Supplementary Information

Structural assignments of yttrium oxide cluster cations studied by ion mobility mass spectrometry

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1. Relative energies of $Y_nO_m^+$ for different spin multiplicities (n = 3, 4)

Table S1. Relative energies of $Y_3O_4^+$ for different spin multiplicities.
Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

spin multiplicity	most stable ΔE /eV	second stable ΔE /eV	third stable ΔE /eV
1	0.00	1.95	1.95
3	3.78	4.68	–
5	7.62	7.48	7.48
7	11.31	–	12.22
9	16.49	–	–
11	–	–	–
13	–	–	–

Table S2. Relative energies of $Y_4O_6^+$ for different spin multiplicities.
Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

spin multiplicity	most stable ΔE /eV	second stable ΔE /eV	third stable ΔE /eV
2	0.00	1.00	1.04
4	3.77	4.14	3.83
6	7.99	8.15	7.86
8	–	–	11.40
10	16.38	16.41	15.78
12	–	–	–
14	–	–	–

2. Analysis of the widths of arrival time distributions (ATDs)

The ATD width w (full width at half maximum) was theoretically expressed as

$$w = 4\sqrt{Dtln2}/v_d,$$

in which D is the diffusion constant, $D = Kk_BTe^{-1}$, t is the drift time, and v_d is the drift velocity [Revercomb and Mason, *Anal. Chem.* **1975**, 47, 970]. Using this equation, the theoretical width for each ion ATD peak was found to be about 70% of the experimental width, and thus the rest was the instrumental broadening of the arrival time. For example, for $Y_4O_7^+$, which is assumed to be one isomer, the theoretical width w was calculated to be 1.51 μs, which was 77 % of the experimental width w_{exp} of 1.97 μs.

In the above equation, the width w is proportional to the drift time t, because $D \propto t^{-1/2}$ and $v_d \propto t^{-1}$. The observed w_{exp} was also found to be proportional to t in the present measurement, and therefore, the ATD widths are mostly explained by w plus instrumental width of one isomer, assuming the same t dependence for the instrumental broadening. As a result, we concluded that most of the ions are explained by one isomer or a few isomers with similar arrival times.

