Electronic Supplementary Material (ESI) for Dalton Transactions.

Covalency in $AnCl_3$ (An = Th–No)

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Supplementary Information

Table SI1: α and β spin 5f electron counts and PBE0 $\langle S^2 \rangle$ values following the ECP geometry optimisations and subsequent single point all electron calculations on $AnCl_3$. $\langle S^2 \rangle$ data are reported as the difference between the formal and actual values. Also reported are the electronic states and point groups. Note that for some molecules the reported point group is of lower symmetry than that implied by the description of the geometries as either trigonal pyramidal or trigonal planar in the main text, but in all cases this is due to very small distortions from either C_{3v} or D_{3h} symmetry.

An	5f electrons α,β	$\langle S^2 \rangle$ small core ECP	$\langle S^2 \rangle$ all electron	Electronic state (point group)
Th	1,0	0.0024	0.0023	$^2A_1$ (C_{3v})
Pa	2,0	0.0070	0.0052	^3A (C_1)
U	3,0	0.0087	0.0086	$^4A_1$ (C_{3v})
Np	4,0	0.0111	0.0122	$^5A_1$ (C_{3v})
Pu	5,0	0.0189	0.0183	^6A (C_1)
Am	6,0	0.0351	0.0339	^7A (C_1)
Cm	7,0	0.0148	0.0152	^8A (C_1)
Bk	7,1	0.0114	0.0116	$^7A_2$ (C_{3v})
Cf	7,2	0.0074	0.0074	^6A (C_1)
Es	7,3	0.0047	0.0047	$^5A_2$ (C_{3v})
Fm	7,4	0.0033	0.0028	^4A (C_1)
Md	7,5	0.0019	0.0024	^3A (C_1)
No	7,6	0.0029	0.0038	$^2A_2'$ (D_{3h})

Table SI2: Average bond lengths (Å) and dihedral angles (°) for $AnCl_3$ with small and large ECP cores for the PBE0 functional, and with small core ECP cores for the PBE functional.

An		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No
Average bond length	PBE0 Small Core	2.545	2.529	2.527	2.521	2.508	2.508	2.496	2.477	2.470	2.452	2.442	2.447	2.476
	PBE0 Large Core	2.643	2.622	2.603	2.585	2.569	2.553	2.537	2.524	2.511	2.499	2.489	2.477	2.467
	PBE Small Core	2.551	2.523	2.518	2.515	2.506	2.517	2.495	2.479	2.474	2.466	2.457	2.482	2.515
	Data from references 22 and 23	2.569	2.551	2.567	2.545	2.533	2.545	2.538	2.500	2.492	2.475	2.466	2.473	2.518
Dihedral angle	PBE0 Small Core	180.0	120.8	123.1	126.4	124.8	140.0	127.6	125.3	149.3	137.6	145.4	176.6	180.0
	PBE0 Large Core	134.1	131.9	131.6	132.1	132.7	133.8	135.2	136.4	138.5	140.3	142.2	145.5	148.6
	PBE Small Core	180.0	122.7	142.3	121.5	117.8	130.3	121.0	117.3	155.0	148.2	150.2	177.1	180.0

Table SI3: An Natural populations in $AnCl_3$ (PBE0/all electron).

An	5f	6d	7s	7p
Th	0.40	1.57	0.60	0.02
Pa	1.89	1.11	0.52	0.04
U	3.17	1.02	0.27	0.02
Np	4.23	0.96	0.21	0.02
Pu	5.22	0.95	0.20	0.02
Am	6.23	0.89	0.19	0.02
Cm	7.11	0.94	0.22	0.02
Bk	8.14	0.93	0.23	0.02
Cf	9.15	0.88	0.21	0.02
Es	10.16	0.89	0.24	0.02
Fm	11.18	0.86	0.26	0.02
Md	12.32	0.76	0.25	0.02
No	13.62	0.61	0.24	0.02

Table SI4: Metal contribution (%) to the An–Cl bonding NBOs (PBE0/all electron).

An	Average	α σ	α π	β σ	β π
Th	10.02	13.00	7.62	12.68	6.78
Pa	10.01	11.88	9.01	11.26	7.91
U	9.48	12.60	7.35	10.91	7.04
Np	9.06	12.26	6.74	11.06	6.18
Pu	8.73	11.69	6.68	10.83	5.71
Am	8.20	9.98	7.78	9.56	5.48
Cm	8.42	11.56	5.92	10.42	5.76
Bk	8.46	11.51	5.59	11.04	5.71
Cf	7.87	9.36	5.81	10.17	6.15
Es	8.34	10.05	5.53	11.43	6.36
Fm	8.43	9.45	4.44	12.08	7.73
Md	8.42	6.67	5.71	11.06	10.25

On the origin of the dips at $AmCl_3$ and $CfCl_3$ in Figure 2.

