SUPPLEMENTARY MATERIAL

Exploring Americium and Curium water clusters: gas-phase structures, solvation number, solvent and entropy effects

Shu-Wen Zhang,[a,b] Yu Cheng,[a,b] Yang-Yang Zhang [a,b]*

[a] School of Rare Earths, University of Science and technology of China, Hefei 230026, China

[b] Fundamental Science Center of Rare Earths, Ganjiang Innovation Academy, Chinese Academy of Sciences, Ganzhou, 341000 Jiangxi, China

Corresponding Authors

*E–mail: yyzhang@gia.cas.cn

Contents

Part A: Results calculated at PBE0-D4/def2−TZVP/ECP60MWB_SEG level

Table S1. The coordination number (CN) of An^{3+} ion with water and the average bond lengths (in Å) of *d*(An–O) among the first solvation shell for the global–minimum structure of $An(H_2O)_n^{3+}$ (An = Am^{3+}, Cm^{3+}; *n*=1–20) clusters in the gas phase at the PBE0-D4/def2–TZVP/ECP60MWB_SEG level.

$Am(H_2O)_n^{3+}$	CN	*d*(Am–O)	$Cm(H_2O)_n^{3+}$	CN	*d*(Cm–O)
$Am(H_2O)^{3+}$	1	2.207	$Cm(H_2O)^{3+}$	1	2.219
$Am(H_2O)_2^{3+}$	2	2.276	$Cm(H_2O)_2^{3+}$	2	2.308
$Am(H_2O)_3^{3+}$	3	2.297	$Cm(H_2O)_3^{3+}$	3	2.294
$Am(H_2O)_4^{3+}$	4	2.336	$Cm(H_2O)_4^{3+}$	4	2.33
$Am(H_2O)_5^{3+}$	5	2.373	$Cm(H_2O)_5^{3+}$	5	2.375
$Am(H_2O)_6^{3+}$	6	2.421	$Cm(H_2O)_6^{3+}$	6	2.417
$Am(H_2O)_7^{3+}$	7	2.452	$Cm(H_2O)_7^{3+}$	7	2.448
$Am(H_2O)_8^{3+}$	6	2.406	$Cm(H_2O)_8^{3+}$	8	2.482
$Am(H_2O)_9^{3+}$	6	2.399	$Cm(H_2O)_9^{3+}$	6	2.393
$Am(H_2O)_{10}^{3+}$	7	2.436	$Cm(H_2O)_{10}^{3+}$	7	2.431
$Am(H_2O)_{11}^{3+}$	7	2.432	$Cm(H_2O)_{11}^{3+}$	7	2.429
$Am(H_2O)_{12}^{3+}$	7	2.43	$Cm(H_2O)_{12}^{3+}$	7	2.426
$Am(H_2O)_{13}^{3+}$	8	2.478	$Cm(H_2O)_{13}^{3+}$	8	2.469
$Am(H_2O)_{14}^{3+}$	8	2.475	$Cm(H_2O)_{14}^{3+}$	8	2.467
$Am(H_2O)_{15}^{3+}$	8	2.47	$Cm(H_2O)_{15}^{3+}$	8	2.463
$Am(H_2O)_{16}^{3+}$	9	2.519	$Cm(H_2O)_{16}^{3+}$	9	2.513
$Am(H_2O)_{17}^{3+}$	9	2.519	$Cm(H_2O)_{17}^{3+}$	9	2.511
$Am(H_2O)_{18}^{3+}$	9	2.517	$Cm(H_2O)_{18}^{3+}$	9	2.521
$Am(H_2O)_{19}^{3+}$	9	2.523	$Cm(H_2O)_{19}^{3+}$	9	2.518
$Am(H_2O)_{20}^{3+}$	9	2.525	$Cm(H_2O)_{20}^{3+}$	9	2.516

Table S2. The coordination number (CN) of An^{3+} ion with water and the average bond length (in Å) of *d*(An–O) (An=Am, Cm) among the first solvation shell for the global–minimum structure of $Am(H_2O)_n^{3+}$ and $Cm(H_2O)_n^{3+}$(*n*=1–20) clusters in the CPCM water solvent model at the PBE0-D4/def2–TZVP/ECP60MWB_SEG level.

$Am(H_2O)_n^{3+}$	CN	*d*(Am–O)	$Cm(H_2O)_n$	CN	*d*(Cm–O)
$Am(H_2O)^{3+}$	1	2.178	$Cm(H_2O)^{3+}$	1	2.196
$Am(H_2O)_2^{3+}$	2	2.253	$Cm(H_2O)_2^{3+}$	2	2.233
$Am(H_2O)_3^{3+}$	3	2.265	$Cm(H_2O)_3^{3+}$	3	2.262
$Am(H_2O)_4^{3+}$	4	2.303	$Cm(H_2O)_4^{3+}$	4	2.298
$Am(H_2O)_5^{3+}$	5	2.341	$Cm(H_2O)_5^{3+}$	5	2.341
$Am(H_2O)_6^{3+}$	6	2.383	$Cm(H_2O)_6^{3+}$	6	2.38
$Am(H_2O)_7^{3+}$	7	2.411	$Cm(H_2O)_7^{3+}$	7	2.407
$Am(H_2O)_8^{3+}$	8	2.447	$Cm(H_2O)_8^{3+}$	8	2.441
$Am(H_2O)_9^{3+}$	9	2.486	$Cm(H_2O)_9^{3+}$	9	2.478
$Am(H_2O)_{10}^{3+}$	9	2.497	$Cm(H_2O)_{10}^{3+}$	9	2.491
$Am(H_2O)_{11}^{3+}$	9	2.499	$Cm(H_2O)_{11}^{3+}$	9	2.493
$Am(H_2O)_{12}^{3+}$	9	2.501	$Cm(H_2O)_{12}^{3+}$	9	2.495
$Am(H_2O)_{13}^{3+}$	9	2.505	$Cm(H_2O)_{13}^{3+}$	8	2.455
$Am(H_2O)_{14}^{3+}$	8	2.463	$Cm(H_2O)_{14}^{3+}$	8	2.453
$Am(H_2O)_{15}^{3+}$	8	2.462	$Cm(H_2O)_{15}^{3+}$	8	2.454
$Am(H_2O)_{16}^{3+}$	9	2.516	$Cm(H_2O)_{16}^{3+}$	9	2.509
$Am(H_2O)_{17}^{3+}$	9	2.512	$Cm(H_2O)_{17}^{3+}$	9	2.506
$Am(H_2O)_{18}^{3+}$	9	2.513	$Cm(H_2O)_{18}^{3+}$	9	2.511
$Am(H_2O)_{19}^{3+}$	9	2.518	$Cm(H_2O)_{19}^{3+}$	9	2.513
$Am(H_2O)_{20}^{3+}$	9	2.519	$Cm(H_2O)_{20}^{3+}$	9	2.51

Table S3. The binding energy (BE) and average binding energy (BE/*n*) (in kcal/mol) for the global–minimum structure of $Am(H_2O)_n^{3+}$(*n*=1–20) calculated in the gas phase and solution at the PBE0-D4/def2–TZVP/ECP60MWB_SEG level with dispersion corrections, respectively.

Reaction	BE (gas)	BE (solution)	BE/*n* (gas)	BE/*n* (solution)
$Am^{3+} + H_2O \rightarrow Am(H_2O)^{3+}$	-110.86	-50.25	-110.86	-50.25
$Am^{3+} + 2\ H_2O \rightarrow Am(H_2O)_2^{3+}$	-199.52	-87.74	-99.76	-43.87
$Am^{3+} + 3\ H_2O \rightarrow Am(H_2O)_3^{3+}$	-277.01	-124.62	-92.34	-41.54
$Am^{3+} + 4\ H_2O \rightarrow Am(H_2O)_4^{3+}$	-343.77	-153.94	-85.94	-38.49
$Am^{3+} + 5\ H_2O \rightarrow Am(H_2O)_5^{3+}$	-398.47	-178.97	-79.69	-35.79
$Am^{3+} + 6\ H_2O \rightarrow Am(H_2O)_6^{3+}$	-446.23	-199.30	-74.37	-33.22
$Am^{3+} + 7\ H_2O \rightarrow Am(H_2O)_7^{3+}$	-485.65	-219.49	-69.38	-31.36
$Am^{3+} + 8\ H_2O \rightarrow Am(H_2O)_8^{3+}$	-520.68	-235.04	-65.09	-29.38
$Am^{3+} + 9\ H_2O \rightarrow Am(H_2O)_9^{3+}$	-555.51	-245.10	-61.72	-27.23
$Am^{3+} + 10\ H_2O \rightarrow Am(H_2O)_{10}^{3+}$	-588.19	-256.85	-58.82	-25.68
$Am^{3+} + 11\ H_2O \rightarrow Am(H_2O)_{11}^{3+}$	-614.52	-267.03	-55.87	-24.28
$Am^{3+} + 12\ H_2O \rightarrow Am(H_2O)_{12}^{3+}$	-645.93	-277.62	-53.83	-23.13
$Am^{3+} + 13\ H_2O \rightarrow Am(H_2O)_{13}^{3+}$	-669.15	-287.56	-51.47	-22.12
$Am^{3+} + 14\ H_2O \rightarrow Am(H_2O)_{14}^{3+}$	-696.08	-298.73	-49.72	-21.34
$Am^{3+} + 15\ H_2O \rightarrow Am(H_2O)_{15}^{3+}$	-716.13	-309.37	-47.74	-20.62
$Am^{3+} + 16\ H_2O \rightarrow Am(H_2O)_{16}^{3+}$	-732.09	-315.40	-45.76	-19.71
$Am^{3+} + 17\ H_2O \rightarrow Am(H_2O)_{17}^{3+}$	-753.04	-325.45	-44.30	-19.14
$Am^{3+} + 18\ H_2O \rightarrow Am(H_2O)_{18}^{3+}$	-774.64	-334.76	-43.04	-18.60
$Am^{3+} + 19\ H_2O \rightarrow Am(H_2O)_{19}^{3+}$	-795.86	-344.12	-41.89	-18.11
$Am^{3+} + 20\ H_2O \rightarrow Am(H_2O)_{20}^{3+}$	-816.51	-353.83	-40.83	-17.69

Table S4. The binding energy (BE) and average binding energy (BE/*n*) (in kcal/mol) for the global–minimum structure of $Cm(H_2O)_n^{3+}$(*n*=1–20) calculated in the gas phase and solution at the PBE0-D4/def2–TZVP/ECP60MWB_SEG level with dispersion corrections, respectively.

