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

High Coordination Number Actinide-Noble Gas Complexes; a Computational Study

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Supplementary Information

Table S1. Average Ac^{3+}-Ne distances (r_{av}), distance ranges (Δr), and average Ac^{3+}-Ne binding energies of $AcNe_n^{3+}$ by BHLYP-D3 method with different basis sets

	Basis set	r_{av} /Å	Δr /Å	$\lvert E_{av}\rvert$ /kJ mol^{-1}
$AcNe^{3+}$	aug-cc-pV5Z	2.678	-	41.365
	Stuttgart RLC	2.685	-	40.439
$AcNe_{16}^{3+}$	aug-cc-pV5Z	2.932	0.215	28.457
	Stuttgart RLC	2.936	0.216	28.411

Table S2. Total energies of U^{3+}, He, and U^{3+}-He by various functionals at equilibrium U^{3+}-He distance. The unit of energy is Hartree. Total energy of U^{3+} by Gaussian 16/BHLYP is -475.2299.

	U^{3+}	He	U^{3+}-He
PBE	-475.3993	-2.8929	-478.3070
B3LYP	-475.3565	-2.9081	-478.2796
PBE0	-475.3745	-2.8951	-478.2834
BHLYP	-475.1612	-2.9057	-478.1472

Table S3. Structural, energetic, and QTAIM parameters for Th-Ng and Ng-Ng BCPs in $ThNg_{12}^{4+}$ complexes. The QTAIM parameters for Ng-Ng BCPs in bare Ng_{12} are listed in parentheses.

	r_{av} /Å	$\lvert E_{av}\rvert$ / kJ mol^{-1}	q_{Ac}	q_{Ng}(av)	Ac-Ng			Ng-Ng		
					ρ_{BCP}	$\nabla^2\rho_{BCP}$	δ	ρ_{BCP}	$\nabla^2\rho_{BCP}$	δ
$ThHe_{12}^{4+}$	2.430	52.573	3.627	0.031	0.027	0.106	0.116	- (*0.003*)	- (*0.016*)	- (*0.011*)
$ThNe_{12}^{4+}$	2.582	78.072	3.510	0.041	0.032	0.136	0.147	- (*0.006*)	- (*0.039*)	- (*0.024*)
$ThAr_{12}^{4+}$	3.116	145.437	3.053	0.079	0.023	0.055	0.194	0.010 (*0.008*)	0.037 (*0.036*)	0.069 (*0.063*)
$ThKr_{12}^{4+}$	3.371	165.687	2.895	0.092	0.019	0.035	0.207	0.009 (*0.008*)	0.031 (*0.029*)	0.086 (*0.077*)
$ThXe_{12}^{4+}$	3.740	185.498	2.676	0.110	0.014	0.018	0.226	0.008 (*0.007*)	0.023 (*0.022*)	0.104 (*0.093*)

Table S4. Average Ac-Ng distance (r_{av}) and QTAIM parameters (au) for Ac-Ng and Ng-Ng BCPs in $AcNg_{12}^{3+}$ complexes when including the second Ng shell. The average distance and BCP properties between Ac and second shell Ng atoms are listed in parentheses.

	r_{av} /Å	Ac-Ng			Ng-Ng		
		ρ_{BCP}	$\nabla^2\rho_{BCP}$	$\frac{G_{BCP}}{\lvert V_{BCP}\rvert}$	ρ_{BCP}	$\nabla^2\rho_{BCP}$	$\frac{G_{BCP}}{\lvert V_{BCP}\rvert}$
$AcNe_{12}^{3+}$	2.760 (*4.307*)	0.021	0.094	1.170	- (*0.003*)	- (*0.015*)	- (*1.684*)
$AcAr_{12}^{3+}$	3.238 (*5.569*)	0.017	0.050	1.120	0.008 (*0.002*)	0.028 (*0.008*)	1.340 (*1.576*)
$AcKr_{12}^{3+}$	3.489 (*6.002*)	0.013	0.034	1.103	0.007 (*0.002*)	0.024 (*0.007*)	1.315 (*1.678*)

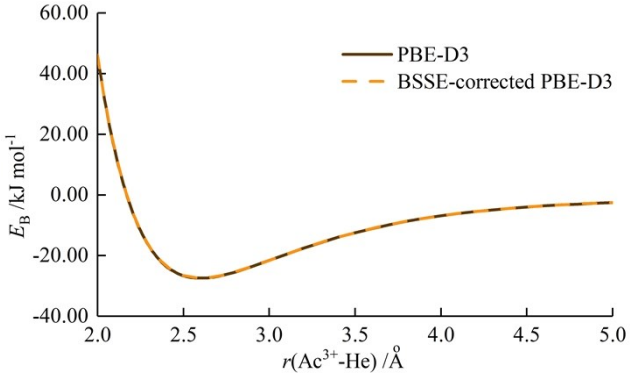


Figure S1. Potential energy curves of Ac^{3+}-He by DFT calculation using PBE-D3 functionals with and without BSSE correction.

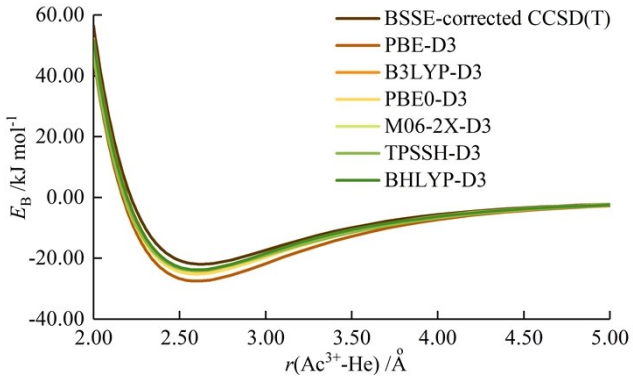


Figure S2. Potential energy curves of Ac^{3+}-He by DFT calculation using various density functionals