As discussed in the main paper, there are dips in the average metal % (m%) at $AmCl_3$ and $CfCl_3$. As shown in table SI4 this decrease is not uniform across all NBOs, being present only in the α and β σ type NBOs. When looking for possible explanations for this, we noticed that $AmCl_3$ and $CfCl_3$ have larger dihedral angles (*i.e.* are more planar) than might be expected on the basis of those of the elements around them – see Figure SI1 below. The reduced % m in the σ type orbitals arises from decreases in both s and d character (Tables SI5 and SI6), the latter consistent with previous conclusions that, for formally d^0 MX_3, pyramidalization comes from an increased participation of the d orbitals of M in the bent structure (M. Kaupp, *Angew. Chem. Int. Ed.*, 2001, **40**, 3534; L. Perrin, L. Maron and O. Eisenstein, *Faraday Discuss.*, 2003, **124**, 25).

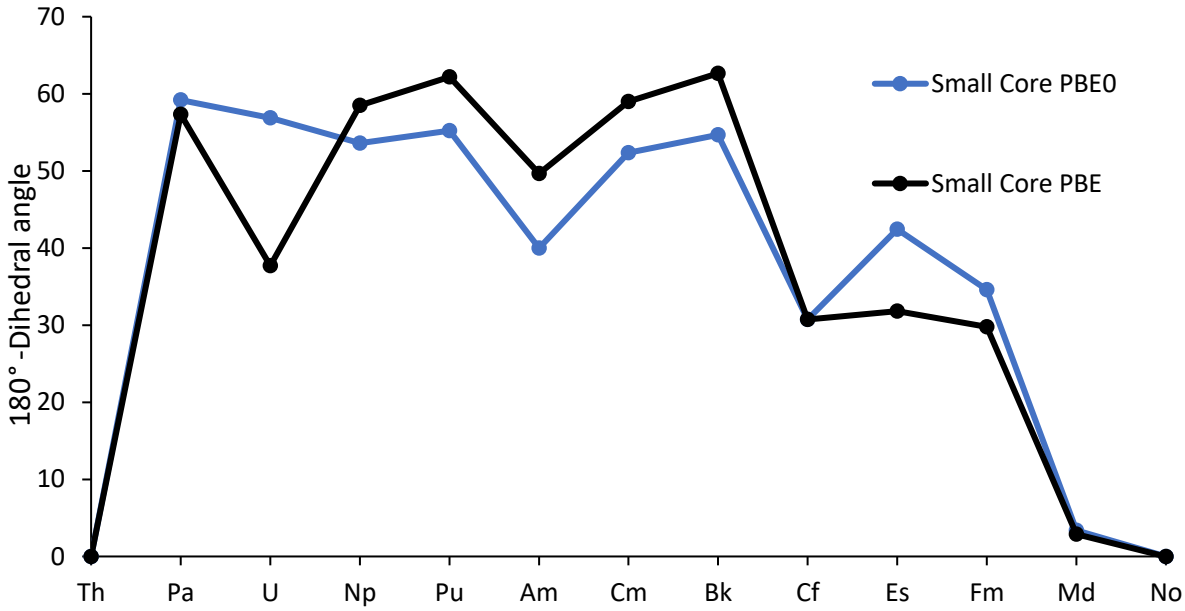

Figure SI1: 180°-the dihedral angle between two Cl-An-Cl planes for $AnCl_3$ (An = Th–No). Dihedral angle data from Table SI2.

Table SI5: NAO contribution (%) to the σ α An-Cl bonding NBOs (PBE0/all electron).

An	s	p	d	f
Th	2.16	0.03	8.88	1.91
Pa	1.90	0.11	7.67	2.14
U	3.78	0.06	7.78	0.93
Np	3.45	0.03	7.81	0.95
Pu	3.37	0.04	7.88	0.35
Am	2.65	0.14	6.98	0.10
Cm	3.70	0.07	7.69	0.07
Bk	3.71	0.06	7.65	0.06
Cf	2.71	0.36	6.18	0.06
Es	3.16	0.16	6.64	0.05
Fm	2.79	0.26	6.12	0.06
Md	1.12	0.85	4.56	0.10

Table SI6: AO contribution (%) to the σ β An-Cl bonding NBOs (PBE0/all electron).

An	s	p	d	f
Th	2.08	0.03	8.74	1.81
Pa	1.70	0.05	7.36	2.10
U	2.52	0.07	6.14	2.14
Np	2.41	0.02	6.70	1.90
Pu	2.60	0.03	6.46	1.72
Am	2.13	0.08	5.69	1.63
Cm	2.59	0.04	6.05	1.71
Bk	2.74	0.05	6.18	2.05
Cf	1.94	0.10	5.87	2.21
Es	2.56	0.06	5.51	3.22
Fm	2.97	0.07	4.68	3.18
Md	3.00	0.06	5.23	2.73

Table SI7: AO contribution (%) to the $\pi\ \alpha$ An-Cl bonding NBOs (PBE0/all electron).