Reaction	BE (gas)	BE (solution)	BE/*n* (gas)	BE/*n* (solution)
$Cm^{3+} + H_2O \rightarrow Cm(H_2O)^{3+}$	-108.40	-48.31	-108.40	-48.31
$Cm^{3+} + 2\ H_2O \rightarrow Cm(H_2O)_2^{3+}$	-191.86	-89.26	-95.93	-44.63
$Cm^{3+} + 3\ H_2O \rightarrow Cm(H_2O)_3^{3+}$	-276.84	-125.22	-92.28	-41.74
$Cm^{3+} + 4\ H_2O \rightarrow Cm(H_2O)_4^{3+}$	-344.43	-154.78	-86.11	-38.69
$Cm^{3+} + 5\ H_2O \rightarrow Cm(H_2O)_5^{3+}$	-398.78	-179.29	-79.76	-35.86
$Cm^{3+} + 6\ H_2O \rightarrow Cm(H_2O)_6^{3+}$	-447.53	-200.84	-74.59	-33.47
$Cm^{3+} + 7\ H_2O \rightarrow Cm(H_2O)_7^{3+}$	-487.13	-221.20	-69.59	-31.60
$Cm^{3+} + 8\ H_2O \rightarrow Cm(H_2O)_8^{3+}$	-522.85	-238.01	-65.36	-29.75
$Cm^{3+} + 9\ H_2O \rightarrow Cm(H_2O)_9^{3+}$	-557.09	-248.98	-61.90	-27.66
$Cm^{3+} + 10\ H_2O \rightarrow Cm(H_2O)_{10}^{3+}$	-589.99	-260.38	-59.00	-26.04
$Cm^{3+} + 11\ H_2O \rightarrow Cm(H_2O)_{11}^{3+}$	-616.32	-270.49	-56.03	-24.59
$Cm^{3+} + 12\ H_2O \rightarrow Cm(H_2O)_{12}^{3+}$	-647.77	-281.07	-53.98	-23.42
$Cm^{3+} + 13\ H_2O \rightarrow Cm(H_2O)_{13}^{3+}$	-672.78	-291.82	-51.75	-22.45
$Cm^{3+} + 14\ H_2O \rightarrow Cm(H_2O)_{14}^{3+}$	-699.09	-302.16	-49.93	-21.58
$Cm^{3+} + 15\ H_2O \rightarrow Cm(H_2O)_{15}^{3+}$	-719.95	-313.24	-48.00	-20.88
$Cm^{3+} + 16\ H_2O \rightarrow Cm(H_2O)_{16}^{3+}$	-736.02	-319.07	-46.00	-19.94
$Cm^{3+} + 17\ H_2O \rightarrow Cm(H_2O)_{17}^{3+}$	-757.00	-328.57	-44.53	-19.33
$Cm^{3+} + 18\ H_2O \rightarrow Cm(H_2O)_{18}^{3+}$	-779.24	-338.41	-43.29	-18.80
$Cm^{3+} + 19\ H_2O \rightarrow Cm(H_2O)_{19}^{3+}$	-798.78	-347.89	-42.04	-18.31
$Cm^{3+} + 20\ H_2O \rightarrow Cm(H_2O)_{20}^{3+}$	-819.60	-357.39	-40.98	-17.87

Part B: Results calculated at PBE-D4/6–31G(d)/ECP(84/85)MWB_AVDZ level

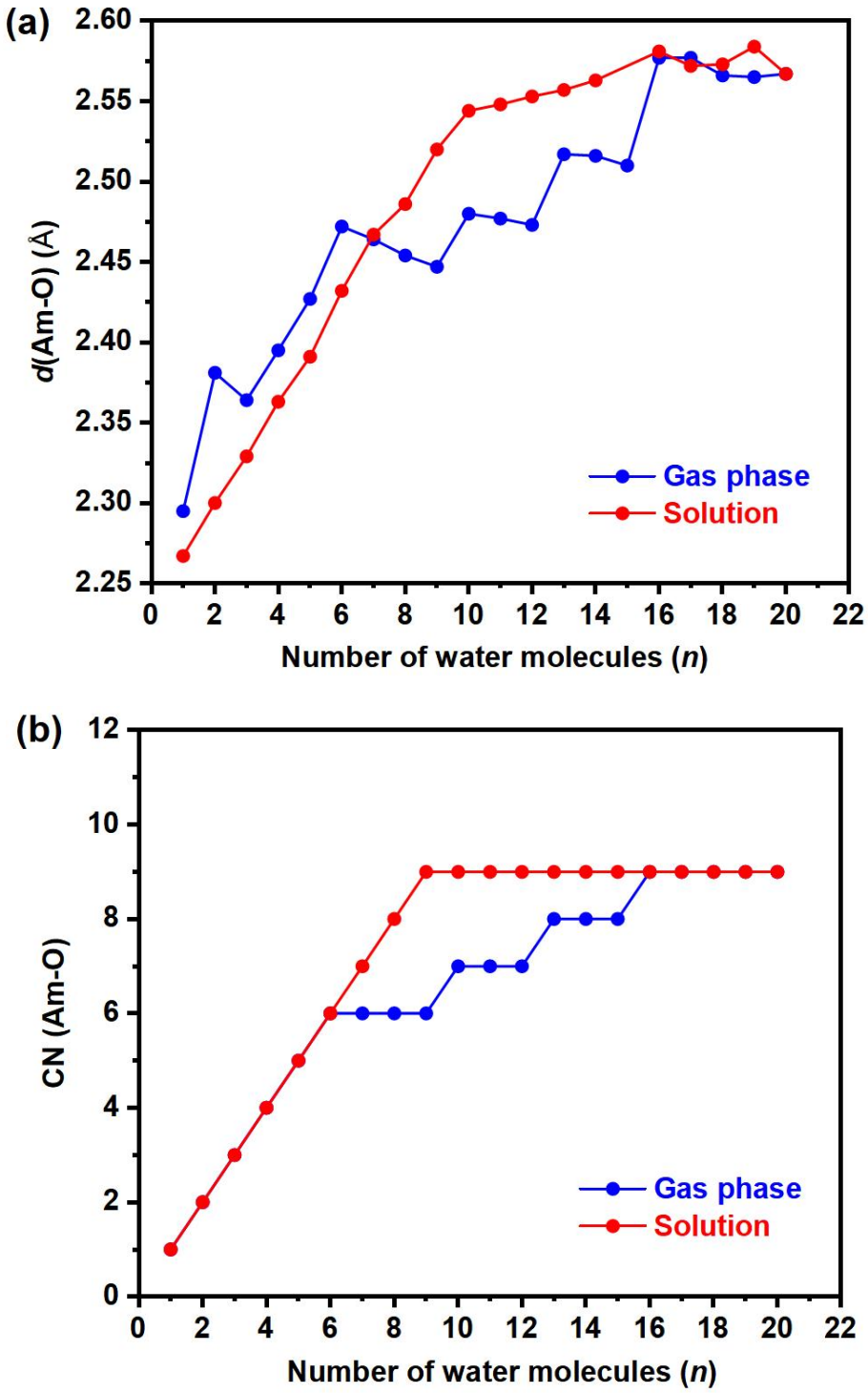


Fig. S1 (a) average bond lengths (in Å) of *d*(Am–O) and (b) coordination number (CN) of Am^{3+} among the first solvation shell changing with the different number of water molecules for the global–minimum structure of $Am(H_2O)_n^{3+}$ (n=1–20) clusters in the gas phase (in blue) and solution (in red) , respectively.

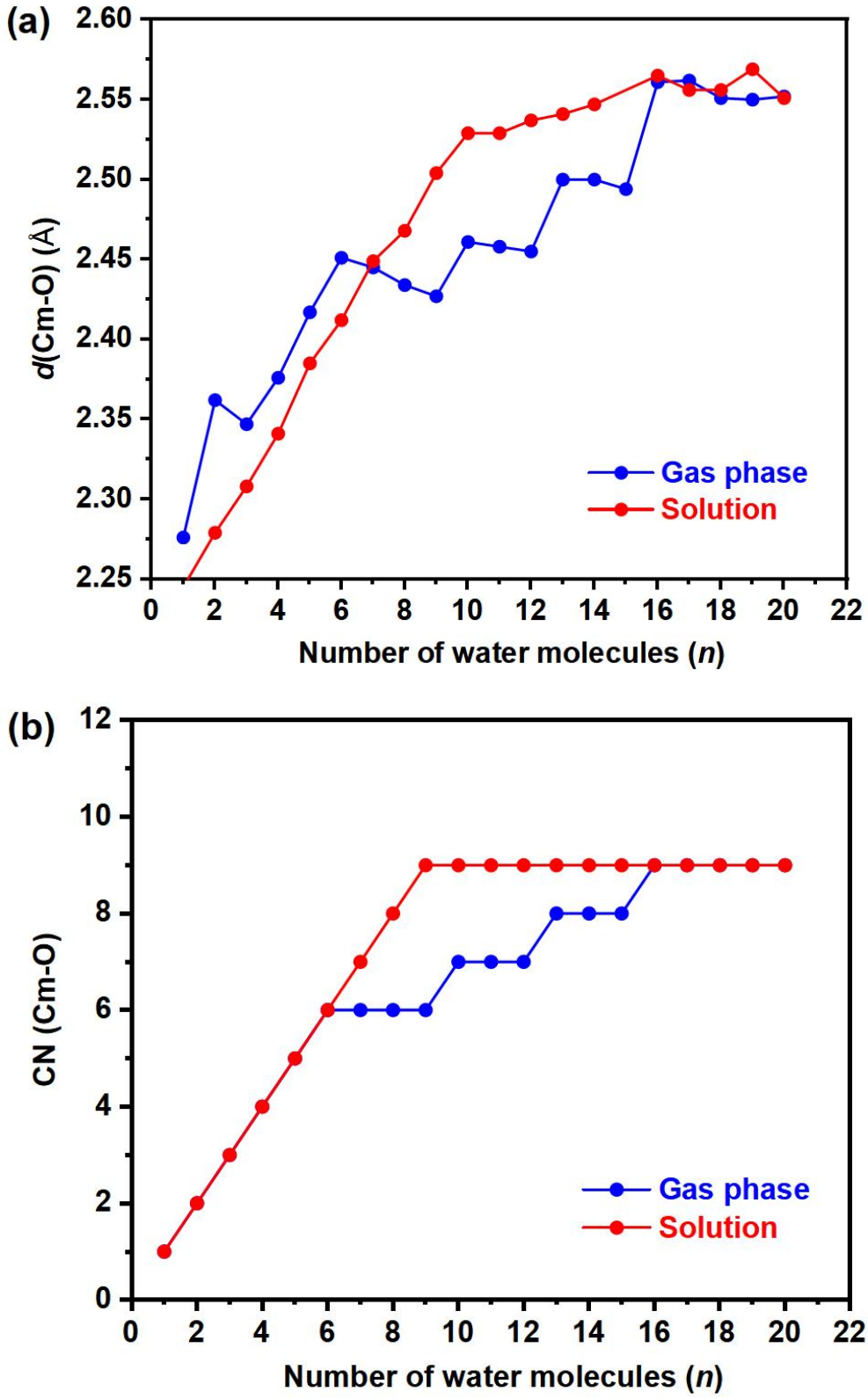


Fig. S2 (a) average bond lengths (in Å) of *d*(Cm–O) and (b) coordination number (CN) of Cm^{3+} among the first solvation shell changing with the different number of water molecules for the global–minimum structure of $Cm(H_2O)_n^{3+}$ (n=1–20) clusters in the gas phase (in blue) and solution (in red) , respectively.