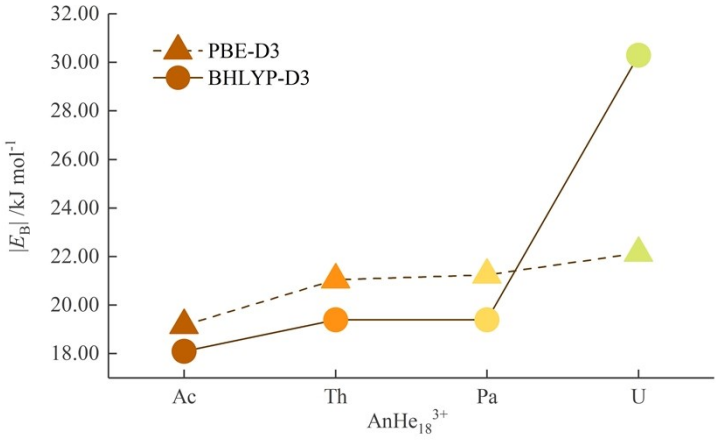


Figure S3. Average An^{3+}-He binding energy of $AnHe_{18}^{3+}$ complexes

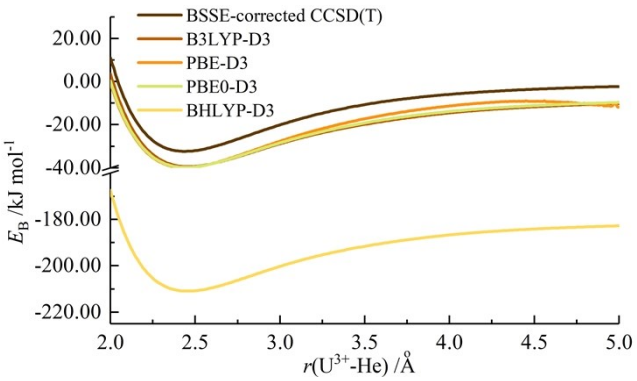


Figure S4. Potential energy curves for U^{3+}-He using various functionals

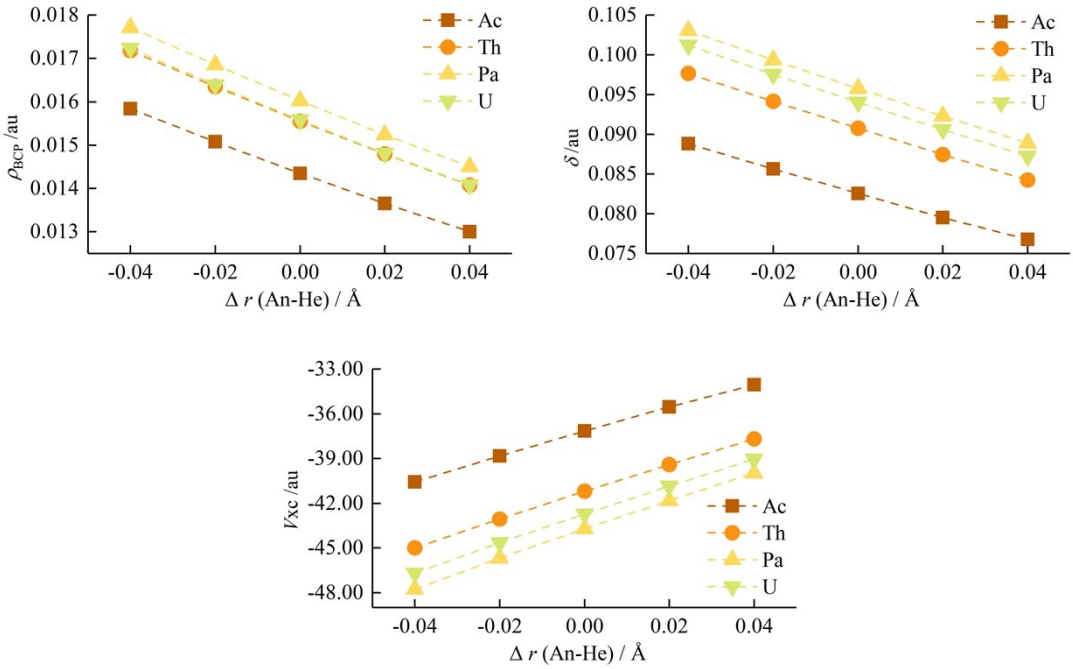


Figure S5. The electron density (ρ) at the An-He BCPs, delocalization index (δ) and IQA exchange-correlation energy (Vxc) for the An-He bond in diatomic An^{3+}-He as a function of the shortening and elongation of An-He bond length from equilibrium ($\triangle r$ (An-He)). The equilibrium An-He distances in the $AnHe_{16}^{3+}$ systems are used as references.

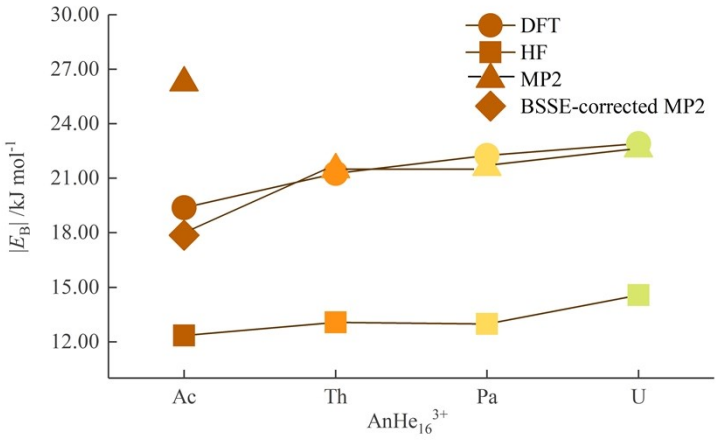
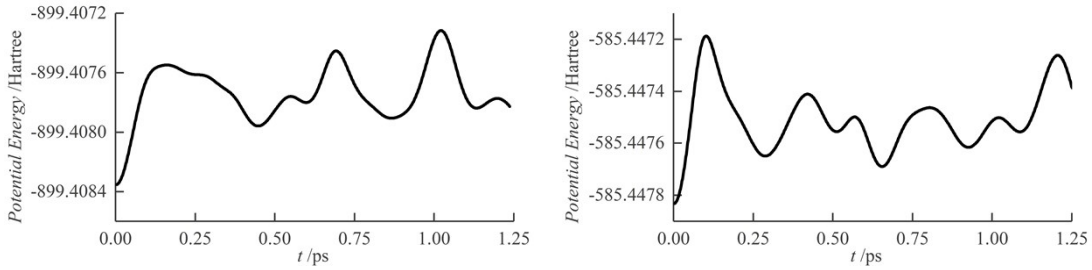
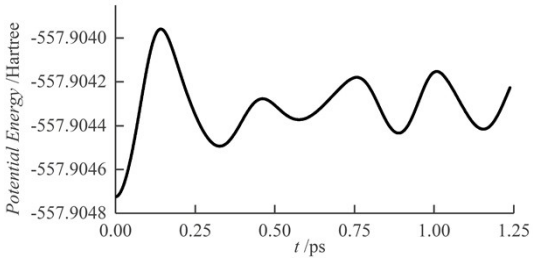


Figure S6. Average binding energies of $AnHe_{16}^{3+}$ (An=Ac-U) obtained from DFT, HF, and MP2 calculation.