An	s	p	d	f
Th	0.00	0.51	4.12	2.95
Pa	0.57	0.28	5.47	2.63
U	0.03	0.19	5.69	1.43
Np	0.25	0.29	5.13	1.04
Pu	0.18	0.27	5.28	0.92
Am	0.00	0.28	4.87	2.57
Cm	0.01	0.30	5.52	0.07
Bk	0.01	0.28	5.22	0.06
Cf	0.07	0.61	5.02	0.05
Es	0.02	0.42	5.01	0.07
Fm	0.06	0.53	4.75	0.07
Md	0.61	1.06	3.89	0.10

Table SI8: AO contribution (%) to the $\pi\ \beta$ An-Cl bonding NBOs (PBE0/all electron).

An	s	p	d	f
Th	0.00	0.37	3.59	2.78
Pa	0.77	0.13	4.81	2.15
U	0.03	0.15	4.90	1.94
Np	0.09	0.19	4.09	1.80
Pu	0.03	0.17	3.97	1.53
Am	0.01	0.27	3.85	1.32
Cm	0.00	0.22	4.25	1.28
Bk	0.00	0.25	4.42	1.02
Cf	0.07	0.28	3.47	2.28
Es	0.00	0.16	3.92	2.24
Fm	0.01	0.18	3.62	3.82
Md	0.05	0.26	5.72	4.16

Table SI9: The Wiberg Bond Index (WBI) and QTAIM metrics (delocalisation Index δ(An,Cl), $(-G/V)_{BCP}$ and bond critical point electron density (ρ_{BCP}), all in au) for the An-Cl bond in $AnCl_3$, where An=Th–Md for the WBI and An=Th–No for the QTAIM metrics (PBE0/all electron).

An	WBI	δ(An,Cl)	$(-G/V)_{BCP}$	ρ_{BCP}
Th	0.97	0.97	0.72	0.084
Pa	0.99	0.97	0.72	0.087
U	0.93	0.91	0.75	0.084
Np	0.89	0.89	0.76	0.083
Pu	0.87	0.89	0.77	0.083
Am	0.83	0.87	0.79	0.081
Cm	0.80	0.84	0.80	0.081
Bk	0.81	0.85	0.80	0.082
Cf	0.79	0.84	0.81	0.082
Es	0.80	0.85	0.81	0.084
Fm	0.81	0.87	0.81	0.084
Md	0.82	0.88	0.83	0.081
No	–	0.79	0.86	0.073

Table SI10: NRT analysis; average α and β spin covalent, ionic and ionic/covalent An-Cl Natural bond orders in $AnCl_3$ (An=Th–Md, PBE0/all electron).

An	α covalent	α ionic	α ionic/covalent	β covalent	β ionic	β ionic/covalent
Th	0.22	1.20	5.58	0.20	1.17	5.80
Pa	0.24	1.17	4.86	0.21	1.15	5.38
U	0.19	0.81	4.39	0.20	1.10	5.59
Np	0.18	0.82	4.70	0.19	1.12	5.96
Pu	0.20	1.07	5.33	0.13	0.70	5.36
Am	0.17	0.95	5.57	0.12	0.71	5.94
Cm	0.14	0.70	5.06	0.13	0.71	5.55
Bk	0.14	0.70	5.17	0.13	0.70	5.23
Cf	0.12	0.71	5.85	0.17	1.12	6.40
Es	0.13	0.70	5.56	0.16	0.84	5.18
Fm	0.12	0.70	5.85	0.17	0.83	4.95
Md	0.09	0.58	6.46	0.17	0.66	3.82

Table SI11: The average energy difference between the α and β 5f and 3p NAOs and the β An and Cl NHOs (Hartrees) in $AnCl_3$ (An = Pu-Md, PBE0/all electron).

An	Pu	Am	Cm	Bk	Cf	Es	Fm	Md
NAO α	0.059	-0.004	-0.084	-0.106	-0.126	-0.145	-0.158	-0.142
NAO β	0.282	0.282	0.257	0.192	0.127	0.060	-0.005	-0.054
σ NHO β	–	0.454	0.435	0.418	0.406	0.367	0.344	0.418
π NHO β	–	0.334	0.314	0.312	0.293	0.290	0.222	0.204

Table SI12: NHO overlap for $AnCl_3$ (An=Th-Md, PBE0/all electron).

An	α σ	α π	β σ	β π
Th	0.58	0.55	0.58	0.55
Pa	0.57	0.52	0.58	0.54
U	0.56	0.48	0.58	0.53
Np	0.56	0.45	0.58	0.48
Pu	0.56	0.42	0.56	0.45
Am	0.59	0.39	0.54	0.44
Cm	0.56	0.42	0.53	0.43
Bk	0.56	0.42	0.53	0.42
Cf	0.55	0.46	0.51	0.40
Es	0.56	0.45	0.52	0.37
Fm	0.55	0.46	0.52	0.35

Table SI13: The PBE $<S^2>$ values following the ECP geometry optimisations and subsequent single point all electron calculations on $AnCl_3$. Data are reported as the difference between the formal and actual values.