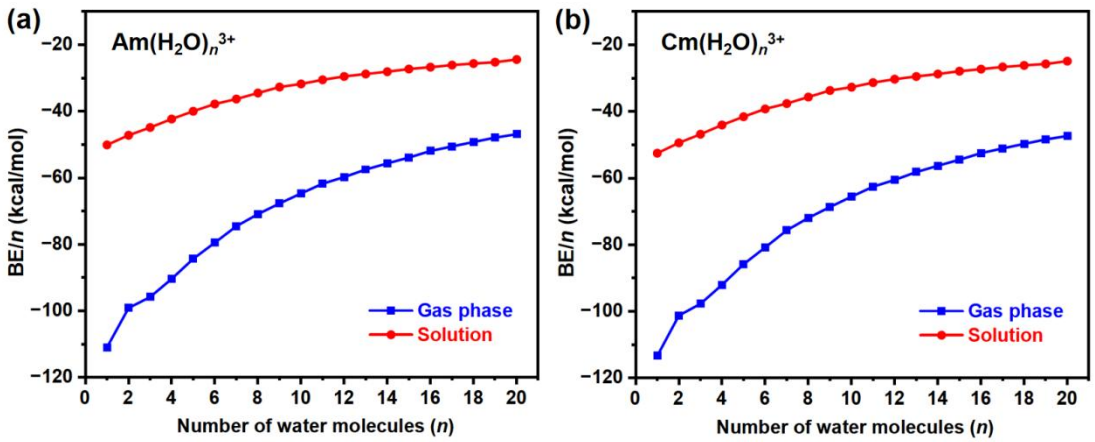


Fig. S3 The average binding energy (BE/*n*) (in kcal/mol) for the global–minimum structure of (a) $Am(H_2O)_n^{3+}$ and (b) $Cm(H_2O)_n^{3+}$(n=1–20) calculated in the gas phase (in blue) and solution (in red) at the DFT PBE/6–31G(d)/RECP level with dispersion corrections, respectively.

Part C: Results calculated at PBE-D4/6–31G(d)/ECP(84/85)MWB_GUESS level

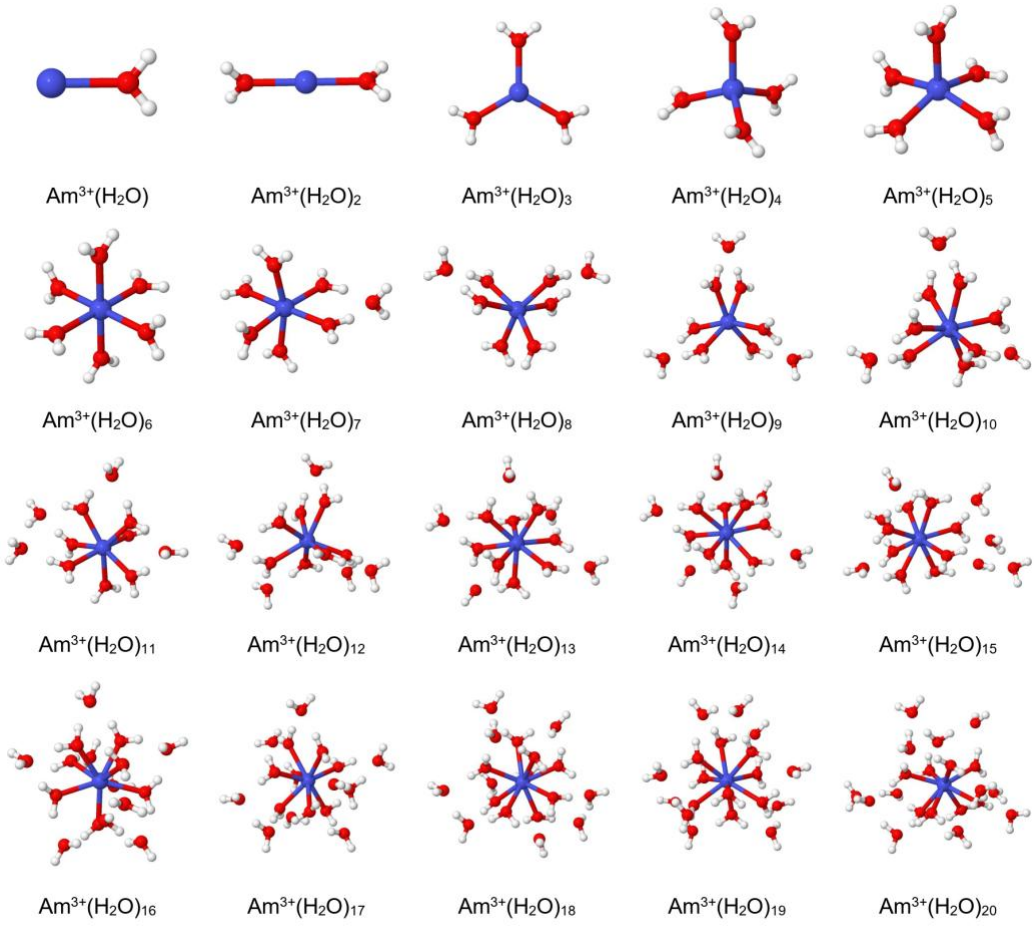


Fig. S4 Global–minimum structures of $Am(H_2O)_n^{3+}$(n=1–20) obtained from global–minimum search in the gas phase at the PBE/6–31G(d)/RECP level with dispersion corrections. Color codes: Am (blue), O (red) and H (white).

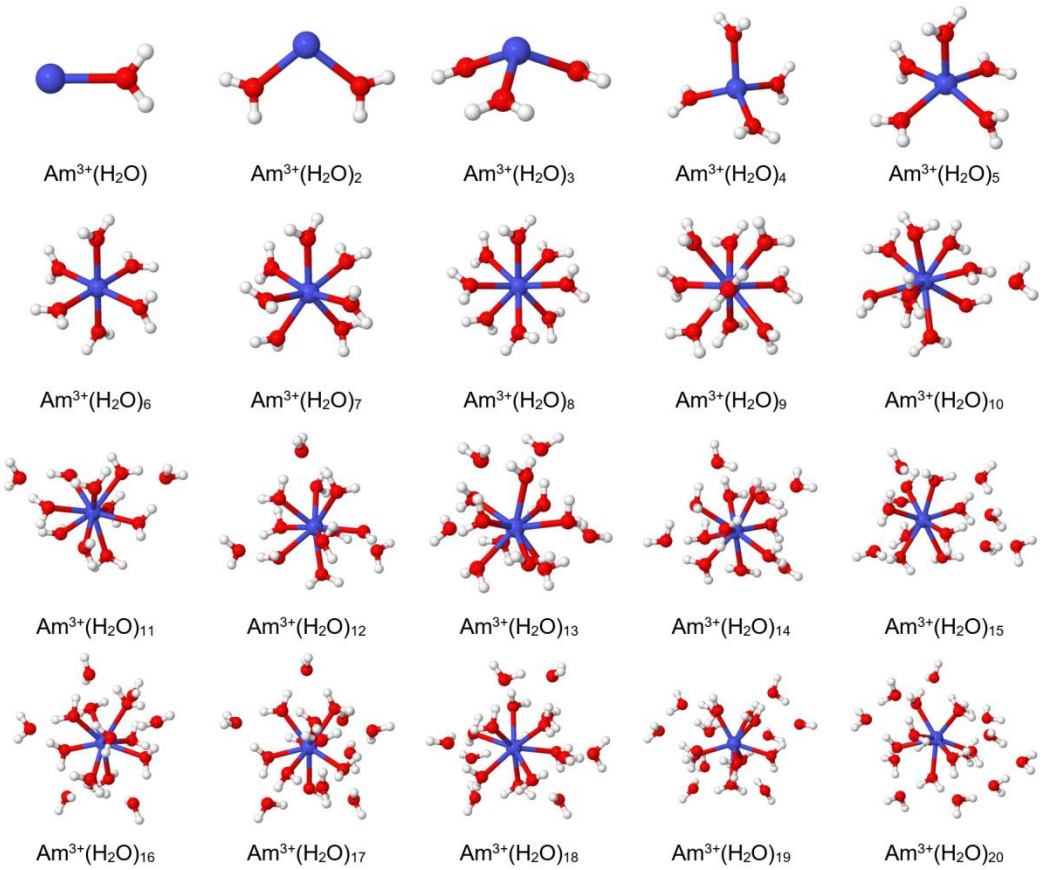


Fig. S5 Global–minimum structures of $Am(H_2O)_n^{3+}$(n=1–20) obtained from global–minimum search in the solution at the PBE/6–31G(d)/RECP level with dispersion corrections. Color codes: Am (blue), O (red) and H (white).

