Supporting Information:

Is the protactinium(V) mono-oxo bond weaker than what we thought?

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Table S1: Integrated crystal orbital bond indices (ICOBIs)[S1] obtained at the optimized structures (see Tables 1 and 2). Mean values are reported when related bonds are crystallography independent.

$[C_8H_{20}N]_2[PaOCl_5]$	Pa–O	Pa–Cl$_{ax}$	Pa–Cl$_{eq}$
PBE+D3(BJ)	2.24	0.98	0.81

$(C_4H_{12}N_2)[UO_2Cl_4]$	U–O$_{yl}$		U–Cl
PBE+D3(BJ)	2.17		0.85

$(C_4H_{12}N_2)_2[UO_2Cl_4(H_2O)]Cl_2$	U–O$_{yl}$	U–O$_w$	U–Cl
PBE+D3(BJ)	2.32	0.36	0.63

For assessing the impact of the "environment", bare $[PaO]^{3+}$ and $[UO_2]^{2+}$ systems have been optimized at the PBE level within large cubic boxes, ensuring more than $10\,\text{Å}$ of distance between two molecular units. The resulting bond distances were 1.822 and 1.811 Å, respectively, together with ICOBIs of 2.97 and 2.66. These values serve as references to assess the impact of coordination in the crystal structures on the bonding of the $[PaO]^{3+}$ and $[UO_2]^{2+}$ subunits. This impact on bonding, referred to as ΔICOBI, was found to be -0.73 for $[PaO]^{3+}$ in $[C_8H_{20}N]_2[PaOCl_5]$ and -0.49 and -0.34 in $(C_4H_{12}N_2)[UO_2Cl_4]$ and $(C_4H_{12}N_2)_2[UO_2Cl_4(H_2O)]Cl_2$, respectively.

Note that the ICOBI is larger in $(C_4H_{12}N_2)_2[UO_2Cl_4(H_2O)]Cl_2$ than in $(C_4H_{12}N_2)[UO_2Cl_4]$ by 0.15, corroborating the water-induced effective bond reinforcement observed by Rajapaksha et al.[S15]. This bond reinforcement is concomitant with a reduction of the U–Cl ICOBI, meaning that it is in fact indirect: by weakening the in-plane bonds with water addition, the uranyl bonds are effectively less destabilized, thus appearing reinforced.

Note that the valence 7p levels of Pa and U are omitted from the ICOBI analysis by absence of such basis functions in the used program[S16] (the procedure requires projection of the plane waves onto a localized basis). Since these atomic levels only have a limited impact on bonding, their omission does not significantly affect our analysis.

Table S2: Benchmark of ten exchange-correlation (XC) functionals based on the Abinit code[S2] for selected protactinium molecular systems. Only the Pa–O bond distance (Å) is reported.

XC functional	$[PaO]^{3+}$	$PaOF_3(H_2O)_3$	$[PaO(C_2O_4)_3]^{3-}$
PW91[S17]	1.710	1.817	1.851
LDA (Wigner)[S18]	1.723	1.832	1.867
PBE[S19]	1.722	1.833	1.869
HTCH93[S20]	1.710	1.813	1.842
HTCH120[S21]	1.710	1.814	1.847
HTCH147[S21]	1.710	1.813	1.845
HTCH407[S22]	1.708	1.811	1.848
GGA (Wu)[S23]	1.715	1.824	1.860
HTBS[S24]	1.743	1.865	1.887
MOHLYP[S25]	1.730	1.842	1.874

Table S3: Role of implicit solvation (C-PCM[S3]) on the Pa–O bond distance (Å) obtained with Gaussian[S4] and the default radii (UFF[S5]).

[PaO]$^{3+}$	Gas phase	C-PCM
B3PW91[S26]	1.689	1.759
B3LYP[S27]	1.697	1.771
PBE[S19]	1.717	1.782
PBE0[S10]	1.681	1.752
PBE0+D3(BJ)[S10,S28]	1.681	1.752
MP2[S29]	1.714	1.766

[PaO(C$_2$O$_4$)$_3$]$^{3-}$	Gas phase	C-PCM
B3PW91[S26]	1.850	1.856
B3LYP[S27]	1.862	1.867
PBE[S19]	1.874	1.881
PBE0[S10]	1.843	1.849
PBE0+D3(BJ)[S10,S28]	1.844	1.849
MP2[S29]	1.857	1.857

The def2-TZVP basis sets[S30] were used on all atoms except for Pa, which was treated with the ECP60MWB energy-consistent pseudopotential[S31] along with its corresponding segmented basis set.[S32] Overall, a bond lengthening of $\sim 0.07\,\text{Å}$ is observed for [PaO]$^{3+}$ and $\sim 0.006\,\text{Å}$ for [PaO(C$_2$O$_4$)$_3$]$^{3-}$, respectively. Notably, there was minimal variation when changing the underlying electronic structure theory method.

Additionally, calculations were conducted in the gas phase using Molpro,[S33] yielding a scalar-relativistic CCSD(T)[S34] value of $1.703\,\text{Å}$ for [PaO]$^{3+}$. The MP2 and B3LYP calculations were also repeated for cross-checking, leading with this setup to 1.714 and $1.698\,\text{Å}$, respectively; values which are identical to those obtained using the Gaussian software.

Table S4: Role of implicit solvation (COSMO[S6]) on the Pa−O bond distance (Å) obtained with ADF[S7] and the default radii.[S8] The ZORA[S9] Hamiltonian was used. Values in red are reported from the main text for convenience.