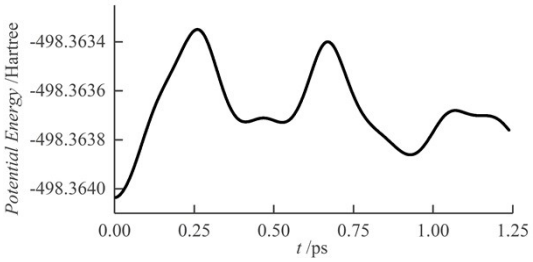


(a) Potential Energy of $AcNe_{15}^{3+}$ vs time

(b) Potential Energy of $AcAr_{10}^{3+}$ vs time



(c) Potential Energy of $AcKr_{10}^{3+}$ vs time



(d) Potential Energy of $AcXe_8^{3+}$ vs time

Figure S7. Evolution of $AcNe_{15}^{3+}$, $AcAr_{10}^{3+}$, $AcKr_{10}^{3+}$, and $AcXe_8^{3+}$ potential energy with time at 10 K. The initial structures are the ones shown in Figure 10, which remain as the potential energy minimum structure during the whole relaxation time.

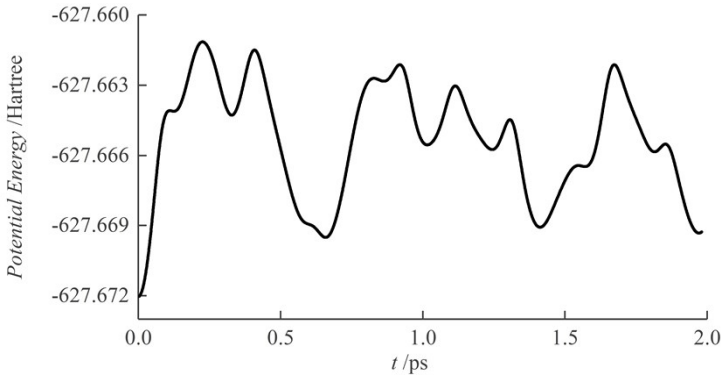


Figure S8. Evolution of $AcAr_{12}^{3+}$ potential energy with time at 100 K. The initial structure is as in Figure 11.

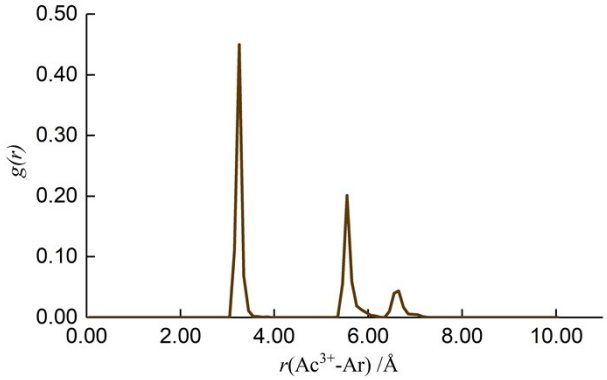
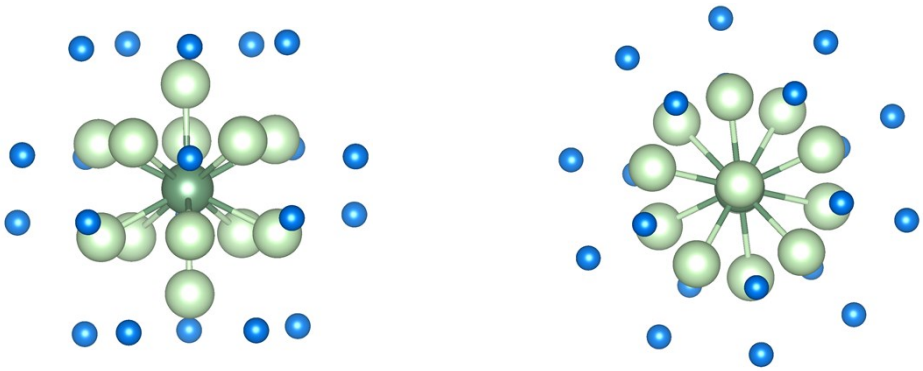


Figure S9. Ac^{3+}-Ar radial distribution function in Ac^{3+}-Ar_{42} obtained from AIMD calculation at 10 K. The time step is 1.21 fs and the total simulation time is 3.63 ps.



(a) Side view (b) Top view

Figure S10. (a) side and (b) top views of optimized $AcAr_{12}^{3+}$ with a second Ar shell. The green and blue balls are the Ar atoms in the first and second shell, respectively.

Cartesian Coordinates (Å) of the optimized $AnNg_n^{q+}$

Cartesian Coordinates (Å) of $AcHe_n^{3+}$ (n=1-18)

n = 1

Ac	-0.0023290	-0.0000000	0.0000000
He	2.6023290	0.0000000	0.0000000

n = 2

Ac	0.0382391	0.2454927	-0.0880064
He	0.2808210	2.3239681	-1.6403215
He	-2.2702233	1.3678086	-0.5402914

n = 3

Ac	0.0409476	0.2438557	-0.0872425
He	0.2805622	2.3241608	-1.6404209
He	-2.2726730	1.3692529	-0.5409558
He	2.2378698	1.5989099	0.3166649

n = 4

Ac	0.0412087	0.2414614	-0.0863626
He	-0.2956683	2.3489158	1.4167260
He	0.2808454	2.3248755	-1.6405016
He	-2.2746778	1.3700397	-0.5415843
He	2.2393304	1.5998027	0.3164942