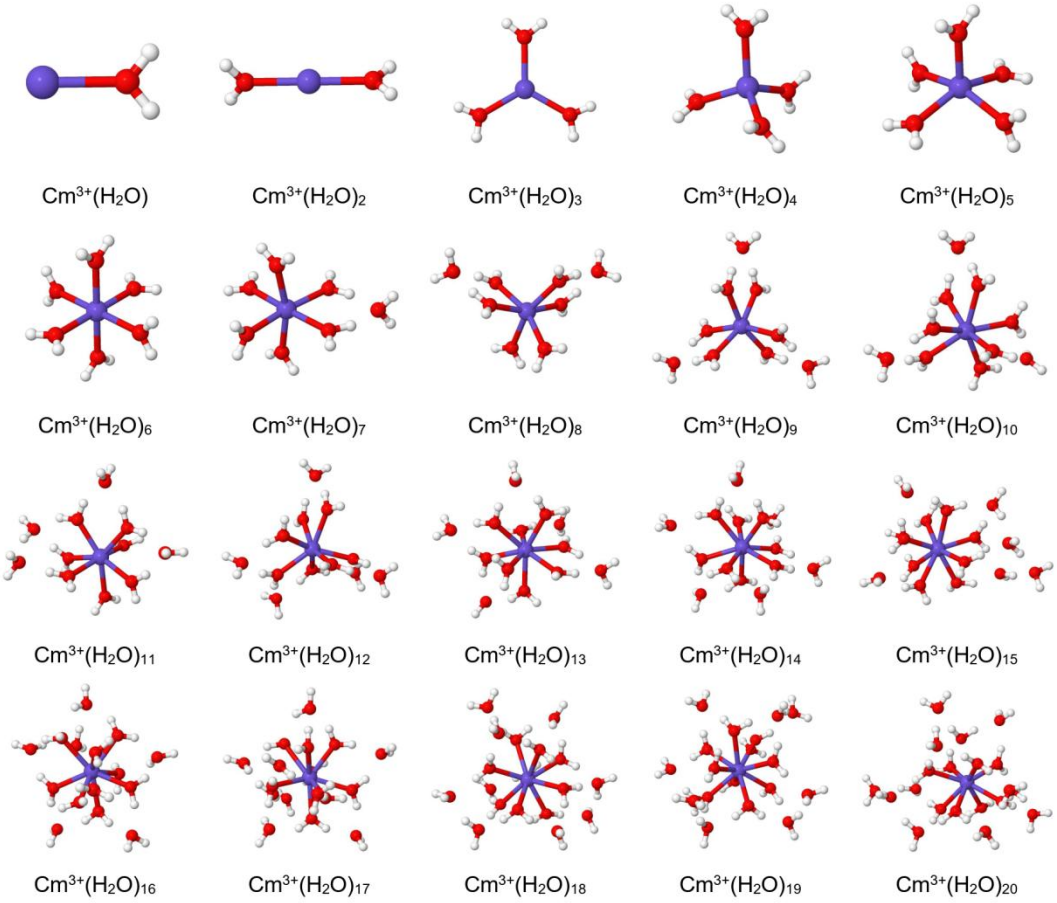


Fig. S6 Global–minimum structures of $Cm(H_2O)_n^{3+}$(n=1–20) obtained from global–minimum search in the gas phase at the PBE/6–31G(d)/RECP level with dispersion corrections. Color codes: Cm (purple), O (red) and H (white).

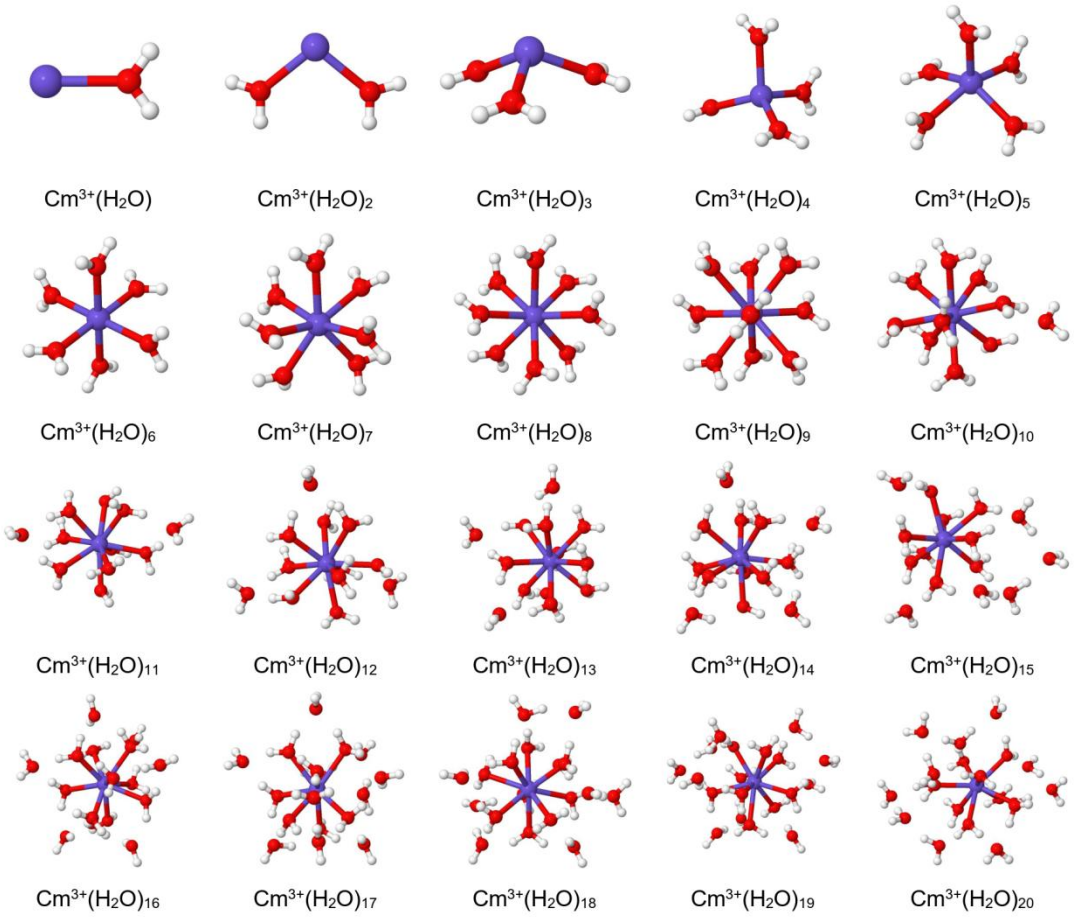


Fig. S7 Global–minimum structures of $Cm(H_2O)_n^{3+}$(n=1–20) obtained from global–minimum search in the solution at the PBE/6–31G(d)/RECP level with dispersion corrections. Color codes: Cm (purple), O (red) and H (white).

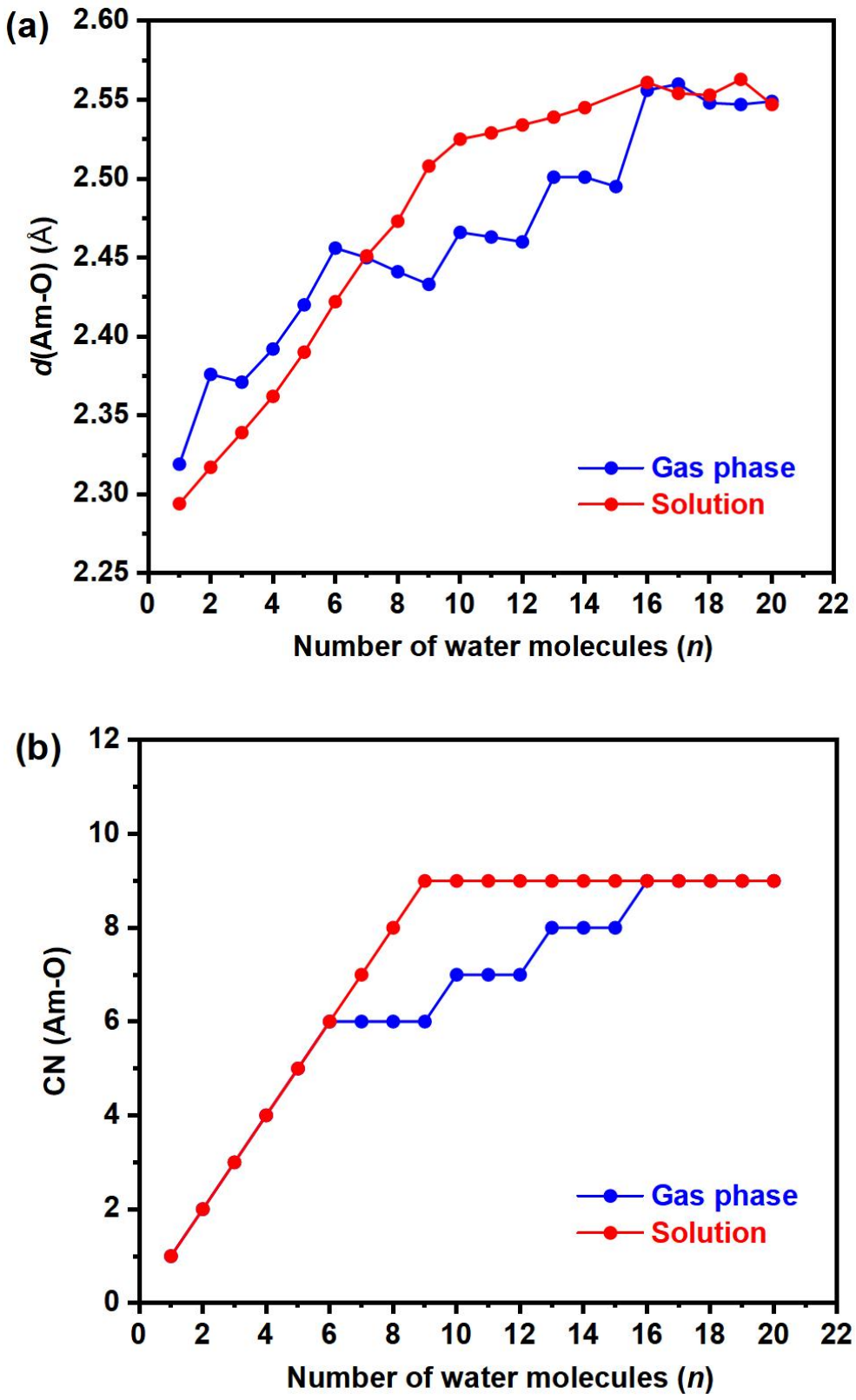


Fig. S8 (a) average bond lengths (in Å) of *d*(Am–O) and (b) coordination number (CN) of Am^{3+} among the first solvation shell changing with the different number of water molecules for the global–minimum structure of $Am(H_2O)_n^{3+}$ (n=1–20) clusters in the gas phase (in blue) and solution (in red) , respectively.