3. Optimized structures of $Y_nO_m^+$ (n = 7–11)

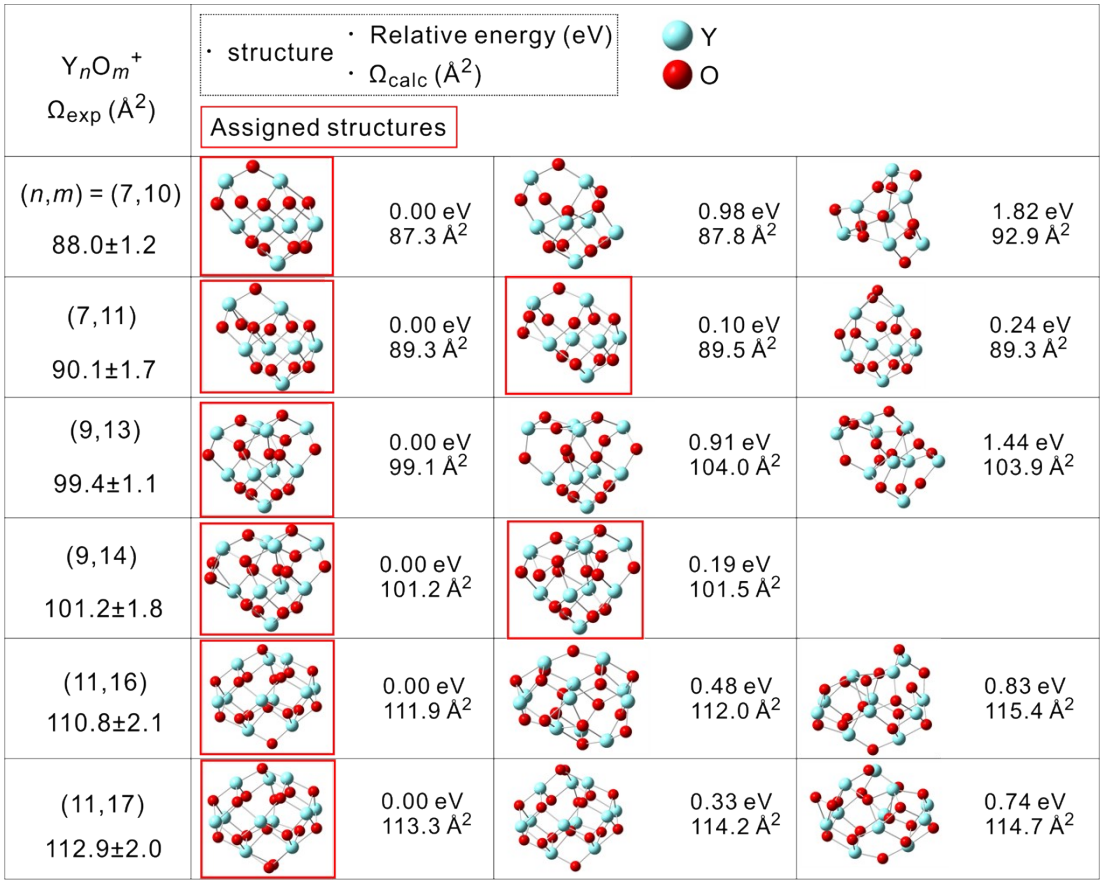


Figure S1. Optimized structures of $YO(Y_2O_3)_3^+$ [(7,10)], $YO_2(Y_2O_3)_3^+$ [(7,11)], $YO(Y_2O_3)_4^+$ [(9,13)], $YO_2(Y_2O_3)_4^+$ [(9,14)], $YO(Y_2O_3)_5^+$ [(11,16)] and $YO_2(Y_2O_3)_5^+$ [(11,17)]. Experimental CCSs (Ω_{exp}) and theoretical CCSs (Ω_{calc}) of each structure, and relative energies are also shown. Assigned structures are indicated by red squares.