n = 5

Ac	0.0447718	0.2361947	-0.0854993
He	-0.2954896	2.3502015	1.4177138
He	0.2812081	2.3262624	-1.6414467
He	-2.2787845	1.3720559	-0.5424984
He	2.2393326	1.6003807	0.3165022
He	2.2131074	-1.2131229	0.2175539

n = 6

Ac	0.0423648	0.2292704	-0.0884083
He	-0.2961524	2.3568516	1.4222588
He	0.2812478	2.3292086	-1.6430198
He	-2.2813962	1.3738372	-0.5433457
He	2.2382895	1.5986912	0.3161002
He	2.2197923	-1.2158868	0.2187403
He	-0.3374344	-1.9626089	1.3172350

n = 7

Ac	0.0001836	0.1662686	-0.0821978

He	-0.3257753	2.3683066	1.3022218
He	0.2541668	2.3457056	-1.5365573
He	-2.2242285	1.4955572	-0.5361210
He	2.2038480	1.5643514	0.2586475
He	2.2328454	-1.1846661	0.2768064
He	-0.2743286	-2.0461600	1.3167610
He	-2.1890790	-1.2348703	-0.5097760

n = 8

Ac	0.0023889	0.1618814	-0.0882796
He	-0.3277025	2.3764885	1.3031599
He	0.2544138	2.3477557	-1.5335135
He	-2.2254818	1.4959249	-0.5366654
He	2.2059382	1.5652380	0.2570001
He	2.2375628	-1.1850270	0.2793210
He	-0.2756846	-2.0524985	1.3169165
He	-2.1938025	-1.2352700	-0.5081545
He	0.3025107	-2.0263010	-1.5226995

n = 9

Ac	0.0032627	0.1618915	-0.0839424
He	-0.3291320	2.3801288	1.3005454
He	0.2553383	2.3540672	-1.5325875
He	-2.2285374	1.4976520	-0.5365297
He	2.2088465	1.5671807	0.2562882
He	2.2405448	-1.1868987	0.2784425
He	-0.2770263	-2.0563509	1.3145702
He	-2.1966664	-1.2369862	-0.5080639
He	0.3035130	-2.0324924	-1.5216379
He	0.9114768	0.1861787	2.3848439

n = 10

Ac	-0.0112610	0.1615869	-0.1020644
He	-0.2984238	2.4070008	1.2518255
He	0.2361037	2.4048464	-1.4797035
He	-2.2332301	1.5163122	-0.5465077
He	2.1859920	1.5746805	0.2916684
He	2.2166317	-1.1954907	0.3119205
He	-0.2407372	-2.0807032	1.2680693
He	-2.2014643	-1.2525256	-0.5223864
He	0.2873813	-2.0848201	-1.4644174
He	0.9506276	0.1834835	2.3435245
He	-1.7764724	0.1492180	1.8459846

n = 11

Ac	-0.0121343	0.1615844	-0.1093546
He	-0.2983404	2.4080075	1.2505757
He	0.2361411	2.4099242	-1.4788010
He	-2.2360685	1.5192315	-0.5458002
He	2.1868477	1.5755202	0.2930426
He	2.2174710	-1.1964321	0.3131736
He	-0.2400501	-2.0816527	1.2666476
He	-2.2042685	-1.2552968	-0.5215475
He	0.2877443	-2.0900115	-1.4632009
He	0.9544980	0.1832084	2.3491796
He	-1.7766928	0.1495057	1.8439986
He	-0.9579454	0.1335887	-2.5795415

n = 12

Ac	-0.0076487	0.1617199	-0.1149765
He	-0.2972288	2.4075779	1.2497841
He	0.2342020	2.4147383	-1.4772994
He	-2.2347518	1.5190476	-0.5475493
He	2.1878242	1.5772023	0.2968274
He	2.2180772	-1.1978053	0.3169811
He	-0.2382546	-2.0812177	1.2656173
He	-2.2031956	-1.2551638	-0.5229165
He	0.2854721	-2.0945548	-1.4618418
He	0.9553944	0.1828111	2.3475051
He	-1.7796014	0.1497451	1.8469783
He	-0.9630870	0.1330767	-2.5807380
He	1.7589467	0.1799774	-2.0817297

n = 13

Ac	0.1430889	0.0802236	-0.1099349
He	-0.1083749	2.4230444	1.1277185
He	-0.1123193	2.4096748	-1.3679471
He	-2.3990659	0.8162248	-0.1215836
He	2.0819640	1.9001960	-0.1075564
He	1.0331209	-2.0160128	1.2547938
He	-1.4727035	-1.6622105	1.1138167
He	-1.4726919	-1.6817400	-1.3031210
He	1.0345059	-1.9968040	-1.5069087
He	1.5983370	0.4760924	2.0750341
He	-1.0127440	0.4490843	2.2626800
He	-1.0025923	0.4092497	-2.4920765
He	1.6056238	0.4901321	-2.2882726
He	2.7156119	-0.5777924	-0.1096471

n = 14

Ac	-0.0001304	0.0412995	-0.1108330
He	0.0007925	2.3269766	1.2732721
He	-0.0015603	2.3200334	-1.5079306
He	-1.9658288	1.8569701	-0.1201861
He	1.9656756	1.8569183	-0.1214458
He	1.2044235	-1.9748077	1.1755683
He	-1.2071576	-1.9694062	1.1824574
He	-1.2052014	-1.9752151	-1.3940135
He	1.2069728	-1.9693690	-1.4015027
He	1.3562616	0.3635058	2.1549904
He	-1.3575843	0.3678229	2.1532874
He	-1.3567655	0.3537916	-2.3780666
He	1.3594131	0.3596447	-2.3750490
He	2.6324498	-0.4388027	-0.1035530
He	-2.6327329	-0.4387832	-0.1069665

n = 15

Ac	-0.0001567	0.0228384	0.0487785
He	0.0002138	2.1877550	1.5890202
He	-0.0013094	2.2615816	-1.4490518
He	-1.9040952	1.9146289	-0.1014281
He	1.9037470	1.9140764	-0.1039430
He	1.2830339	-2.0311052	1.1724658
He	-1.2843819	-2.0292901	1.1739505
He	-1.1721091	-1.9889449	-1.3070401
He	1.1712266	-1.9863997	-1.3106940
He	1.9363407	0.5064938	1.8572119
He	-1.9368282	0.5045326	1.8575917
He	-1.2807427	0.3024918	-2.2792402
He	1.2847597	0.3067519	-2.2768571
He	2.6339141	-0.4034734	-0.2742906
He	-2.6345849	-0.4013578	-0.2764451
He	0.0008191	-0.5293311	2.6816190

n = 16

Ac	-0.0000710	0.1863385	0.1165788
He	0.0006637	2.8855453	0.4999944
He	-0.0004864	1.6578461	2.3971746
He	-0.0002068	2.1719645	-1.7244554
He	-2.0228192	1.9124858	-0.2756364
He	2.0230095	1.9121147	-0.2768496
He	1.2897774	-1.9274026	1.1589433