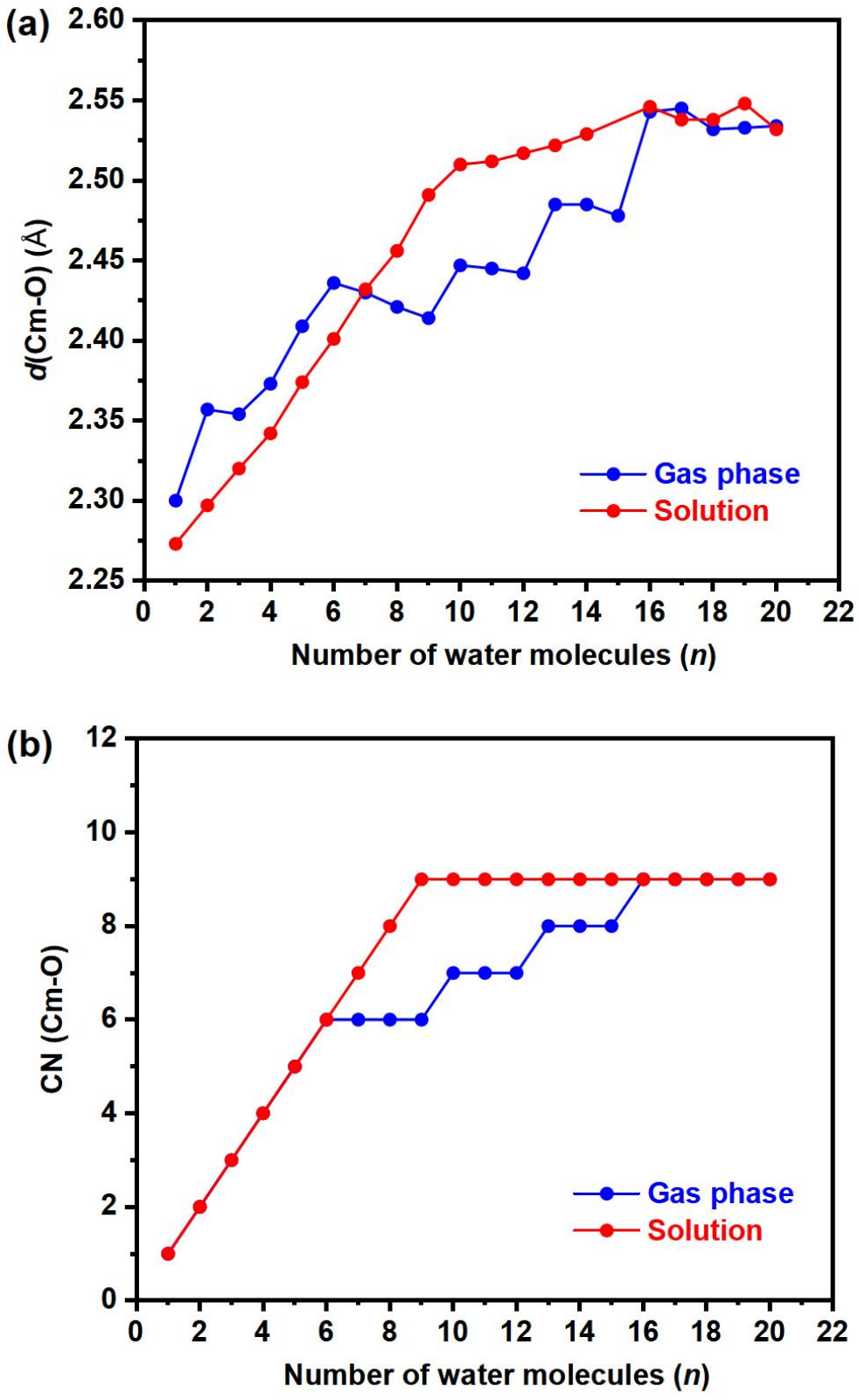


Fig. S9 (a) average bond lengths (in Å) of *d*(Cm–O) and (b) coordination number (CN) of Cm^{3+} among the first solvation shell changing with the different number of water molecules for the global–minimum structure of $Cm(H_2O)_n^{3+}$ (n=1–20) clusters in the gas phase (in blue) and solution (in red) , respectively.

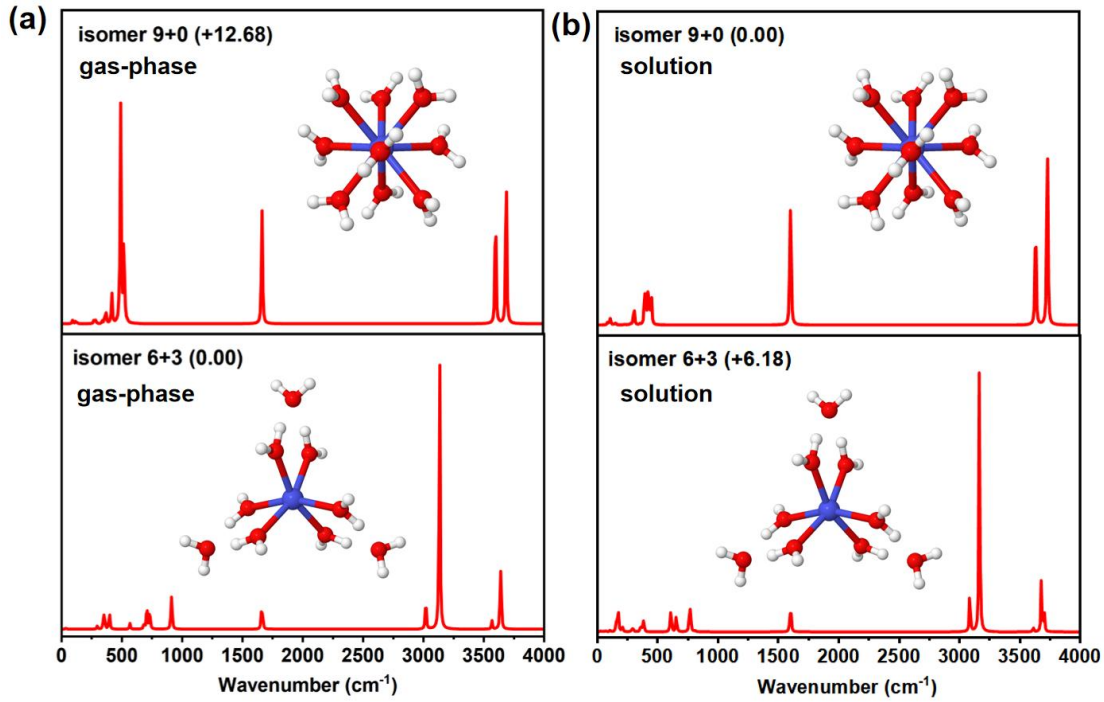


Fig. S10 The simulated infrared spectrum of two isomers of $Am(H_2O)_9^{3+}$ cluster calculated in the (a) gas–phase and (b) solution with CPCM solvation model at the PBE/6–31G(d)/RECP level with dispersion corrections. The relative energies of these two optimized structures (in kcal/mol) are also shown in the bracket.

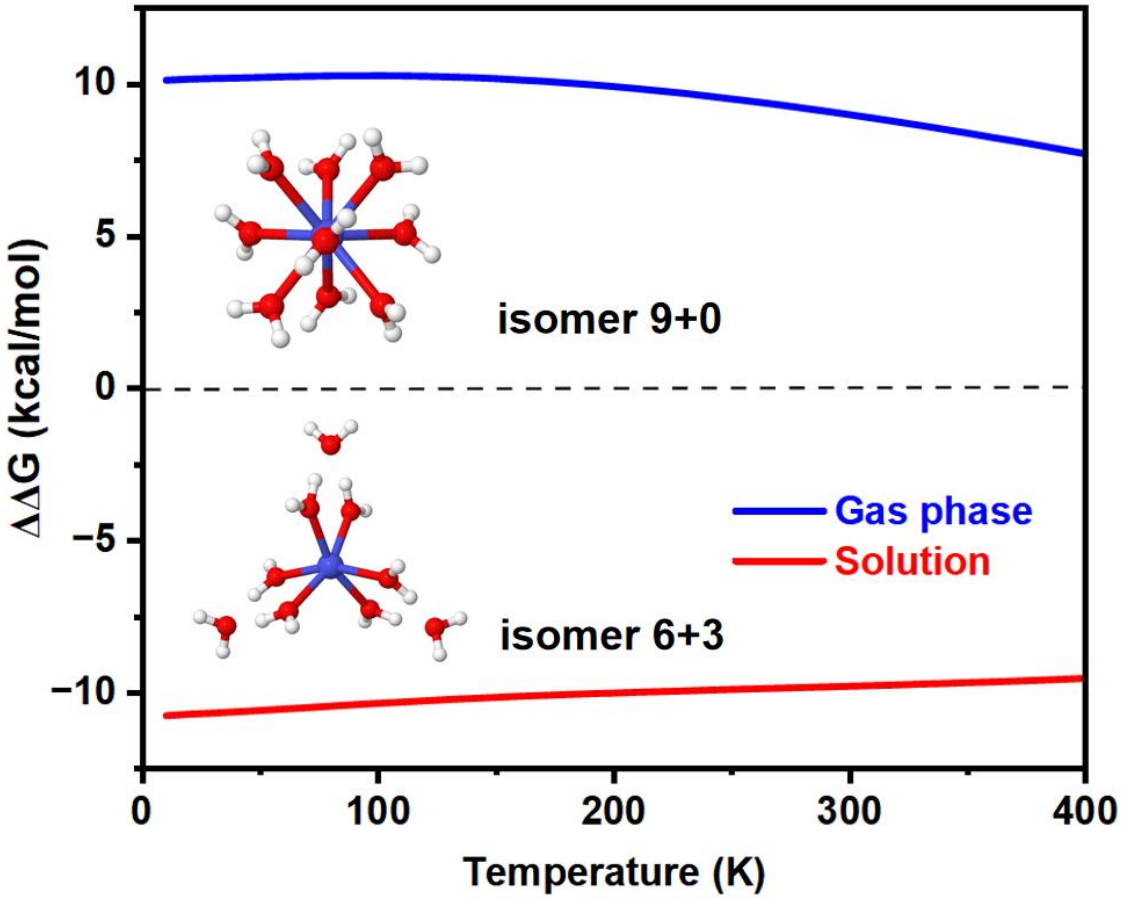


Fig. S11 Difference of Gibbs free energy (in kcal/mol) between the two isomers of $Am(H_2O)_9^{3+}$ cluster $\Delta\Delta G = \Delta G_{(9+0)} - \Delta G_{(6+3)}$ calculated in the gas–phase (in blue) and solution (in red) at the PBE/6–31G(d)/RECP level with dispersion corrections, respectively.