An	Small core ECP	All electron
Th	0.0020	0.0020
Pa	0.0048	0.0066
U	0.0099	0.0098
Np	0.0160	0.0178
Pu	0.0392	0.0373
Am	0.0970	0.0906
Cm	0.0142	0.0145
Bk	0.0114	0.0131
Cf	0.0074	0.0060
Es	0.0041	0.0036
Fm	0.0030	0.0029
Md	0.0011	0.0011
No	0.0008	0.0010

Table SI14: An Natural populations in $AnCl_3$ (PBE/all electron).

An	5f	6d	7s	7p
Th	0.50	1.55	0.64	0.02
Pa	1.97	1.17	0.56	0.04
U	3.29	1.08	0.33	0.02
Np	4.37	1.02	0.26	0.02
Pu	5.38	1.00	0.25	0.02
Am	6.41	0.91	0.22	0.02
Cm	7.21	1.00	0.25	0.02
Bk	8.26	0.97	0.30	0.02
Cf	9.36	0.89	0.23	0.02
Es	10.42	0.84	0.24	0.02
Fm	11.54	0.78	0.29	0.02
Md	12.65	0.67	0.27	0.02
No	13.71	0.59	0.28	0.02

Table SI15: Metal contribution (%) to the An–Cl bonding NBOs (PBE/all electron).

An	Average	α σ	α π	β σ	β π
Th	10.72	13.58	8.50	13.21	7.57
Pa	10.89	14.29	8.29	12.30	8.67
U	10.80	13.99	8.96	12.06	8.20
Np	10.27	12.77	8.95	12.13	7.24
Pu	10.20	12.42	9.93	11.91	6.53
Am	9.40	10.65	11.79	9.92	5.21
Cm	9.59	12.56	6.46	12.11	7.21
Bk	9.73	12.28	5.98	12.90	7.76
Cf	9.30	10.08	5.68	12.35	9.09
Es	9.73	8.42	5.88	13.63	11.00
Fm	10.14	9.52	4.65	12.71	13.69
Md	9.59	7.65	3.90	12.64	14.16

Table SI16: AO contribution (%) to the σ α An-Cl bonding NBOs (PBE/all electron).

An	s	p	d	f
Th	2.18	0.03	9.08	2.27
Pa	2.95	0.03	8.87	2.36
U	3.98	0.04	8.57	1.36
Np	3.85	0.03	8.52	0.34
Pu	3.80	0.04	8.36	0.16
Am	3.04	0.06	7.29	0.10
Cm	4.10	0.04	8.32	0.07
Bk	4.03	0.04	8.12	0.06
Cf	3.11	0.14	6.81	0.04
Es	2.50	0.34	5.80	0.05
Fm	3.04	0.08	5.58	0.04
Md	1.96	0.20	5.41	0.04

Table SI17: AO contribution (%) to the σ β An-Cl bonding NBOs (PBE/all electron).

An	s	p	d	f
Th	2.17	0.03	8.88	2.11
Pa	1.89	0.05	7.85	2.47
U	2.79	0.07	6.70	2.46
Np	2.85	0.04	6.93	2.29
Pu	2.90	0.04	6.75	2.20
Am	2.24	0.05	5.35	2.19
Cm	2.86	0.04	6.46	2.73
Bk	3.87	0.02	6.48	2.49
Cf	1.89	0.05	5.95	4.38
Es	2.38	0.03	3.86	7.29
Fm	1.81	0.30	4.72	5.82
Md	3.17	0.07	6.26	2.91

Table SI18: AO contribution (%) to the π α An-Cl bonding NBOs (PBE/all electron).

An	s	p	d	f
Th	0.00	0.47	4.54	3.44
Pa	0.01	0.11	4.86	3.25
U	0.05	0.18	6.31	2.39
Np	0.18	0.27	5.84	2.63
Pu	0.03	0.19	4.50	5.15
Am	0.00	0.32	7.38	3.85
Cm	0.00	0.25	6.14	0.05
Bk	0.00	0.21	5.70	0.05
Cf	0.04	0.41	5.17	0.05
Es	0.19	0.55	5.07	0.05
Fm	0.03	0.25	4.32	0.04
Md	0.12	1.12	2.56	0.06

Table SI19: AO contribution (%) to the π β An-Cl bonding NBOs (PBE/all electron).

An	s	p	d	f
Th	0.00	0.38	3.92	0.00
Pa	0.74	0.16	5.17	2.56
U	0.10	0.12	5.41	2.55
Np	0.00	0.16	4.61	2.45
Pu	0.00	0.16	4.07	2.28
Am	0.00	0.17	2.28	2.78
Cm	0.01	0.20	4.59	2.40
Bk	0.14	0.19	4.47	2.94
Cf	0.05	0.19	3.90	4.88
Es	0.00	0.22	5.46	5.17
Fm	0.00	0.17	6.49	6.88
Md	0.44	0.28	7.13	5.89

Table SI20: The Wiberg Bond Index (WBI) and QTAIM metrics (delocalisation Index δ(An,Cl), $(-G/V)_{BCP}$ and bond critical point electron density (ρ_{BCP}), all in au) for the An-Cl bond in $AnCl_3$, where An=Th–Md for the WBI and An=Th–No for the QTAIM metrics (PBE/all electron).