He	-1.2898895	-1.9277329	1.1586820
He	-1.1332802	-1.8990901	-1.2121794
He	1.1334295	-1.8988687	-1.2118810
He	2.0248620	0.5064316	1.8563042
He	-2.0247705	0.5056592	1.8560319
He	-1.2707729	0.2420227	-2.2501737
He	1.2705802	0.2417365	-2.2500682
He	2.6235168	-0.3755776	-0.2664213
He	-2.6237859	-0.3752392	-0.2667455
He	-0.0001413	-0.6618888	2.6892008

n = 17

Ac	0.0000107	0.0308856	0.1565480
He	0.0005040	2.6592700	0.8006187
He	0.0003953	-2.6546656	0.7089590
He	-0.0003566	1.2430349	2.6186469
He	-0.0000211	2.0915685	-1.6448259
He	-1.9030192	1.9130352	-0.3691315
He	1.9032501	1.9125788	-0.3696690
He	1.9051031	-1.5252328	1.3268214
He	-1.9048150	-1.5257342	1.3258914
He	-1.1931852	-1.9755522	-1.2128824
He	1.1927797	-1.9753516	-1.2134734
He	2.0768475	0.8026000	1.7081145
He	-2.0770117	0.8018824	1.7079725
He	-1.1868764	0.1464384	-2.2746605
He	1.1869317	0.1466514	-2.2746034
He	2.6443696	-0.2664080	-0.4610180
He	-2.6445110	-0.2659112	-0.4611351
He	-0.0003851	-1.0574103	2.6352856

n = 18

Ac	0.0000118	0.0000090	-0.0000451
He	-0.0000029	2.8009788	-0.0014354
He	-0.0000047	-2.8263926	0.0003837
He	-0.0000111	1.8200657	2.0328342
He	-0.0000040	1.8187695	-2.0337611
He	-2.0327915	1.8191737	-0.0002060
He	2.0327995	1.8191796	-0.0002063
He	1.4292665	-1.8162637	1.4312339
He	-1.4292618	-1.8162570	1.4312305
He	-1.4299741	-1.8167675	-1.4304128
He	1.4299768	-1.8167725	-1.4304178
He	1.9085923	0.5120517	1.9097714

He	-1.9085887	0.5120496	1.9097655
He	-1.9086173	0.5115316	-1.9096302
He	1.9086180	0.5115279	-1.9096319
He	2.7043184	-0.5104605	0.0001254
He	-2.7043077	-0.5104579	0.0001273
He	-0.0000088	-0.5102862	2.7077333
He	-0.0000107	-0.5116793	-2.7074586

Cartesian Coordinates (Å) of $ThHe_{18}^{q+}$ (q=3, 4)

$ThHe_{18}^{3+}$

Th	0.0003130	0.0200369	0.0147806
He	0.0280231	2.6782793	-0.4339479
He	-0.0281616	-2.6153862	0.5855044
He	-0.1127778	2.0345873	1.7477625
He	0.1476722	1.3113897	-2.2932266
He	-1.9950524	1.7308297	-0.4388175
He	2.0369528	1.6994387	-0.3508238
He	1.6448820	-1.4085998	1.5658043
He	-1.7055973	-1.4281033	1.4745790
He	-1.6664130	-1.9033270	-0.8417927
He	1.6557887	-1.9422023	-0.7303804
He	1.8400205	0.8601829	1.7572442
He	-1.9994090	0.8011723	1.6328566
He	-1.7695385	0.0941036	-1.9909280
He	1.9517721	0.0065871	-1.8428762
He	3.1614649	-0.3244829	0.1575708
He	-3.1549132	-0.3009135	-0.0792697
He	-0.0683923	-0.2623922	2.6439607
He	0.0538323	-1.3080232	-2.2843361

$ThHe_{18}^{4+}$

Th	-0.0000321	0.0037873	-0.0000048
He	0.0000031	2.6593151	-0.0007429
He	0.0000005	-2.6843630	0.0004364
He	-0.0000037	1.6874199	1.8648168
He	-0.0000018	1.6864772	-1.8657890
He	-1.8649678	1.6869803	-0.0003230
He	1.8649806	1.6870001	-0.0003248
He	1.3103783	-1.6849335	1.3115522
He	-1.3103729	-1.6849199	1.3115431
He	-1.3105970	-1.6854031	-1.3107873
He	1.3106002	-1.6854109	-1.3107928
He	1.7742940	0.4678604	1.7739492
He	-1.7742917	0.4678560	1.7739322

He	-1.7743640	0.4670802	-1.7740620
He	1.7743657	0.4670814	-1.7740789
He	2.5108167	-0.4671788	0.0002087
He	-2.5107998	-0.4671720	0.0002102
He	-0.0000046	-0.4651265	2.5118551
He	-0.0000036	-0.4663500	-2.5115984

Cartesian Coordinates (Å) of $AnHe_{17}^{q+}$ (An=Th, q=4; An=Pa, q=5; An=U, q=6)

$ThHe_{17}^{4+}$

Th	-0.0154794	0.1311564	-0.0005670
He	-0.0333124	2.6591750	0.0164723
He	-0.3233917	1.6989723	1.9278647
He	0.2734643	1.7297360	-1.9064689
He	-1.9485532	1.6988488	0.2796589
He	1.8954301	1.7286899	-0.2591395
He	1.0433601	-1.8987448	1.0433311
He	-1.1245661	-1.8318462	1.0950030
He	-1.0453777	-1.9012589	-1.0698692
He	1.1194268	-1.8033962	-1.1215208
He	1.6711782	0.8693882	1.7204546
He	-1.8277624	0.1270908	1.7854177
He	-1.7106098	0.8745167	-1.7114102
He	1.7956087	0.1735717	-1.7894206
He	2.4171055	-0.4587444	0.1901123
He	-2.4398873	-0.4895016	-0.2043820
He	0.1519504	-0.4912967	2.4266468
He	-0.1772593	-0.4607093	-2.4340123