Calculation level: B3LYP / Y: LANL2DZ, O: D95V

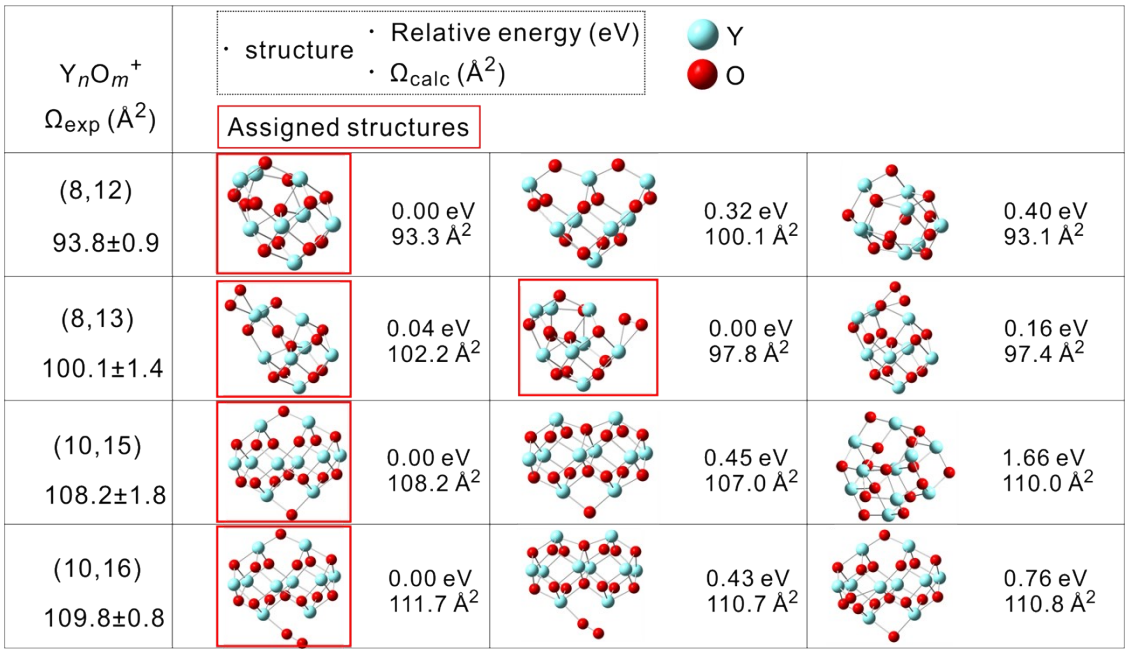


Figure S2. Optimized structures of $(Y_2O_3)_4^+$ ($Y_8O_{12}^+$), $O(Y_2O_3)_4^+$ ($Y_8O_{13}^+$), $(Y_2O_3)_5^+$ ($Y_{10}O_{15}^+$), and $O(Y_2O_3)_5^+$ ($Y_{10}O_{16}^+$). Experimental CCSs (Ω_{exp}), theoretical CCSs (Ω_{calc}) of each structure, and relative energies are also shown. Assigned structures are indicated by red squares. Calculation level: B3LYP / Y: LANL2DZ, O: D95V

For $Y_8O_{13}^+$, using B3LYP / Y: SDD, O: aug-cc-pVTZ level, the energy order of the leftmost structure and the middle structure in Fig. S2 are reversed, and the leftmost structure become the most stable. The energy difference is 0.07 eV.

4. NBO charge of $Y_nO_m^+$ (n = 3, 4)

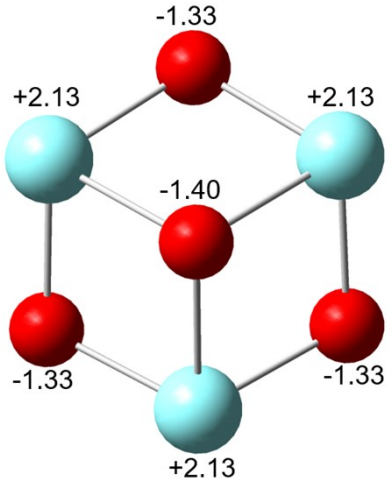


Figure S3. NBO charge of $Y_3O_4^+$.

Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

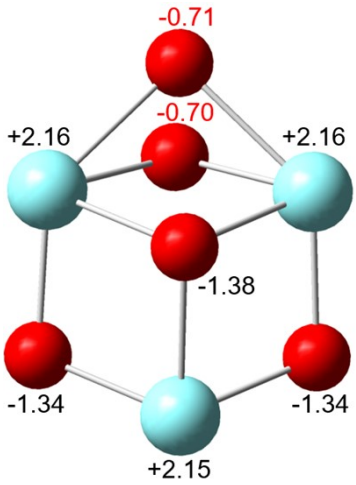


Figure S4. NBO charge of $Y_3O_5^+$.

Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

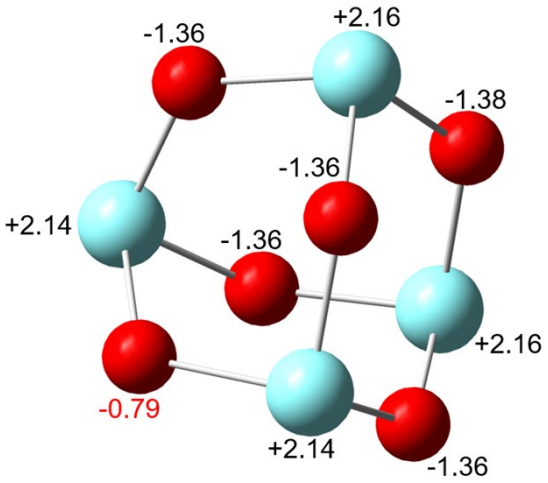


Figure S5. NBO charge of $Y_4O_6^+$.

Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

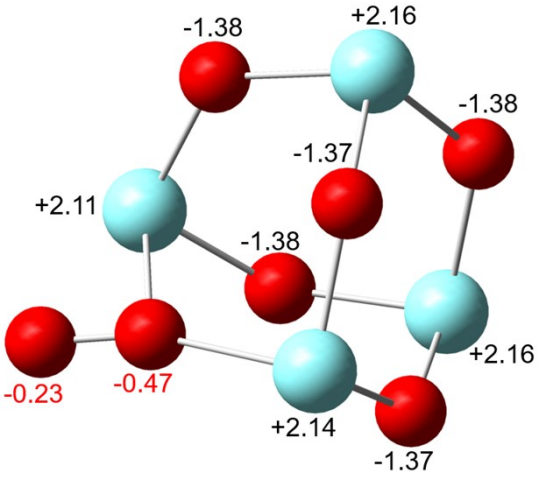


Figure S6. NBO charge of $Y_4O_7^+$.

Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

5. NBO spin population of $Y_nO_m^+$ (n = 4)

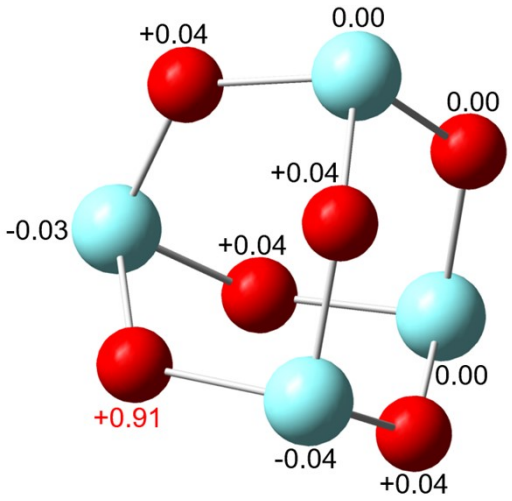


Figure S7. NBO spin population of $Y_4O_6^+$.

Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

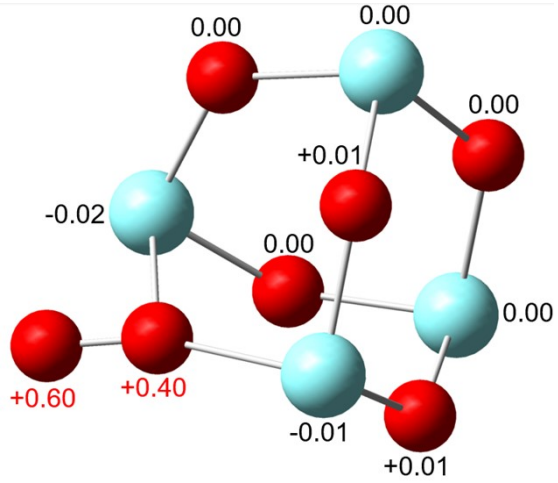


Figure S8. NBO spin population of $Y_4O_7^+$.

Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

6. Bond length of $Y_nO_m^+$ (n = 3, 4)

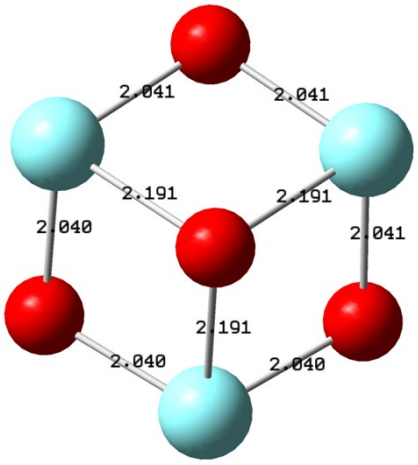


Figure S9. Bond length of $Y_3O_4^+$ in Å.

Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

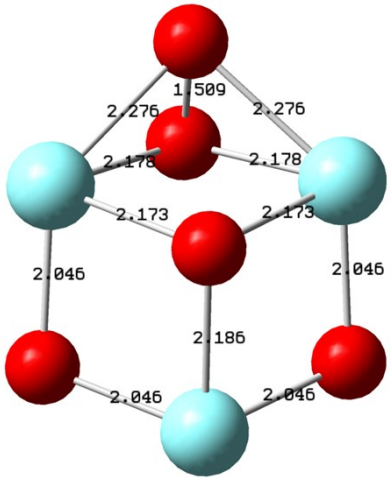


Figure S10. Bond length of $Y_3O_5^+$ in Å.

Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

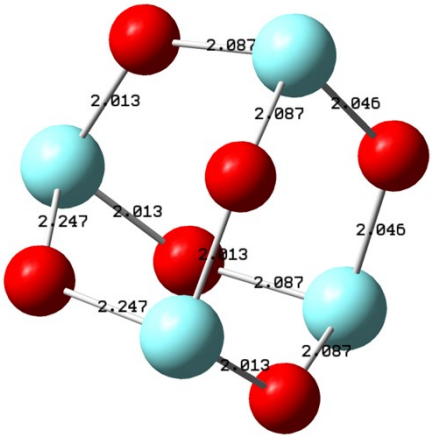


Figure S11. Bond length of $Y_4O_6^+$ in Å.

Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

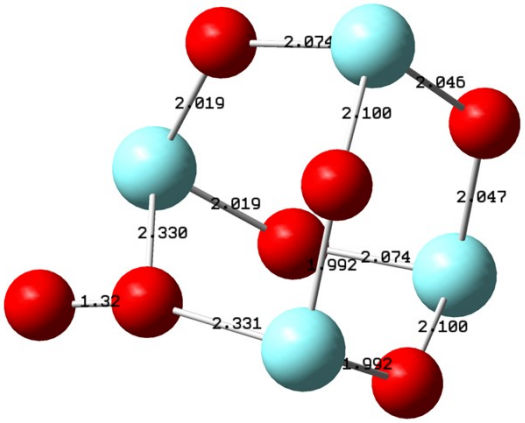
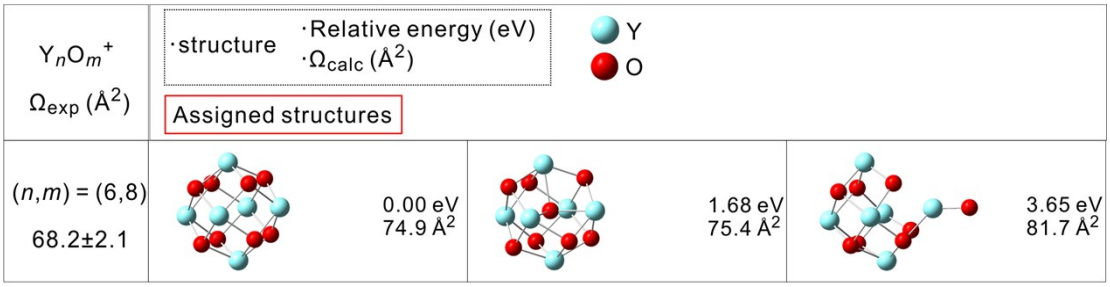


Figure S12. Bond length of $Y_4O_7^+$ in Å.

Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ

7. Experimental CCS, optimized structures, relative energies and theoretical CCSs of $Y_6O_8^+$



Calculation level: B3LYP/SDD(Y), aug-cc-pVTZ(O)

Figure S13. Optimized structures of $Y_6O_8^+$. Experimental CCS (Ω_{exp}), theoretical CCSs (Ω_{calc}) of each structure, and relative energies are also shown. Calculation level: B3LYP / Y: SDD, O: aug-cc-pVTZ.

