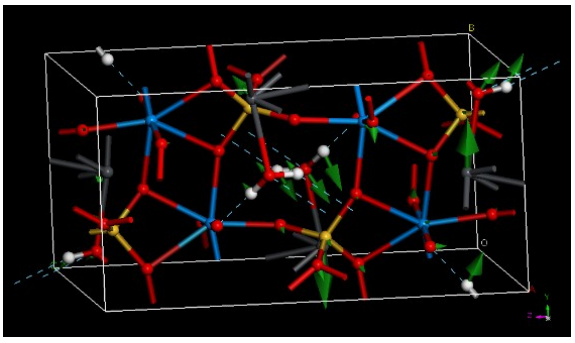


Figure S.2. Resolution of the composite bands in the experimental Raman spectrum of kasolite mineral into single band contributions (A) Region: 840-950 cm^{-1}; (B) Region: 710-840 cm^{-1}; (C) Region: 520-580 cm^{-1}; (D) Region: 390-510 cm^{-1}; (E) Region: 275-310 cm^{-1}; (F) Region: 180-210 cm^{-1}; (G) Region: 150-180 cm^{-1}; (H) Region: 90-110 cm^{-1}.