$PaHe_{17}^{5+}$

Pa	-0.0074424	-0.0454443	0.0111894
He	0.1232187	-2.4153917	-0.0118233
He	-0.1414568	1.7660083	1.5053967
He	-0.1051486	1.7957722	-1.4487106
He	-1.5305990	1.7705814	0.0108044
He	1.2570564	1.9662193	0.0479676
He	1.1355174	-1.4798012	1.4849261
He	-1.0147340	-1.5995311	1.4618838
He	-0.9788289	-1.5686490	-1.4959360
He	1.1719374	-1.4491876	-1.4626352
He	1.6846711	0.6117932	1.5055033
He	-1.7876657	0.3975223	1.4890587
He	-1.7513313	0.4285439	-1.5014012
He	1.7203044	0.6429599	-1.4262425
He	2.2907215	-0.6521837	0.0335150

He	-2.2186680	-0.8916022	-0.0252327
He	-0.0221310	-0.0714171	2.4145647
He	0.0371787	-0.0223766	-2.3921913

UHe_{17}^{6+}

U	0.0039430	-0.0058398	-0.0028691
He	0.0011812	2.3154442	0.0107271
He	-0.2956298	1.4236771	1.7506397
He	0.2850061	1.4405704	-1.7431702
He	-1.7524203	1.4260362	0.2507761
He	1.7539298	1.4371554	-0.2547634
He	0.9640934	-1.8749027	0.9642279
He	-1.0153288	-1.7852324	0.9997214
He	-0.9351695	-1.8843933	-0.9765670
He	1.0406823	-1.7706934	-1.0133626
He	1.5429009	0.7028398	1.5740994
He	-1.6912947	-0.0106288	1.6496408
He	-1.5443095	0.6985247	-1.5795239
He	1.6923929	0.0132864	-1.6637931
He	2.2131858	-0.5453781	0.1911358
He	-2.1989725	-0.5660834	-0.2063068
He	0.1552028	-0.5598733	2.2066553
He	-0.1487358	-0.5509225	-2.2138991

Cartesia*n* Coordi*n*ates (Å) of A*n*He_{16}^{3+} (A*n*=Th-U)

$ThHe_{16}^{3+}$

Th	0.0254051	-0.0218638	0.0094330
He	-0.1782360	1.6599194	2.0372880
He	0.2042833	-1.7852892	1.9451895
He	-1.6129509	-0.1972652	2.0470910
He	1.6483173	0.1061865	2.0625969
He	1.3497690	-1.0809653	-1.9756790
He	-1.0315535	-1.4407961	-1.9506450
He	-1.0197891	0.8949010	-2.2030757
He	1.3261926	1.2885340	-1.8777635
He	2.0670120	-1.7253645	0.4146971
He	-1.7110178	-1.9742758	0.5055312
He	-1.9693025	1.6689305	0.5078277
He	1.5933490	2.0607323	0.5935217
He	2.6937808	0.2941151	-0.2623216
He	-2.5444818	-0.1881468	-0.6303654
He	0.2318726	-2.6595264	-0.4440350
He	-0.2436681	2.5431359	-0.6597915

$PaHe_{16}^{3+}$

Pa	0.0378538	0.0146467	0.0079519
He	-0.0256383	1.3839512	2.2573920
He	0.1368500	-1.7758256	1.8685232
He	-1.6659741	-0.2061589	1.9537183
He	1.7069567	-0.0524821	2.0157497
He	1.3219633	-1.0482914	-1.9417568
He	-1.0096935	-1.5293322	-1.8341614
He	-0.9012300	0.6558891	-2.3335907
He	1.3609366	1.2867232	-1.8373129
He	2.0671424	-1.6815394	0.3265547
He	-1.7315334	-1.8925104	0.4093556
He	-1.7072277	1.8340478	0.7457816
He	1.2742569	2.2185377	0.5481769
He	2.6257696	0.4501780	-0.1218766
He	-2.4689862	0.0879888	-0.5858193
He	0.2426847	-2.7296095	-0.3696993
He	-0.4351486	2.4267487	-0.9894875

UHe_{16}^{3+}

U	-0.0112333	0.0103284	0.0062710
He	1.6232539	1.8771590	0.9014782
He	-1.4310616	0.3312864	2.2108052
He	-0.6633128	2.2381632	1.1148273
He	0.8061922	0.3776776	2.4860927
He	-0.6290860	-2.4810004	-0.6164208
He	-1.8552952	-0.7467697	-1.6113509
He	0.7147035	-1.3594940	-2.1297462
He	1.6017716	-2.0789566	-0.1002521
He	-1.9056838	-1.5615925	0.9836798
He	-1.4213408	1.9613028	-1.0692050
He	0.8857837	2.1740575	-1.2076147
He	2.4351159	-0.2826525	0.9670723
He	0.2802868	-1.7937375	1.8121570
He	-0.2262120	0.6474258	-2.5574981
He	-2.5905674	0.5179066	0.2074266
He	2.1860654	0.2458516	-1.3032303

Cartesia*n* Coordi*n*ates (Å) of Ac*n*g*n*$^{3+}$ (*n*g=*n*e-Xe)

$Ac*n*e_{15}^{3+}$

Ac	0.0649089	0.0374574	-0.0842097
*n*e	-0.7301278	2.3808119	1.5004672
*n*e	-0.2941238	2.3970812	-1.5590759
*n*e	-2.4540755	1.5129865	-0.1705287

*n*e	1.6001231	2.4558837	0.4254928
*n*e	1.5890502	-1.7620539	1.6627125
*n*e	-0.8151548	-2.4290434	1.1894670
*n*e	-0.6758719	-2.3538666	-1.4566864
*n*e	1.9594319	-1.8652829	-0.9806477
*n*e	1.0340101	0.6682458	2.5117670
*n*e	-1.5858081	-0.0590368	2.2040448
*n*e	-1.7458412	0.1592806	-2.3081171
*n*e	2.1182923	1.1501184	-1.7935565
*n*e	2.8988724	0.1769591	0.5271491
*n*e	-2.6250572	-1.0840760	-0.1079119
*n*e	0.6398915	-0.5977066	-2.9156596