An	WBI	δ(An,Cl)	$(-G/V)_{BCP}$	ρ_{BCP}
Th	1.04	1.04	0.73	0.084
Pa	1.09	1.06	0.72	0.088
U	1.07	1.02	0.74	0.087
Np	1.01	1.00	0.76	0.085
Pu	1.00	0.99	0.77	0.084
Am	0.94	0.97	0.80	0.079
Cm	0.91	0.93	0.79	0.082
Bk	0.94	0.97	0.79	0.084
Cf	0.91	0.96	0.81	0.081
Es	0.91	0.97	0.82	0.081
Fm	0.96	1.02	0.83	0.080
Md	0.88	0.96	0.85	0.074
No	–	0.79	0.88	0.067

Table SI21: NRT analysis; average α and β spin covalent, ionic and ionic/covalent An-Cl Natural bond orders in $AnCl_3$ (An=Th–Md, PBE/all electron).

An	α covalent	α ionic	α ionic/covalent	β covalent	β ionic	β ionic/covalent
Th	0.24	1.20	5.07	1.42	0.23	5.29
Pa	0.28	1.14	4.14	1.33	0.24	4.61
U	0.22	0.78	3.63	1.40	0.24	4.94
Np	0.28	1.20	4.23	1.31	0.22	4.97
Pu	0.24	1.02	4.35	1.31	0.21	5.33
Am	0.20	0.80	3.96	1.30	0.18	6.18
Cm	0.16	0.68	4.25	1.32	0.21	5.15
Bk	0.15	0.68	4.60	1.45	0.25	4.86
Cf	0.12	0.71	5.71	1.30	0.24	4.47
Es	0.12	0.88	7.32	1.16	0.24	3.85
Fm	0.12	0.71	6.09	1.44	0.32	3.42
Md	0.08	0.59	7.23	1.00	0.25	2.98

Table SI22: The average energy difference between the α and β 5f and 3p NAOs and the β An and Cl NHOs (Hartrees) in $AnCl_3$ (An = Pu-Md, PBE/all electron).

An	Pu	Am	Cm	Bk	Cf	Es	Fm	Md
NAO α	0.062	0.034	-0.027	-0.043	0.014	-0.046	-0.038	-0.090
NAO β	0.162	0.160	0.117	0.080	0.057	0.031	0.013	0.000
σ NHO β	–	0.355	0.316	0.310	0.261	0.224	0.174	0.274
π NHO β	–	0.217	0.210	0.182	0.159	0.166	0.147	0.168

Table SI23: NHO overlap for $AnCl_3$ (An=Th-Md, PBE/all electron).

An	α σ	α π	β σ	β π
Th	0.57	0.54	0.57	0.54
Pa	0.56	0.53	0.57	0.54
U	0.55	0.50	0.56	0.53
Np	0.54	0.46	0.56	0.48
Pu	0.55	0.40	0.54	0.44
Am	0.56	0.38	0.54	0.39
Cm	0.54	0.41	0.50	0.40
Bk	0.54	0.41	0.51	0.38
Cf	0.53	0.44	0.47	0.34
Es	0.52	0.46	0.42	0.34
Fm	0.54	0.44	0.36	0.33

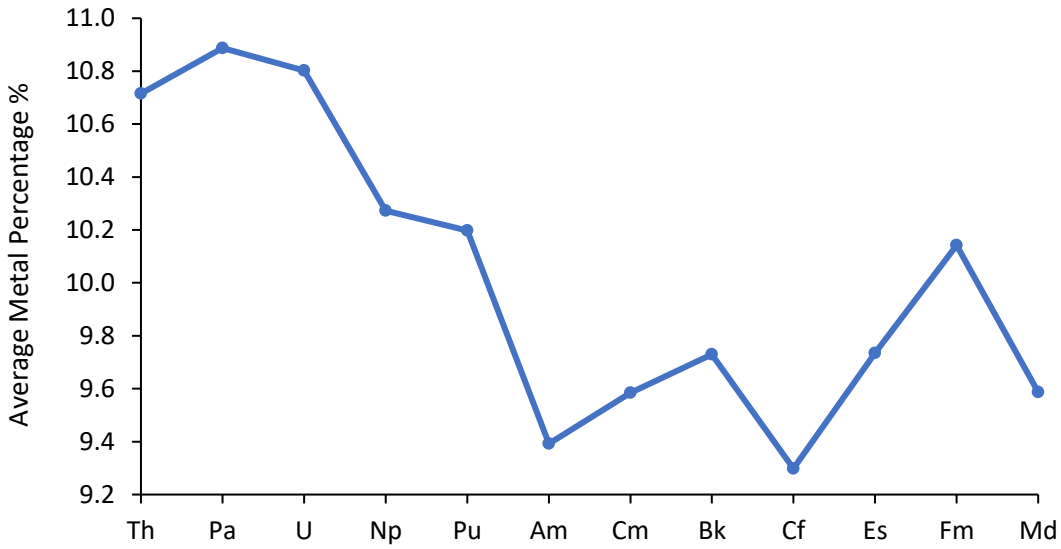

Figure SI2: Average metal contribution (%) to the metal–chlorine NBOs in $AnCl_3$, computed at the PBE level. $NoCl_3$ is omitted as it did not converge on σ type + π type NBOs for all three An-Cl bonds.