8. Atomic coordinates (Å) and natural charge for assigned structures of $YO(Y_2O_3)_x^+$ and $YO_2(Y_2O_3)_x^+$ (x = 1–5).

Singlet was used for odd number of Y atoms as spin multiplicity.

Calculation level: B3LYP / Y: SDD, O: aug-cc pVTZ

$YO(Y_2O_3)_1^+$ [(3,4)]

	x	y	z	charge
Y	-6.033929	-0.547892	-3.181722	2.13056
Y	-2.841521	-0.710987	-3.167272	2.13065
Y	-4.579009	-3.393752	-3.119195	2.13063
O	-2.884038	-2.601706	-3.933653	-1.33221
O	-4.384814	0.333565	-3.998523	-1.33219
O	-4.488966	-1.526931	-1.975998	-1.39525
O	-6.176253	-2.432988	-3.949458	-1.33218

$YO_2(Y_2O_3)_1^+$ [(3,5)]

	x	y	z	charge
Y	-6.100232	-1.308426	-2.754679	2.16306
Y	-2.994614	-0.686735	-3.281380	2.14665
Y	-4.032055	-3.725036	-3.265431	2.16299
O	-2.693886	-2.490187	-4.198675	-1.34309
O	-4.865667	0.047733	-3.661788	-1.34313
O	-4.183459	-1.979298	-1.980263	-1.38294
O	-5.794651	-2.882862	-4.227777	-0.69735
O	-6.283697	-3.566220	-2.974528	-0.70618

$YO(Y_2O_3)_2^+$ [(5,7)]

	x	y	z	charge
Y	-0.961502	1.406355	2.851185	2.11389
Y	-2.669607	-0.726731	0.075302	2.13635
Y	0.524600	-1.046059	0.215080	2.13643
Y	-2.602055	2.967909	0.008445	2.15484
Y	1.194247	2.589216	0.174754	2.15490
O	-3.181013	1.086149	-0.642990	-1.37808
O	-0.631170	3.252458	-0.488477	-1.39337
O	1.445797	0.624021	-0.438065	-1.37826
O	-1.091366	-1.545704	-0.928122	-1.34050
O	-1.085307	-0.380056	1.595759	-1.45191
O	0.784721	2.183651	2.175712	-1.37711
O	-2.456356	2.505322	2.033718	-1.37718

$YO_2(Y_2O_3)_2^+$ [(5,8)]

	x	y	z	charge
Y	-0.759013	0.558447	2.782506	2.14446
Y	-2.823404	-0.789461	-0.364787	2.14972
Y	0.409511	-1.080097	-0.135381	2.11895
Y	-2.388444	2.875360	0.456017	2.17036
Y	1.334122	2.385353	-0.104492	2.16841
O	-3.146466	1.221325	-0.521000	-1.39593
O	-0.466480	3.288194	-0.219472	-1.39396
O	1.219577	0.595295	-1.004808	-1.35674
O	-1.204301	-1.484411	-1.372247	-1.34752
O	-1.396384	-0.758897	1.260389	-1.42066
O	1.054898	1.385092	1.863513	-0.75678
O	-1.981828	2.124436	2.352772	-1.38832
O	1.264702	-0.097097	1.952349	-0.69200