$AcAr_{10}^{3+}$

Ac	-0.3567782	0.7265734	-0.2300788
Ar	-0.5772107	3.5234594	1.3052302
Ar	-0.3854128	2.1160940	-3.0604747
Ar	-3.0111041	2.3904742	-0.8202945
Ar	2.0763068	2.7343745	-0.7034171
Ar	2.5104530	-0.6485413	-0.6297476
Ar	-0.1893949	-2.1482962	1.0277506
Ar	-2.9904791	-1.0247935	-0.7495303
Ar	-0.1631655	-1.3232921	-2.6547252
Ar	1.3773972	0.7955615	2.3861020
Ar	-2.2092375	0.5558364	2.2981995

$AcKr_{10}^{3+}$

Ac	-0.0004260	0.0232246	-0.0506911
Kr	-0.2416594	3.0302771	1.5774009
Kr	-0.0277725	1.4908501	-3.0446000
Kr	-2.8415353	1.7956987	-0.6702414
Kr	2.6037483	2.1658224	-0.5413135
Kr	3.0858528	-1.4466482	-0.4970818
Kr	0.1760212	-3.0247055	1.2550756
Kr	-2.8384850	-1.8494789	-0.6301640
Kr	0.2060649	-2.1790022	-2.6192606
Kr	1.8485724	0.1064053	2.7030297
Kr	-1.9679374	-0.1529032	2.6154212

$AcXe_{8}^{3+}$

Ac	-0.0001944	0.0004863	0.0003323
Xe	-0.2006829	3.3142520	1.0918181
Xe	0.8797183	1.9738265	-2.7414508
Xe	-3.0764723	1.0938363	-1.2427562

Xe	3.1388785	-1.1303005	-1.0391934
Xe	0.1324823	-3.2807289	1.1931258
Xe	-0.7227900	-2.0475573	-2.7328110
Xe	2.0805535	0.2256210	2.7958932
Xe	-2.2312394	-0.1464035	2.6833455

$AcAr_{12}^{3+}$

Ac	-0.0064321	0.1613828	-0.1126065
Ar	-0.3569055	2.9493779	1.5683140
Ar	0.2761831	2.9423875	-1.8170246
Ar	-2.7651033	1.8465367	-0.6342013
Ar	2.7116720	1.9203437	0.3924955
Ar	2.7523255	-1.5238930	0.4086246
Ar	-0.2891103	-2.6194634	1.5923734
Ar	-2.7245511	-1.5977689	-0.6176913
Ar	0.3439262	-2.6270428	-1.7930608
Ar	1.1755828	0.1899758	2.9434158
Ar	-2.2100788	0.1450782	2.3070474
Ar	-1.1882409	0.1325036	-3.1686210
Ar	2.1968810	0.1777352	-2.5324220

$AcKr_{12}^{3+}$

Ac	-0.0064609	0.1613050	-0.1126145
Kr	-0.3826153	3.1589140	1.6936062
Kr	0.2963391	3.1517449	-1.9443858
Kr	-2.9725790	1.9724941	-0.6733540
Kr	2.9154266	2.0507721	0.4309139
Kr	2.9597370	-1.6495599	0.4472938
Kr	-0.3093927	-2.8281639	1.7202355
Kr	-2.9282337	-1.7284680	-0.6560840
Kr	0.3696194	-2.8368753	-1.9179210
Kr	1.2634013	0.1918925	3.1753014
Kr	-2.3749951	0.1437606	2.4899818
Kr	-1.2759134	0.1304088	-3.4006078
Kr	2.3618155	0.1789283	-2.7157221

$AcXe_{12}^{3+}$

Ac	-0.0063746	0.1612593	-0.1125097
Xe	-0.4210592	3.4620122	1.8753730
Xe	0.3274809	3.4530775	-2.1298069
Xe	-3.2720626	2.1551167	-0.7297988
Xe	3.2106775	2.2418562	0.4863145
Xe	3.2590979	-1.8324598	0.5047673
Xe	-0.3403766	-3.1304085	1.9045021

Xe	-3.2236764	-1.9192436	-0.7114511
Xe	0.4081659	-3.1393375	-2.1006408
Xe	1.3922992	0.1952062	3.5080264
Xe	-2.6123648	0.1419400	2.7522930
Xe	-1.4052203	0.1274805	-3.7330450
Xe	2.5995621	0.1806539	-2.9773807

Cartesian Coordinates (Å) of the potetial energy minimum structure of $AcAr_n^{3+}$ by AIMD

$AcAr_{10}^{3+}$

Ac	-0.341723	0.724974	-0.228494
Ar	-0.573627	3.531934	1.320062
Ar	-0.405558	2.102679	-3.047847
Ar	-3.007184	2.397427	-0.842387
Ar	2.079925	2.732924	-0.712099
Ar	2.516414	-0.645057	-0.638566
Ar	-0.186009	-2.157332	1.031794
Ar	-2.998035	-1.028356	-0.735354
Ar	-0.155496	-1.306967	-2.653594
Ar	1.372507	0.786558	2.391087
Ar	-2.219839	0.558666	2.284410

$AcAr_{11}^{3+}$

Ac	0.130921	-0.274761	-0.058243
Ar	-0.019834	2.442194	1.620510
Ar	0.348832	3.947579	-1.545343
Ar	-2.245538	1.614507	-0.959315
Ar	2.654103	1.521801	-0.399833
Ar	2.944645	-1.861379	-0.067842
Ar	-0.066866	-3.140085	1.194310
Ar	-2.552767	-1.763997	-0.889436
Ar	0.463312	-2.548805	-2.293389
Ar	1.562438	-0.443207	2.741835
Ar	-2.002680	-0.320781	2.255836
Ar	0.458741	0.777742	-3.031223

$AcAr_{14}^{3+}$

Ac	-0.379845	-0.113810	-0.141952
Ar	0.310617	3.233884	2.976142
Ar	0.318553	3.462513	-2.945343
Ar	-1.765577	2.717495	0.022367
Ar	1.692561	2.220635	-0.029788
Ar	1.829447	-3.793907	2.927315
Ar	-1.186119	-2.684237	1.510482

