Electronic Supplementary Information (ESI)*

Borohydrides oxidation by photoexcited $[UO_2(CO_3)_3]^{4-}$

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*Note after publication:

Originally-published Fig.S4 contained the structure and the spin density of the lowest triplet state of the wrong adduct $[(UO_2(CO_3)_3^{4-})(BH_3\mathbf{NC}^-)]$ instead of the correct $[(UO_2(CO_3)_3^{4-})(BH_3\mathbf{CN}^-)]$. Now, Fig.S4 has been replaced with correct figure. The structures and spin densities of the above two adducts are very similar and this change does not alter any discussions in the main text. The ESI was updated and republished on 05/06/2019. The authors apologize for this error and inconvenience to the readers.

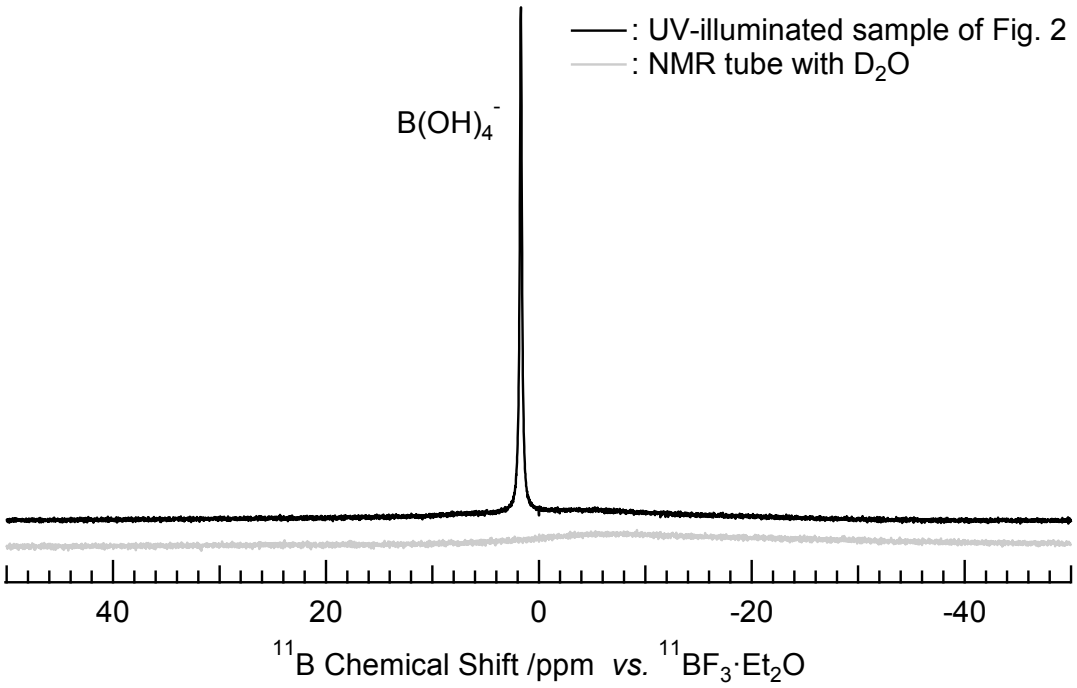

Fig. S1. ^{11}B NMR spectrum of the sample solution of Fig. 2 after UV-illumination together with that of a borosilicate NMR tube with D_2O.