$YO(Y_2O_3)_3^+$ [(7,10)]

	x	y	z	charge
Y	-6.209608	-0.448189	0.482667	2.13074
Y	-5.306570	3.187378	-0.304444	2.13079
Y	-2.105797	2.017826	-0.811625	2.12055
Y	-2.890426	-1.139338	-0.129304	2.12049
Y	-3.655093	1.267572	2.031832	2.12059
Y	-4.425364	0.416417	-2.792450	2.13076
O	-3.248373	3.018725	0.772685	-1.41049
O	-2.007735	0.593943	0.808563	-1.37114
O	-5.585733	1.543576	1.089884	-1.37818
O	-4.200509	-0.814983	1.601621	-1.41051
O	-4.006316	2.308881	-1.808569	-1.37825
O	-7.107716	3.095365	-1.307788	-1.38765
O	-2.319335	0.096348	-1.851377	-1.41051
O	-4.806048	-0.908366	-1.112025	-1.37812
Y	-7.925364	1.410863	-2.196939	2.14622
O	-6.366855	0.763309	-3.400194	-1.38764
O	-7.867958	0.037023	-0.645747	-1.38764

$YO_2(Y_2O_3)_3^+$ [(7,11)] - 1 (The leftmost structure in Fig. S1)

	x	y	z	charge
Y	-5.956247	-0.539420	0.669248	2.12887
Y	-5.522851	2.945831	-0.208416	2.07999
Y	-2.249802	2.053923	-0.903865	2.13659
Y	-2.736444	-1.151889	-0.133848	2.13104
Y	-3.525722	1.321673	2.086751	2.13092
Y	-4.666904	0.261438	-2.618181	2.08018
O	-3.387895	3.001572	0.729965	-1.39385
O	-1.941781	0.677517	0.739114	-1.37967
O	-5.591018	1.441852	1.483770	-1.37856
O	-4.018803	-0.803273	1.650537	-1.40247
O	-4.190998	2.198384	-1.755105	-1.35365
O	-7.112892	3.457070	-1.510506	-1.36655
O	-2.458472	0.089612	-1.884138	-1.39383
O	-4.722741	-1.278871	-0.959844	-1.37867
Y	-7.708034	1.795576	-2.555140	2.14580
O	-6.307908	0.929349	-3.778175	-1.36661
O	-7.693256	0.215413	-0.789179	-0.64231
O	-6.361618	0.853884	-1.026786	-0.77721

$YO_2(Y_2O_3)_3^+$ [(7,11)] – 2 (The structure in the middle in Fig. S1)

	x	y	z	charge
Y	-6.179747	-0.509932	0.467266	2.14067
Y	-5.302425	3.180797	-0.299558	2.09081
Y	-2.119646	2.011057	-0.821490	2.12330
Y	-2.847743	-1.153099	-0.108672	2.12437
Y	-3.667004	1.261300	2.025568	2.12341
Y	-4.412506	0.345135	-2.782700	2.14039
O	-3.296372	3.039562	0.753060	-1.40642
O	-2.007130	0.617672	0.814891	-1.37089
O	-5.564100	1.484113	1.041158	-1.36966
O	-4.170225	-0.833279	1.611289	-1.41040
O	-4.027110	2.226961	-1.785996	-1.36953
O	-7.518699	3.142331	-0.636172	-0.70809
O	-2.293483	0.075471	-1.839083	-1.41031
O	-4.763851	-0.996779	-1.109086	-1.38462
Y	-7.891291	1.495996	-2.158095	2.15866
O	-6.360720	0.753304	-3.330358	-1.38185
O	-7.801103	0.058943	-0.676555	-1.38163
O	-6.809394	3.479469	-1.931447	-0.70820

$YO(Y_2O_3)_4^+$ [(9,13)]