Ar	-1.288349	-2.500567	-2.046038
Ar	1.709723	-2.508248	-0.376321
Ar	1.537511	-0.312975	2.330371
Ar	-1.796525	0.502967	2.674790
Ar	-1.918681	0.795271	-2.825804
Ar	1.434847	-0.000023	-2.719706
Ar	4.207572	-0.135650	-0.248764
Ar	-3.531940	-0.566206	-0.098750

Cartesian Coordinates (Å) of the structure of Ac^{3+}-Ng_{32}

Ac^{3+}-Ne_{32}

Ac	-0.2557642	-0.0021300	-0.0329163
Ne	-0.5587989	2.4423933	1.2109196
Ne	0.1072413	2.2481639	-1.5910966
Ne	-2.5446496	1.4116516	-0.6442176
Ne	2.0276362	1.4707031	0.4508044
Ne	2.0205464	-1.4308226	0.5947508
Ne	-0.6078562	-2.2751687	1.4909097
Ne	-2.5461581	-1.4652977	-0.5151873
Ne	0.0347948	-2.4397809	-1.2981961
Ne	0.5736939	0.1409147	2.5966771
Ne	-2.2009524	0.1632670	1.9211082
Ne	-1.0798125	-0.1336120	-2.6639635
Ne	1.7171178	-0.1846285	-1.9559249
Ne	1.2801902	4.0384617	0.0407959
Ne	1.5769574	2.6317245	2.8445563
Ne	-1.7467442	3.9799563	-0.6637484
Ne	2.7650903	2.2964542	-2.0042965
Ne	-1.1711443	1.8477249	3.7648016
Ne	-2.1065118	2.3120114	-3.1393394
Ne	-3.2128448	2.6454968	1.6604578
Ne	0.7796577	1.2790707	-4.0194054
Ne	-3.7718832	-0.1156363	-2.5068390
Ne	4.0243624	-0.0324760	-0.5623095
Ne	3.2663247	0.1182222	2.4267481
Ne	-4.5225767	0.0234492	0.5627881
Ne	-1.2320700	-1.3482242	3.9414087
Ne	-2.1126821	-2.6102901	-2.9189513
Ne	-3.2592551	-2.3132736	1.9408914
Ne	0.6816771	-1.8182225	-3.8400590
Ne	1.5613575	-2.3093511	3.1014562
Ne	-1.8181337	-4.0401160	-0.1452003
Ne	2.6914635	-2.6831633	-1.7017224

Ne	1.2381888	-4.0092768	0.5478735

Ac^{3+}-Ar_{32}

Ac	-0.2869763	0.0034966	-0.0206506
Ar	-0.6848861	2.8416309	1.4318416
Ar	0.1343762	2.6249213	-1.8432795
Ar	-3.0250010	1.7059192	-0.7820436
Ar	2.4031841	1.7208497	0.5343885
Ar	2.4122436	-1.6791274	0.7353064
Ar	-0.6811930	-2.6339024	1.7715830
Ar	-3.0028658	-1.7213505	-0.5963264
Ar	0.1091246	-2.8368218	-1.4993672
Ar	0.7482411	0.1849346	3.0412916
Ar	-2.5760142	0.1331575	2.2227824
Ar	-1.2985175	-0.1674447	-3.0701423
Ar	2.0338151	-0.1677577	-2.2581531
Ar	1.8234909	5.1483608	-0.0491050
Ar	2.0586531	3.4730209	3.6118636
Ar	-2.2183979	5.1639672	-0.9733312
Ar	3.6626104	2.9229422	-2.5915375
Ar	-1.3680322	2.2886956	4.8939843
Ar	-2.5058031	3.0748522	-4.1388007
Ar	-4.1005689	3.3711427	2.3053111
Ar	1.1289502	1.5952150	-5.1304956
Ar	-4.9089071	-0.0953479	-3.2456084
Ar	5.2576482	-0.0114779	-0.6817396
Ar	4.3754911	0.0747965	3.0824206
Ar	-5.8517235	0.0467285	0.7502471
Ar	-1.3946356	-1.6656344	5.1315374
Ar	-2.5371818	-3.4503448	-3.7810384
Ar	-4.1244735	-3.0971456	2.5443368
Ar	1.0027096	-2.1869921	-4.9334258
Ar	2.0451623	-3.0377075	4.0143078
Ar	-2.2266267	-5.1884937	-0.2297617
Ar	3.4827764	-3.4691305	-2.1989730
Ar	1.7117896	-5.1277573	0.8461517

Ac^{3+}-Kr_{32}

Ac	-0.2550842	-0.0047875	-0.0332154
Kr	-0.6597942	3.0721779	1.5611173
Kr	0.2014729	2.8396181	-1.9918405
Kr	-3.1242047	1.8044087	-0.8456495
Kr	2.6472456	1.8444258	0.5551451
Kr	2.6129393	-1.8134464	0.7798306

Kr	-0.7096990	-2.8513897	1.9249203
Kr	-3.1566542	-1.8543899	-0.6222835
Kr	0.1506242	-3.0819534	-1.6294704
Kr	0.8265478	0.1920485	3.2810461
Kr	-2.7350639	0.1679868	2.4123693
Kr	-1.3343449	-0.2014433	-3.3460415
Kr	2.2287480	-0.1784094	-2.4800493
Kr	1.8725234	5.6049991	0.1171367
Kr	2.3287038	3.6872510	3.9299939
Kr	-2.2930274	5.5753706	-0.8904920
Kr	3.9557948	3.2631845	-2.7867410
Kr	-1.5596967	2.4912376	5.2698989
Kr	-2.7802687	3.2135557	-4.4209815
Kr	-4.4082258	3.6442548	2.2962395
Kr	1.0903874	1.7907766	-5.5997145
Kr	-5.1925671	-0.1684782	-3.4446648
Kr	5.7004662	-0.1088426	-0.7849952
Kr	4.6871793	0.1624069	3.3697408
Kr	-6.2089738	0.0985033	0.7311184
Kr	-1.5970580	-1.8039328	5.5315703
Kr	-2.8405547	-3.6923921	-4.0003958
Kr	-4.4659367	-3.2706292	2.7225349
Kr	1.0490622	-2.5019919	-5.3357022
Kr	2.2718442	-3.2215473	4.3554621
Kr	-2.3854005	-5.6133676	-0.1854534
Kr	3.8948660	-3.6609196	-2.3581187
Kr	1.7866119	-5.5860900	0.8112592