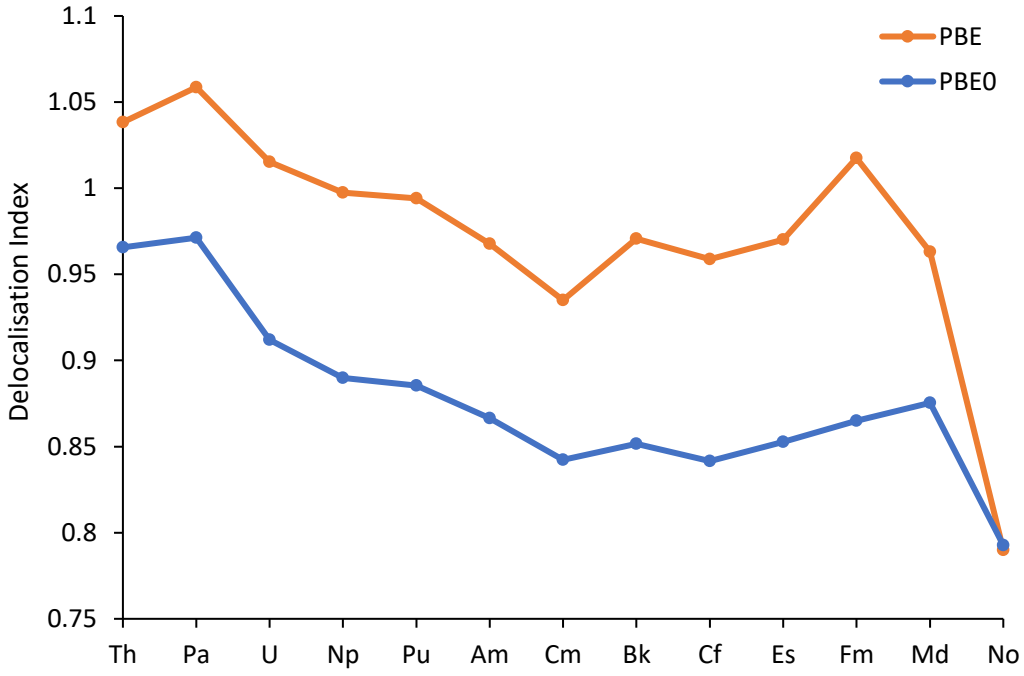

Figure SI3: Delocalisation Index of $AnCl_3$ (An=Th-No) for both the PBE and PBE0 functionals

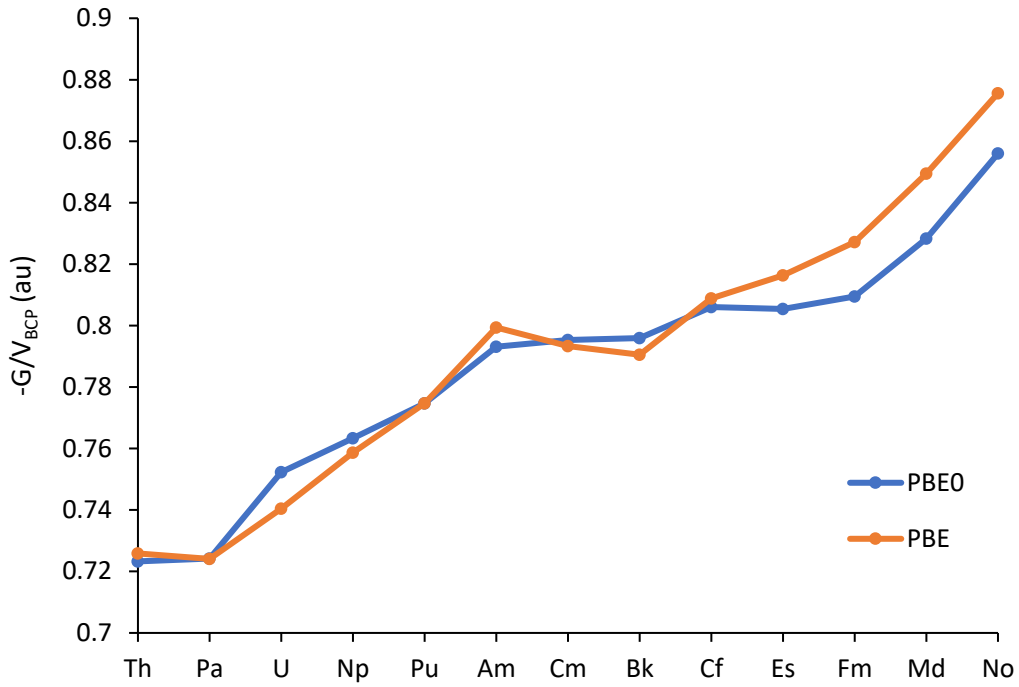

Figure SI4: $(-G/V)_{BCP}$ for $AnCl_3$ (An=Th-No) for PBE and PBE0 functionals.