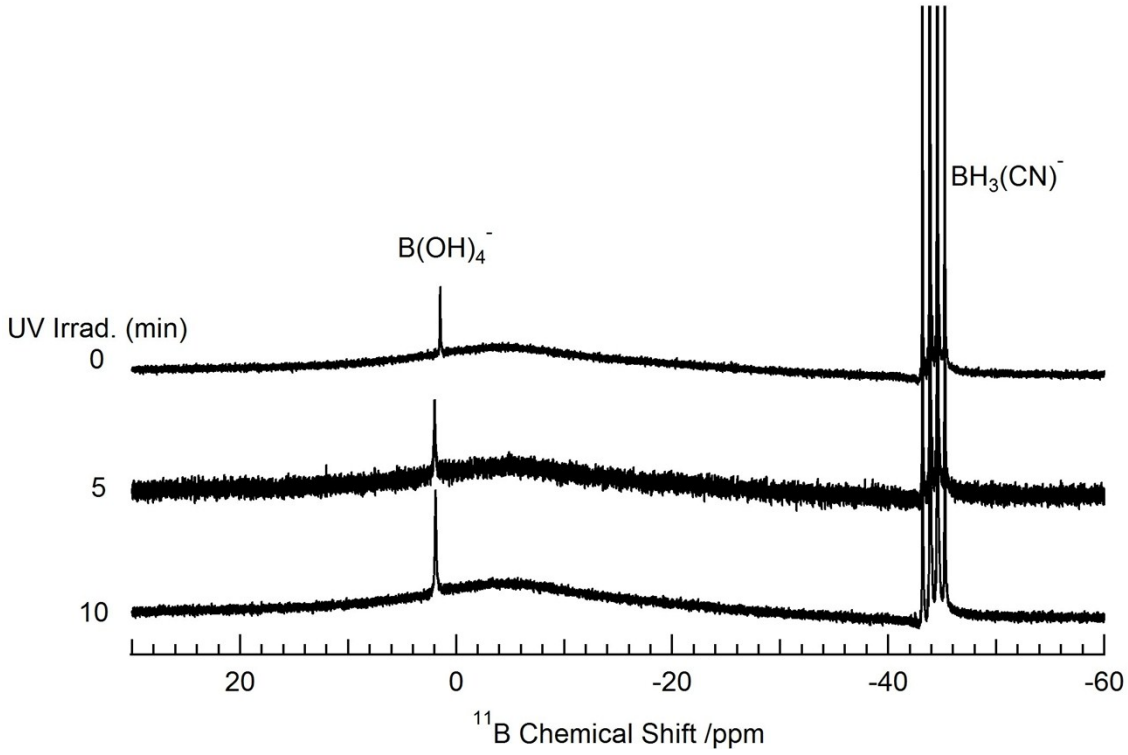

Fig. S2. ^{11}B NMR spectra of the sample solution of Fig. 4 at different UV irradiation time. $B(OH)_4^-$ as an impurity in $NaBH_3CN$ (Purity: 98.5 mol%) was also present in the initial state. The broad band centred at −5 ppm arises from a borosilicate NMR tube (see Fig. S1).

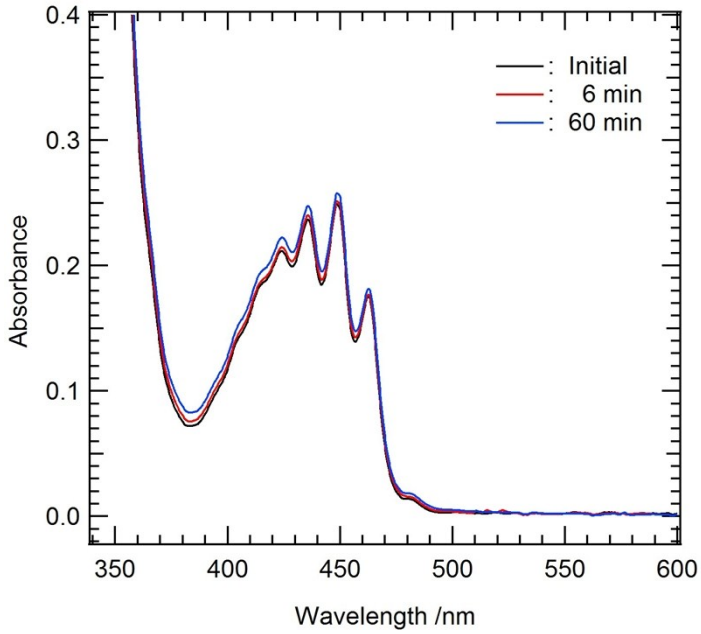

Fig. S3. UV-vis absorption spectra of aqueous solution containing $[U^{VI}O_2(CO_3)_3]^{4-}$ (10.3 mM), Na_2CO_3 (0.960 M), and $NaBH_3CN$ (0.693 M) at different time. The sample solution was held at 70°C in the dark.

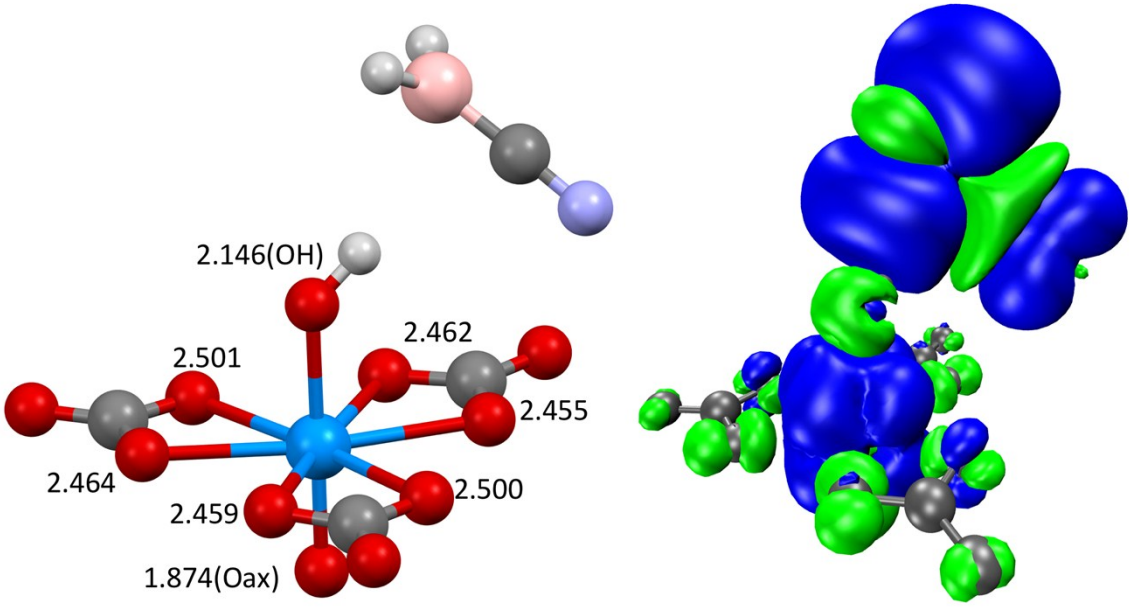

Fig. S4. Optimized structure (left) and spin density α–β (right) of the lowest triplet state of the uranyl triscarbonate-cyanoborohydride adduct. Hydrogen abstraction by photoexcited $[UO_2(CO_3)_3]^{4-}$ and charge transfer is observed as similar to borohydride system (Fig. 5). Distances from uranium are shown in Å. Isovalue of the surface is 0.0003 a.u.