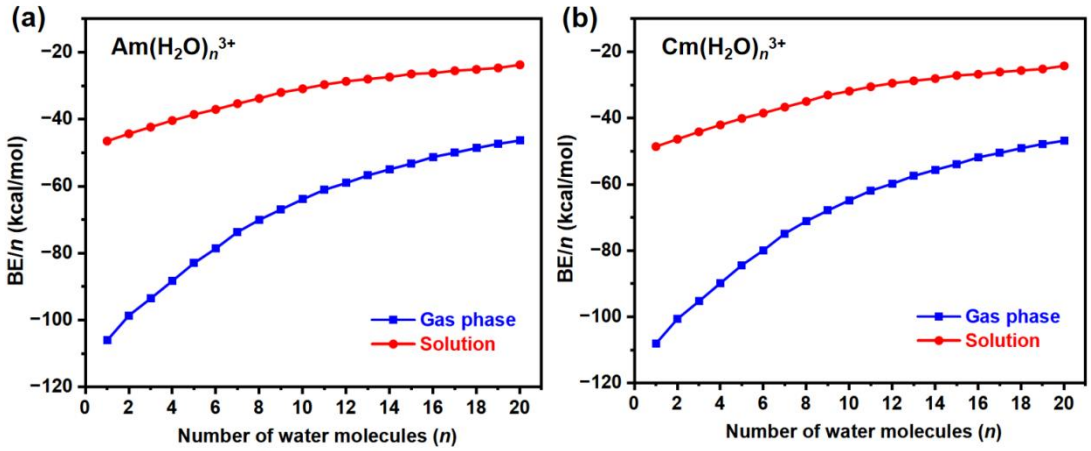


Fig. S12 The average binding energy (BE/*n*) (in kcal/mol) for the global–minimum structure of (a) $Am(H_2O)_n^{3+}$ and (b) $Cm(H_2O)_n^{3+}$(*n*=1–20) calculated in the gas phase (in blue) and solution (in red) at the DFT PBE/6–31G(d)/RECP level with dispersion corrections, respectively.

Part D: Supplementary results calculated at the force field level

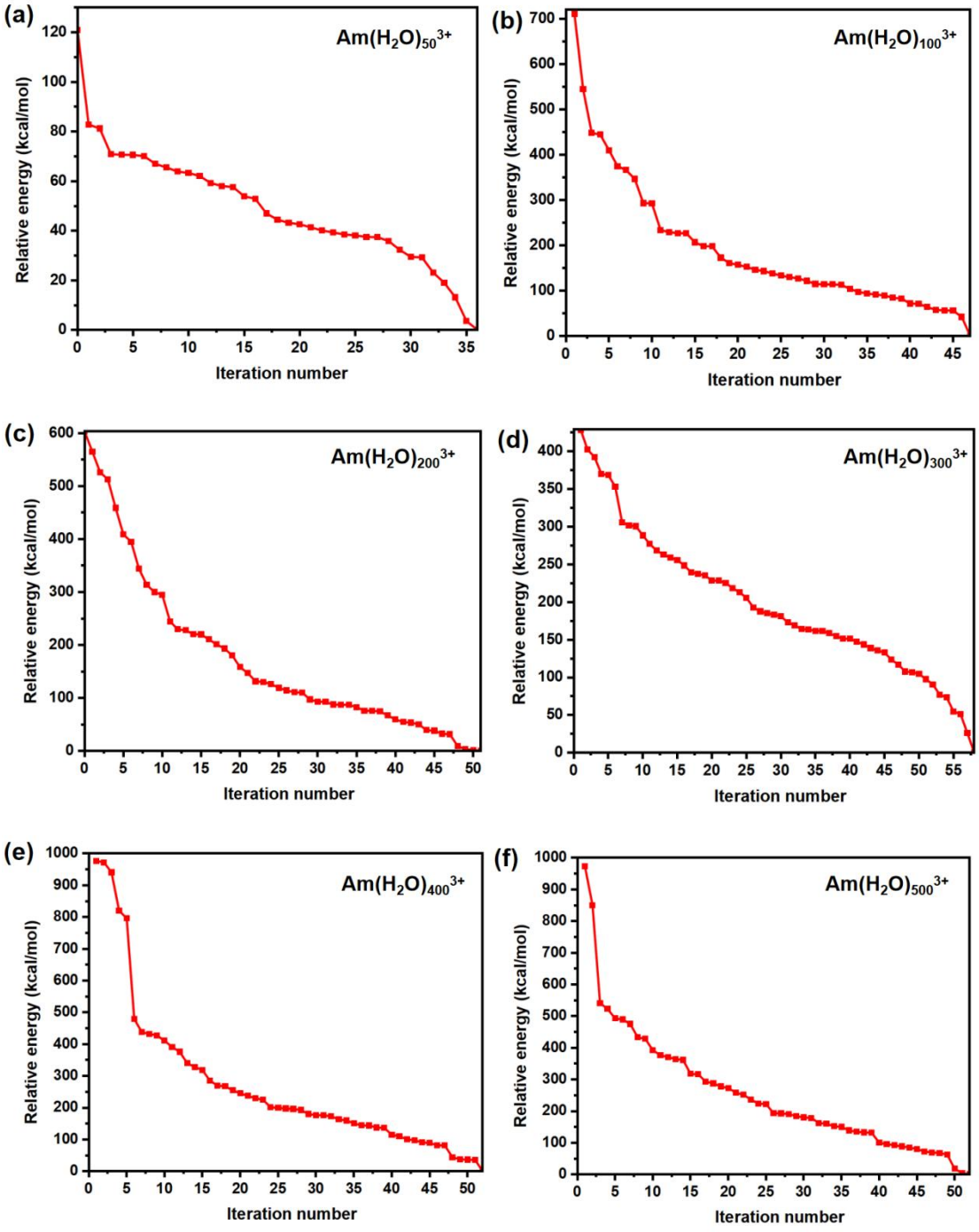
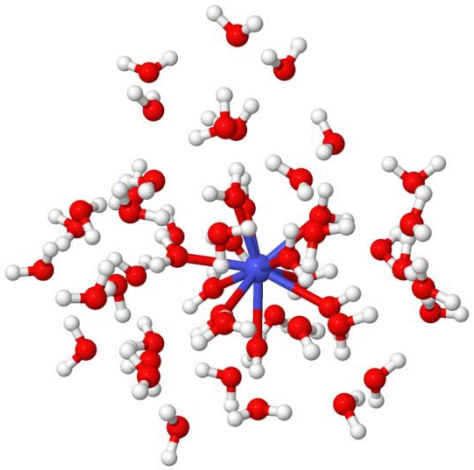
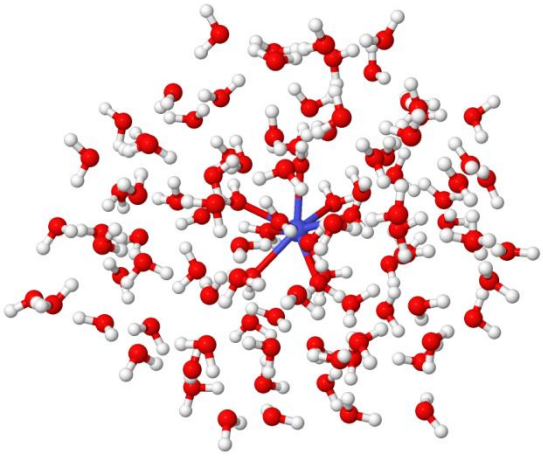


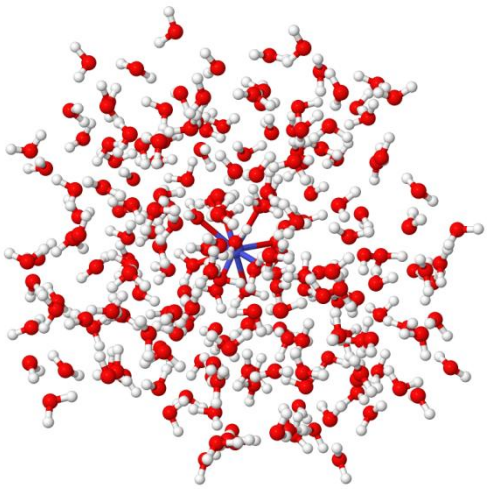
Fig. S13 The evolution of relative energy (in kcal/mol) of the isomers of (a) $Am(H_2O)_{50}^{3+}$ (b) $Am(H_2O)_{100}^{3+}$ (c) $Am(H_2O)_{200}^{3+}$ (d) $Am(H_2O)_{300}^{3+}$ (e) $Am(H_2O)_{400}^{3+}$ (f) $Am(H_2O)_{500}^{3+}$ clusters during the global–minimum structure search by using the TGMin (v3.0) package at the force field level.