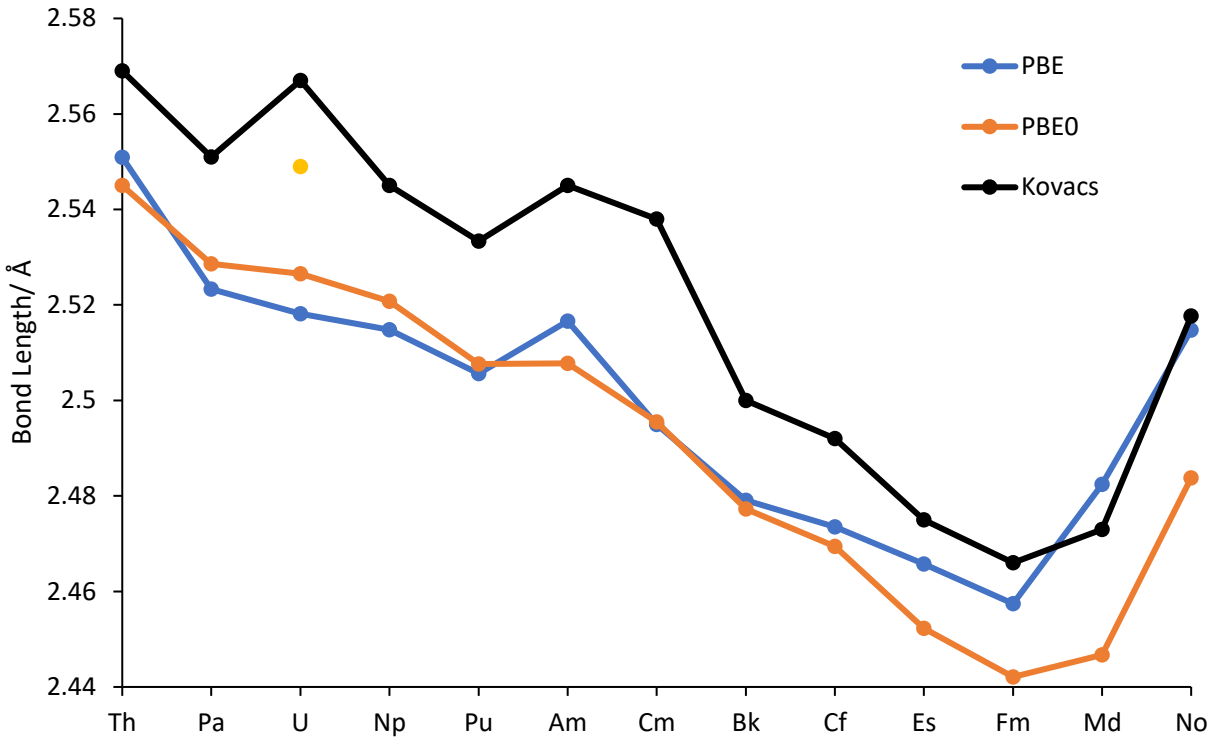

Figure SI5: An–Cl bond lengths computed with small core ECPs using the PBE and PBE0 functionals (data in Table SI2). The experimental value for UCl_3 is shown as the orange dot, and the black line provides the B3LYP data from Kovács *et al.*[21,22]

Converged cartesian atomic coordinates (Å)

PBE0

Th	0.00000000	0.00000000	0.00000200
Cl	0.00000000	2.54503700	-0.00000400
Cl	-2.20406700	-1.27251900	-0.00000400
Cl	2.20406700	-1.27251900	-0.00000400
Pa	0.00470200	0.00000000	-0.29903800
Cl	-1.20819800	2.05117300	0.53066600
Cl	2.39132000	-0.00005300	0.53940000
Cl	-1.20829300	-2.05111700	0.53066700
U	0.00000000	0.00000000	0.28172000
Cl	0.00000000	2.39979800	-0.50820100
Cl	-2.07828600	-1.19989900	-0.50820100
Cl	2.07828600	-1.19989900	-0.50820100
Np	0.00000000	0.00000000	0.26036300
Cl	0.00000000	2.41123400	-0.47477900
Cl	-2.08819000	-1.20561700	-0.47477900
Cl	2.08819000	-1.20561700	-0.47477900
Pu	-0.01024800	0.00009800	-0.26968300
Cl	-2.39920100	0.00701000	0.50904100
Cl	1.23432800	2.03671800	0.49114400
Cl	1.22153700	-2.04427300	0.49100300
Am	-0.00001300	-0.02173500	-0.17870300
Cl	-2.17780900	-1.15531400	0.34153300
Cl	0.00056900	2.43299000	0.31558800
Cl	2.17731400	-1.15621400	0.34151600
Cm	0.00000400	-0.00000700	-0.24573000
Cl	-1.79527800	-1.58202200	0.46255900
Cl	-0.47248000	2.34575200	0.46253100
Cl	2.26773800	-0.76369000	0.46256300
Bk	0.00000000	0.00000000	0.25474300
Cl	0.00000000	2.36441000	-0.48451200
Cl	-2.04763900	-1.18220500	-0.48451200
Cl	2.04763900	-1.18220500	-0.48451200