$[PaO]^{3+}$	Relativity	Gas phase	COSMO
B3LYP[S27]	Scalar	1.705	1.729
	Spin-orbit	1.707	1.731
PBE0[S10]	Scalar	1.688	1.710
	Spin-orbit	1.690	1.713

$[PaO(C_2O_4)_3]^{3-}$	Relativity	Gas phase	COSMO
B3LYP[S27]	Scalar	1.871	1.878
	Spin-orbit	1.873	1.881
PBE0[S10]	Scalar	1.852	1.858
	Spin-orbit	1.854	1.862

The TZ2P basis sets[S13] were used on all atoms. By comparing Table S3 and Table S4, it is clear that the COSMO model leads to a lesser impact of solvation on the Pa-O bond distance than the C-PCM one. Test calculations have shown that this is essentially due to the use of the default UFF radii (rescaled by the 1.1 default α value). Despite this moderate discrepancy, the previous trend holds (solvation-induced bond lengthening).

Table S5: Role of implicit solvation (COSMO[S6]) on the U–O bond distance(s) (Å) obtained with ADF[S7] and the default radii. The ZORA[S9] Hamiltonian was used. Values in red are reported from the main text for convenience.

$[UO_2]^{2+}$	Relativity	Gas phase	COSMO
PBE0[S10]	Scalar	1.684	1.702
	Spin-orbit	1.687	1.705

$[UO_2Cl_4]^{2-}$	Relativity	Gas phase	COSMO
PBE0[S10]	Scalar	1.763	1.766
	Spin-orbit	1.767	1.771

$[UO_2(C_2O_4)_3]^{4-}$	Relativity	Gas phase	COSMO
PBE0[S10]	Scalar	1.779(3)	1.7815(15)
	Spin-orbit	1.783(3)	1.786(2)

The TZ2P basis sets[S13] were used on all atoms. As other deviation values reported in parenthesis in the main text for mean distances, the standard deviations have been computed using the following formula:

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (d_i - \overline{d})^2} \tag{1}$$

where N is the number of distances entering the calculation of the mean $\overline{d}$ value. In other words, no Bessel's correction was applied.

Table S6: QTAIM bonding indicators obtained at the An–O (An = Pa, U) bond critical points and Bader charges, based on ADF[S7] calculations with the COSMO implicit solvation[S6] and the PBE0 exchange-correlation functional.[S10] Distances and delocalisation indices are reported from the main text for convenience.

System	d (Å)	ρ, a.u.	$\nabla^2\rho$	G, a.u.	V, a.u.	$|V|/G$	H, a.u.	q(An), a.u.	q(X), a.u.	δ
$[PaO]^{3+}$	1.710	0.36	0.33	0.58	-1.07	1.84	-0.50	3.69	-0.69	2.33
$[PaO(C_2O_4)_3]^{3-}$	1.858	0.25	0.36	0.34	-0.59	1.74	-0.25	3.09	-1.14	1.69
$[UO_2]^{2+}$	1.702	0.36	0.39	0.59	-1.10	1.86	-0.49	3.53	-0.77	2.15
$[UO_2Cl_4]^{2-}$	1.766	0.30	0.36	0.46	-0.83	1.80	-0.37	2.93	-0.97	1.89
$[UO_2(C_2O_4)_3]^{4-}$	1.7815(15)	0.29	0.36	0.44	-0.79	1.80	-0.35	2.41	-0.73	1.84

Table S7: Mayer[S11] and Wiberg[S12] bond indices of the Pa–O and Pa–Cl bonds within the $[PaO(Cl)_5]^{2-}$ cluster, at the PBE+D3(BJ) solid-state geometry. Calculations were performed with ADF[S7] and the TZ2P basis sets.[S13]

	Pa−O	Pa−Cl$_{ax}$	Pa−Cl$_{eq}$
Mayer	2.02	0.91	0.79
Wiberg	2.07	1.03	0.91

Table S8: Pa (5f and 6d orbitals) and O atomic orbital contributions to the σ and π Pa−O natural localized molecular orbitals (NLMOs)[S14] within $[PaO(Cl)_5]^{2-}$ cluster (same computational details as in Table S7).

	σ			π	
Pa(5f)	Pa(6d)	O(s/p)	Pa(5f)	Pa(6d)	O(s/p)
16.2	6.4	76.4	10.7	9.3	79.7

Table S9: Pa (5f and 6d orbitals) and Cl atomic orbital contributions to the σ and π Pa−Cl natural localized molecular orbitals (NLMOs)[S14] within $[PaO(Cl)_5]^{2-}$ cluster (same computational details as in Table S7).

	σ			π		
	Pa(5f)	Pa(6d)	Cl(s/p)	Pa(5f)	Pa(6d)	Cl(s/p)
Cl$_{ax}$	8.1	6.2	83.5	3.7	3.9	92.2
Cl$_{eq}$	4.7	7.2	85.3			

To cross-check our previous analysis of the solid-state $[C_8H_{20}N]_2[PaOCl_5]$ compound based on ICOBIs (see Table S1 and the related discussion), we have also performed bonding analyses within the molecular quantum chemistry framework, based on the $[PaO(Cl)_5]^{2-}$ cluster, defined at the solid-state geometry. Clearly, the deviation to the ideal triple bond is confirmed with both the Mayer[S11] and Wiberg[S12] bond indices and the specificity of the Pa−Cl$_{ax}$ bond is also reproduced. We have also computed atomic contributions per shell to the σ and π bonds between the atoms of interest, when applicable (see Tables S8 and S9). While both the Pa−O and Pa−Cl$_{ax}$ bonds display actual π character, it is absent from the Pa−Cl$_{eq}$ bonds. This, together with the shorter Pa−Cl$_{eq}$ bond distance (compared to the Pa−Cl$_{ax}$ ones), is in fact a signature for the inverse *trans* effect, expected for $[C_8H_{20}N]_2[PaOCl_5]$.[S35]

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