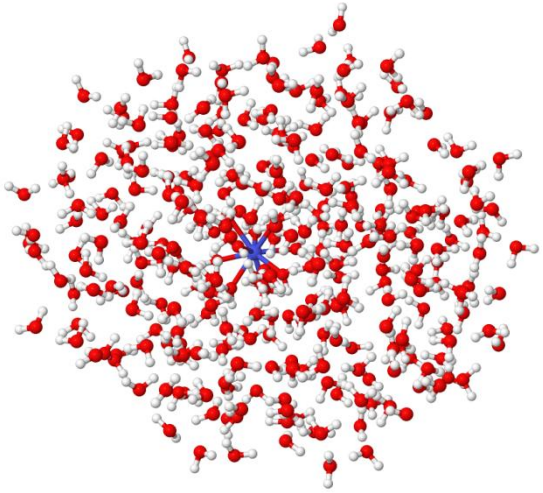
$Am(H_2O)_{50}^{3+}$



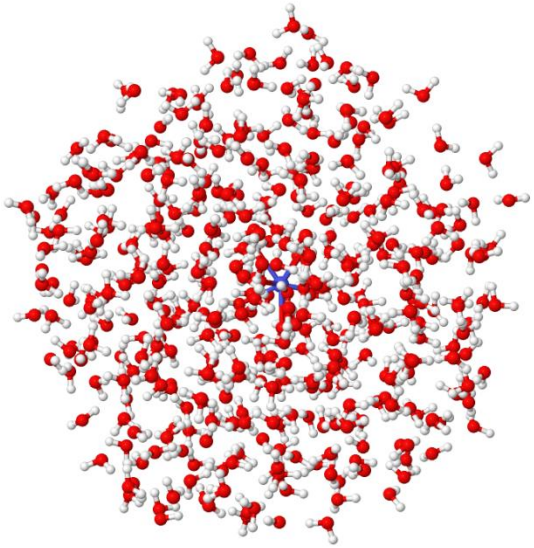
$Am(H_2O)_{100}^{3+}$



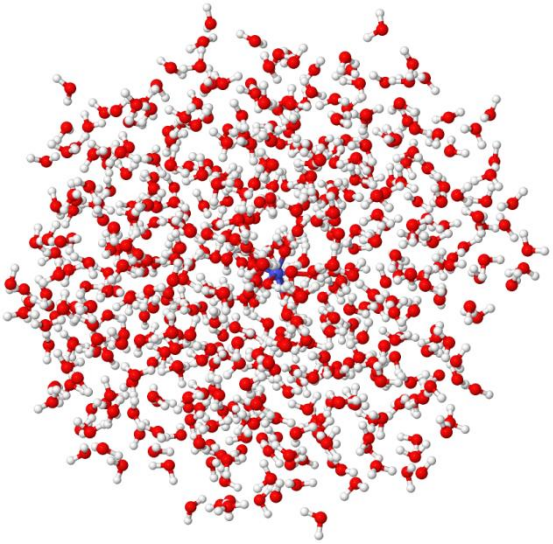
$Am(H_2O)_{200}^{3+}$



$Am(H_2O)_{300}^{3+}$



$Am(H_2O)_{400}^{3+}$



$Am(H_2O)_{500}^{3+}$

Fig. S14 The global–minimum structure of $Am(H_2O)_n^{3+}$ (n = 50, 100, 200, 300, 400, 500) clusters searched by using the TGMin (v3.0) package at the force field level.

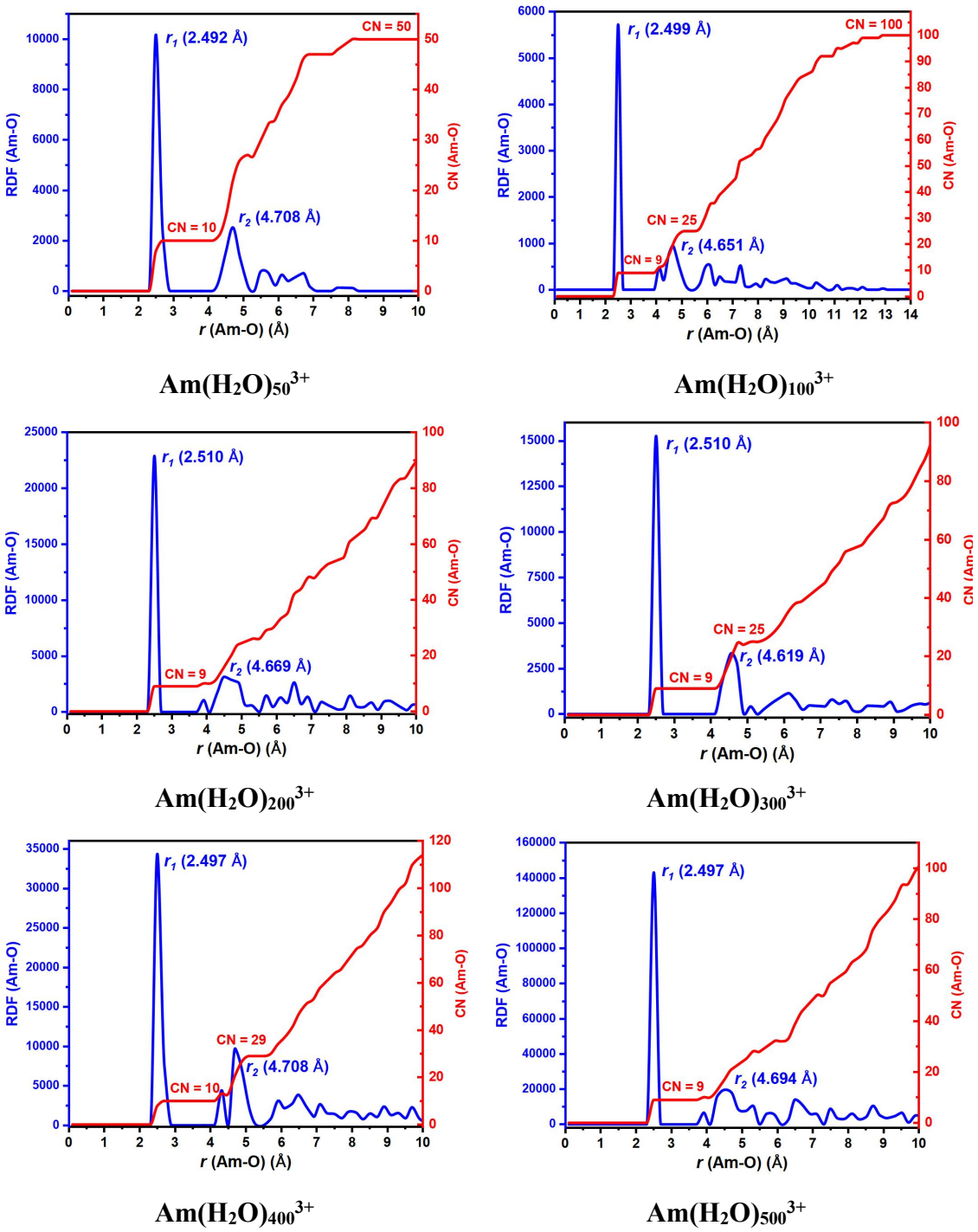


Fig. S15 The radial distribution function (RDF) and coordination number (CN) of Am–O for the global–minimum structure of (a) $Am(H_2O)_{50}^{3+}$ (b) $Am(H_2O)_{100}^{3+}$ (c) $Am(H_2O)_{200}^{3+}$ (d) $Am(H_2O)_{300}^{3+}$ (e) $Am(H_2O)_{400}^{3+}$ and (f) $Am(H_2O)_{500}^{3+}$ clusters .

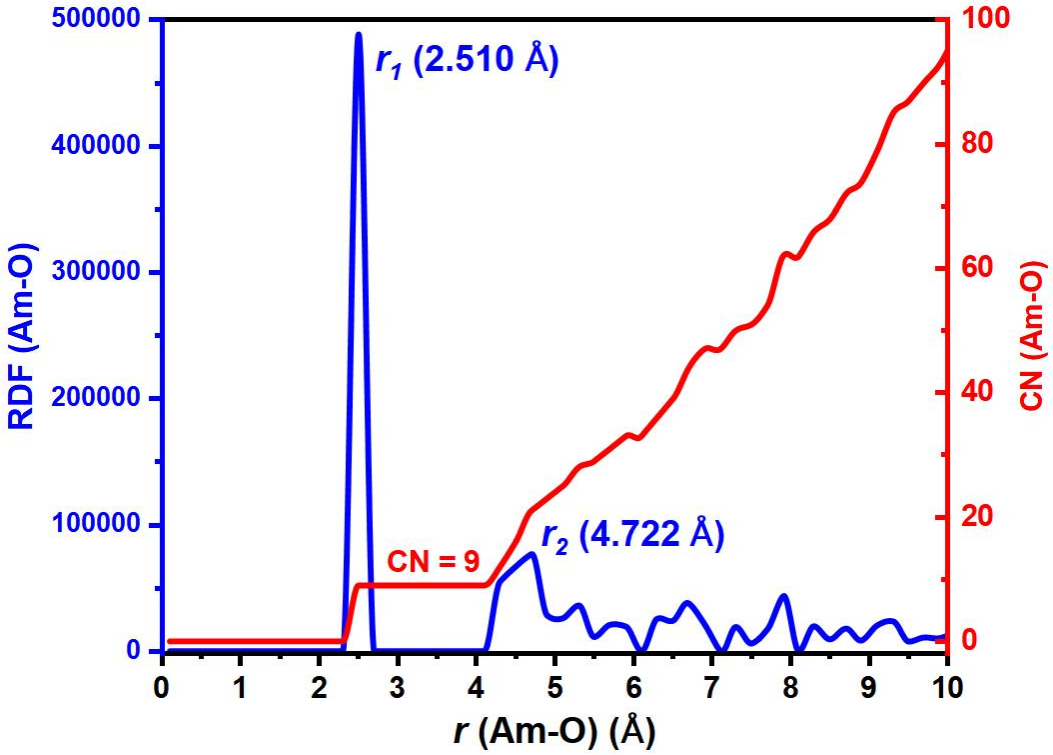


Fig. S16 The radial distribution function (RDF) and coordination number (CN) of Am–O for the global–minimum structure of $Am(H_2O)_{600}^{3+}$ cluster.

Part E: Raw data of the calculated frequencies in numerical form

Table S5. The raw data of the calculated frequencies in numerical form of two isomers of $Am(H_2O)_9^{3+}$ clusters calculated in the gas–phase.