Cf	-0.00939100	-0.00013800	-0.13567600
Cl	-2.45223800	-0.01060600	0.26652500
Cl	1.24350800	2.08743200	0.25775200
Cl	1.26286800	-2.07603200	0.25785200
Es	0.00000000	0.00000000	0.18684400
Cl	0.00000000	2.38989300	-0.36269800
Cl	-2.06970800	-1.19494700	-0.36269800
Cl	2.06970800	-1.19494700	-0.36269800
Fm	-0.00002800	0.00000500	-0.14832100
Cl	1.32420800	2.00438500	0.29079000
Cl	1.07392900	-2.14889400	0.29079600
Cl	-2.39797100	0.14448200	0.29089000
Md	0.01331800	-0.00001300	0.01413700
Cl	-1.26921600	2.08259900	-0.02754900
Cl	2.46067100	-0.00073400	-0.02889000
Cl	-1.27057900	-2.08178600	-0.02755000
No	0.00000000	0.00000000	0.00000000
Cl	0.00000000	2.48375700	0.00000000
Cl	2.15099600	-1.24187800	0.00000000
Cl	-2.15099600	-1.24187800	0.00000000

PBE

Th	0.00000000	0.00000000	0.00000000
Cl	0.00000000	2.55092500	0.00000100
Cl	-2.20916500	-1.27546200	0.00000100
Cl	2.20916500	-1.27546200	0.00000100
Pa	-0.00001600	0.00000400	-0.28599900
Cl	-2.22004800	-0.89698600	0.51031900
Cl	0.33321900	2.37102000	0.51049900
Cl	1.88691600	-1.47405700	0.51011700
U	-0.00008300	-0.00007600	-0.32374600
Cl	1.78395800	-1.52796700	0.58385400
Cl	0.43180500	2.30879700	0.58374100
Cl	-2.21531600	-0.78042100	0.58444400
Np	-0.00006100	-0.00004400	-0.28800600
Cl	0.72478600	2.26656200	0.52511200
Cl	1.60093900	-1.76064200	0.52517600
Cl	-2.32538900	-0.50568200	0.52527400
Pu	-0.00543400	-0.00000100	-0.30880400
Cl	-2.35392100	-0.00011700	0.57660700
Cl	1.19187800	2.01738100	0.56544800
Cl	1.19208700	-2.01725900	0.56544900
Am	-0.02547500	-0.00011100	-0.22111700
Cl	1.29844400	2.04483100	0.39983800
Cl	1.30415000	-2.04133200	0.39997500
Cl	-2.46023100	-0.00288100	0.43584300
Cm	-0.00002500	-0.00000300	-0.28266400
Cl	-2.03913500	-1.18447400	0.53224100
Cl	-0.00616000	2.35821300	0.53209400
Cl	2.04543700	-1.17372300	0.53188700
Bk	0.00000000	0.00000000	0.30022000
Cl	0.00000000	2.32101400	-0.57100600
Cl	-2.01005700	-1.16050700	-0.57100600
Cl	2.01005700	-1.16050700	-0.57100600

Cf	0.01569300	-0.00001000	-0.18657500
Cl	2.43234900	-0.00045200	0.37182200
Cl	-1.26098000	2.04489100	0.35185800
Cl	-1.26183300	-2.04438000	0.35187200
Es	0.00000000	-0.01920200	-0.13436400
Cl	-0.00001100	2.41406900	0.24841200
Cl	-2.15495900	-1.15113300	0.26704000
Cl	2.15497200	-1.15111400	0.26702300
Fm	-0.00005900	-0.00033200	0.22812900
Cl	2.00636300	-1.24864100	-0.44745300
Cl	-2.08624600	-1.11005000	-0.44754500
Cl	0.08022800	2.36064500	-0.44693700
Md	-0.01280400	-0.00197800	0.02046700
Cl	-2.49021300	-0.11691000	-0.04177000
Cl	1.17518100	2.17789800	-0.03979900
Cl	1.39110600	-2.04923600	-0.04003200
No	0.00001000	-0.00008600	0.00000000
Cl	2.21954000	-1.18228600	-0.00000500
Cl	-2.13406800	-1.33036500	-0.00000500
Cl	-0.08553300	2.51316900	0.00001200