Isomer 9+0 of $Am(H_2O)_9^{3+}$
---------- VIBRATIONAL FREQUENCIES ---------- Scaling factor for frequencies = 1.000000000 (already applied!) 0: 0.00 cm**-1 1: 0.00 cm**-1 2: 0.00 cm**-1 3: 0.00 cm**-1 4: 0.00 cm**-1 5: 0.00 cm**-1 6: 38.75 cm**-1 7: 40.35 cm**-1 8: 74.43 cm**-1 9: 74.88 cm**-1 10: 79.68 cm**-1 11: 83.35 cm**-1 12: 83.58 cm**-1 13: 87.58 cm**-1 14: 89.15 cm**-1 15: 102.61 cm**-1 16: 102.94 cm**-1 17: 103.86 cm**-1 18: 107.16 cm**-1 19: 108.87 cm**-1 20: 117.65 cm**-1 21: 213.55 cm**-1 22: 215.96 cm**-1 23: 217.92 cm**-1 24: 232.14 cm**-1 25: 234.58 cm**-1 26: 245.26 cm**-1 27: 247.92 cm**-1 28: 254.97 cm**-1 29: 257.78 cm**-1 30: 265.53 cm**-1 31: 270.67 cm**-1 32: 282.74 cm**-1 33: 287.10 cm**-1 34: 296.67 cm**-1 35: 324.00 cm**-1

36:	347.38 cm**-1
37:	351.60 cm**-1
38:	352.39 cm**-1
39:	361.97 cm**-1
40:	362.54 cm**-1
41:	400.65 cm**-1
42:	409.68 cm**-1
43:	412.13 cm**-1
44:	426.26 cm**-1
45:	426.78 cm**-1
46:	471.74 cm**-1
47:	484.90 cm**-1
48:	487.81 cm**-1
49:	500.50 cm**-1
50:	515.70 cm**-1
51:	525.93 cm**-1
52:	527.69 cm**-1
53:	528.84 cm**-1
54:	538.25 cm**-1
55:	543.03 cm**-1
56:	543.98 cm**-1
57:	1652.46 cm**-1
58:	1654.41 cm**-1
59:	1654.97 cm**-1
60:	1656.98 cm**-1
61:	1658.21 cm**-1
62:	1658.27 cm**-1
63:	1661.11 cm**-1
64:	1662.24 cm**-1
65:	1669.01 cm**-1
66:	3594.58 cm**-1
67:	3594.76 cm**-1
68:	3596.32 cm**-1
69:	3596.49 cm**-1
70:	3596.66 cm**-1
71:	3596.88 cm**-1
72:	3597.30 cm**-1
73:	3597.50 cm**-1
74:	3603.55 cm**-1
75:	3678.32 cm**-1
76:	3678.61 cm**-1
77:	3683.47 cm**-1
78:	3684.20 cm**-1
79:	3684.28 cm**-1
80:	3684.54 cm**-1
81:	3684.70 cm**-1
82:	3684.94 cm**-1
83:	3685.73 cm**-1

Isomer 6+3 of $Am(H_2O)_9^{3+}$

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.000000000 (already applied!)

0:	0.00 cm**-1
1:	0.00 cm**-1
2:	0.00 cm**-1
3:	0.00 cm**-1
4:	0.00 cm**-1
5:	0.00 cm**-1
6:	31.65 cm**-1
7:	32.26 cm**-1
8:	35.95 cm**-1
9:	40.58 cm**-1
10:	41.22 cm**-1
11:	46.26 cm**-1
12:	87.25 cm**-1
13:	89.59 cm**-1
14:	90.17 cm**-1
15:	128.30 cm**-1
16:	129.55 cm**-1
17:	130.64 cm**-1
18:	185.09 cm**-1
19:	188.84 cm**-1
20:	189.34 cm**-1
21:	290.62 cm**-1
22:	291.16 cm**-1
23:	307.56 cm**-1
24:	312.19 cm**-1
25:	312.54 cm**-1
26:	330.82 cm**-1
27:	331.32 cm**-1
28:	338.39 cm**-1
29:	338.89 cm**-1
30:	349.08 cm**-1
31:	349.63 cm**-1
32:	350.30 cm**-1
33:	370.85 cm**-1
34:	371.44 cm**-1
35:	378.46 cm**-1
36:	379.85 cm**-1
37:	382.80 cm**-1
38:	383.28 cm**-1
39:	383.51 cm**-1
40:	384.04 cm**-1
41:	389.70 cm**-1
42:	562.91 cm**-1
43:	563.23 cm**-1

44:	574.04 cm**-1
45:	690.44 cm**-1
46:	690.61 cm**-1
47:	719.84 cm**-1
48:	738.56 cm**-1
49:	739.90 cm**-1
50:	751.10 cm**-1
51:	872.11 cm**-1
52:	872.26 cm**-1
53:	874.71 cm**-1
54:	910.85 cm**-1
55:	914.23 cm**-1
56:	914.59 cm**-1
57:	1653.00 cm**-1
58:	1653.32 cm**-1
59:	1653.51 cm**-1
60:	1655.92 cm**-1
61:	1656.43 cm**-1
62:	1656.54 cm**-1
63:	1733.40 cm**-1
64:	1733.62 cm**-1
65:	1736.95 cm**-1
66:	2986.53 cm**-1
67:	2987.25 cm**-1
68:	2996.44 cm**-1
69:	3112.31 cm**-1
70:	3113.02 cm**-1
71:	3141.50 cm**-1
72:	3563.95 cm**-1
73:	3564.28 cm**-1
74:	3564.60 cm**-1
75:	3632.00 cm**-1
76:	3632.20 cm**-1
77:	3632.82 cm**-1
78:	3633.02 cm**-1
79:	3634.03 cm**-1
80:	3637.95 cm**-1
81:	3641.93 cm**-1
82:	3642.45 cm**-1
83:	3642.76 cm**-1

Table S6. The raw data of the calculated frequencies in numerical form of two isomers of $Am(H_2O)_9^{3+}$ cluster calculated in the solution with CPCM solvation model.

Isomer 9+0 of $Am(H_2O)_9^{3+}$

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VIBRATIONAL FREQUENCIES
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Scaling factor for frequencies =    1.000000000    (already applied!)

    0:         0.00 cm**-1
    1:         0.00 cm**-1
    2:         0.00 cm**-1
    3:         0.00 cm**-1
    4:         0.00 cm**-1
    5:         0.00 cm**-1
   15:        24.00 cm**-1
   16:        33.32 cm**-1
   17:        63.90 cm**-1
   18:        67.84 cm**-1
   19:        70.75 cm**-1
   20:        83.36 cm**-1
   21:        96.62 cm**-1
   22:       101.88 cm**-1
   23:       106.17 cm**-1
   24:       113.14 cm**-1
   25:       115.61 cm**-1
   26:       122.56 cm**-1
   27:       133.45 cm**-1
   28:       134.49 cm**-1
   29:       146.05 cm**-1
   30:       198.48 cm**-1
   31:       206.82 cm**-1
   32:       207.28 cm**-1
   33:       222.85 cm**-1
   34:       233.48 cm**-1
   35:       243.94 cm**-1
   36:       247.48 cm**-1
   37:       253.92 cm**-1
   38:       257.72 cm**-1
   39:       265.30 cm**-1
   40:       266.97 cm**-1
   41:       268.80 cm**-1
   42:       272.67 cm**-1
   43:       277.67 cm**-1
   44:       278.25 cm**-1
   45:       279.70 cm**-1
   46:       319.89 cm**-1
   47:       328.70 cm**-1
```

48:	390.80 cm**-1
49:	395.27 cm**-1
50:	404.61 cm**-1
51:	415.91 cm**-1
52:	419.59 cm**-1
53:	427.13 cm**-1
54:	439.17 cm**-1
55:	452.19 cm**-1
56:	453.89 cm**-1
57:	1589.27 cm**-1
58:	1590.95 cm**-1
59:	1591.37 cm**-1
60:	1595.65 cm**-1
61:	1596.74 cm**-1
62:	1599.01 cm**-1
63:	1602.21 cm**-1
64:	1603.19 cm**-1
65:	1606.58 cm**-1
66:	3627.00 cm**-1
67:	3627.55 cm**-1
68:	3627.78 cm**-1
69:	3628.04 cm**-1
70:	3628.35 cm**-1
71:	3628.60 cm**-1
72:	3629.48 cm**-1
73:	3629.61 cm**-1
74:	3631.29 cm**-1
75:	3720.41 cm**-1
76:	3721.69 cm**-1
77:	3722.39 cm**-1
78:	3722.49 cm**-1
79:	3722.75 cm**-1
80:	3723.32 cm**-1
81:	3724.70 cm**-1
82:	3725.19 cm**-1
83:	3725.30 cm**-1

Isomer 6+3 of $Am(H_2O)_9^{3+}$

VIBRATIONAL FREQUENCIES

Scaling factor for frequencies = 1.000000000 (already applied!)

0:	0.00 cm**-1
1:	0.00 cm**-1
2:	0.00 cm**-1
3:	0.00 cm**-1
4:	0.00 cm**-1
5:	0.00 cm**-1

```
 6:      19.37 cm**-1
 7:      25.28 cm**-1
 8:      29.04 cm**-1
 9:      31.14 cm**-1
10:      43.28 cm**-1
11:      51.13 cm**-1
12:      55.17 cm**-1
13:      75.16 cm**-1
14:      88.96 cm**-1
15:      99.57 cm**-1
16:     104.37 cm**-1
17:     112.47 cm**-1
18:     188.20 cm**-1
19:     191.59 cm**-1
20:     193.05 cm**-1
21:     215.50 cm**-1
22:     222.45 cm**-1
23:     226.56 cm**-1
24:     229.98 cm**-1
25:     231.46 cm**-1
26:     248.40 cm**-1
27:     286.78 cm**-1
28:     289.15 cm**-1
29:     294.55 cm**-1
30:     296.89 cm**-1
31:     297.65 cm**-1
32:     308.82 cm**-1
33:     337.27 cm**-1
34:     338.43 cm**-1
35:     346.65 cm**-1
36:     352.50 cm**-1
37:     355.35 cm**-1
38:     358.62 cm**-1
39:     370.70 cm**-1
40:     371.94 cm**-1
41:     385.39 cm**-1
42:     398.59 cm**-1
43:     400.95 cm**-1
44:     402.34 cm**-1
45:     615.65 cm**-1
46:     629.93 cm**-1
47:     636.63 cm**-1
48:     656.31 cm**-1
49:     664.38 cm**-1
50:     671.46 cm**-1
51:     779.72 cm**-1
52:     784.81 cm**-1
53:     787.80 cm**-1
54:     851.99 cm**-1
55:     853.56 cm**-1
```

56:	857.82 cm**-1
57:	1588.53 cm**-1
58:	1588.84 cm**-1
59:	1589.65 cm**-1
60:	1600.84 cm**-1
61:	1609.79 cm**-1
62:	1610.88 cm**-1
63:	1666.98 cm**-1
64:	1668.31 cm**-1
65:	1669.55 cm**-1
66:	3029.35 cm**-1
67:	3031.03 cm**-1
68:	3035.37 cm**-1
69:	3119.13 cm**-1
70:	3121.65 cm**-1
71:	3135.44 cm**-1
72:	3605.61 cm**-1
73:	3607.53 cm**-1
74:	3607.57 cm**-1
75:	3652.08 cm**-1
76:	3653.89 cm**-1
77:	3656.23 cm**-1
78:	3656.43 cm**-1
79:	3656.91 cm**-1
80:	3658.25 cm**-1
81:	3695.15 cm**-1
82:	3696.51 cm**-1
83:	3696.79 cm**-1