	x	y	z	charge
Y	-1.977829	1.627313	-2.930487	2.13492
Y	-0.550796	0.155235	2.761136	2.14612
Y	0.241206	1.706984	-0.037395	2.04626
Y	-3.721599	-2.241390	2.055412	2.13681
Y	2.034107	-0.971035	0.901789	2.12219
Y	-2.873390	-1.318380	-1.718618	2.05236
Y	0.268086	-1.257920	-1.869996	2.03613
O	-0.613828	2.569757	-1.791169	-1.34011
O	1.291658	0.828331	1.842958	-1.38902
O	1.584621	0.165631	-0.882396	-1.36099
O	-3.433721	0.922946	-1.588433	-1.37099
O	-2.690474	-0.478676	2.578713	-1.38952
O	-2.320829	-3.636234	1.742124	-1.36323
O	-1.345798	-2.752104	-1.325578	-1.37017
O	1.326255	-2.560573	-0.392212	-1.39388
O	0.287369	-1.717700	2.046076	-1.38221
O	-1.338689	1.789851	1.527731	-1.36833
O	-1.387814	-0.403743	-3.184811	-1.38310
O	-3.972642	-1.316138	0.186748	-1.36996
O	-1.185618	-0.202877	-0.362974	-1.32238
Y	-2.969417	0.726244	0.610602	1.98578
Y	-0.539398	-3.214504	0.646868	2.14331

$YO_2(Y_2O_3)_4^+$ [(9,14)] #1 (the leftmost structure in Fig. S1)

	x	y	z	charge
Y	-1.968180	1.622535	-2.935001	2.13715
Y	-0.540679	0.212402	2.765970	2.14981
Y	0.249173	1.720159	-0.056408	2.04458
Y	-3.672802	-2.233561	2.061777	2.17114
Y	2.027038	-0.956047	0.911485	2.12291
Y	-2.888488	-1.303592	-1.715920	2.06244
Y	0.251630	-1.261991	-1.858460	2.03893
O	-0.598679	2.581575	-1.813547	-1.34018
O	1.305729	0.859961	1.837624	-1.38809
O	1.585897	0.152906	-0.881204	-1.36009
O	-3.444325	0.936007	-1.601408	-1.37178
O	-2.678033	-0.451390	2.561341	-1.38738
O	-2.665880	-3.965430	1.159654	-0.69584
O	-1.352638	-2.710787	-1.282834	-1.36470
O	1.296686	-2.583931	-0.352608	-1.38950
O	0.265249	-1.657436	2.027102	-1.37321
O	-1.327094	1.826422	1.517870	-1.36794
O	-1.394030	-0.415706	-3.187939	-1.38335
O	-3.953031	-1.283633	0.213997	-1.37423
O	-1.190281	-0.146338	-0.389996	-1.32272
Y	-2.962048	0.762319	0.599775	1.99227
Y	-0.531613	-3.219355	0.680652	2.09939
O	-1.975934	-3.575023	2.450384	-0.69960

$YO_2(Y_2O_3)_4^+$ [(9,14)] #2 (the structure in the middle in Fig. S1)

	x	y	z	charge
Y	-1.968800	1.619227	-2.905983	2.13969
Y	-0.567024	0.063798	2.781416	2.10044
Y	0.236581	1.694490	0.008118	2.05011
Y	-3.555768	-2.343957	2.142783	2.16524
Y	2.021860	-1.009448	0.888621	2.11807
Y	-2.845386	-1.338487	-1.685879	2.05880
Y	0.285423	-1.241124	-1.894379	2.03912
O	-0.636683	2.572623	-1.733828	-1.33930
O	1.283778	0.750982	1.901939	-1.38770
O	1.578728	0.167224	-0.858582	-1.35973
O	-3.477484	0.923479	-1.603659	-1.37089
O	-2.874643	-0.256891	2.669882	-0.74498
O	-2.261974	-3.756101	1.594243	-1.36352
O	-1.295781	-2.765278	-1.366722	-1.36847
O	1.380919	-2.585926	-0.469832	-1.39731
O	0.208338	-1.772380	1.901007	-1.37041
O	-1.346896	1.727565	1.539556	-1.36950
O	-1.388815	-0.407486	-3.191863	-1.38268
O	-3.849899	-1.313618	0.278815	-1.38329
O	-1.217932	-0.163408	-0.423726	-1.32421
Y	-3.000491	0.770917	0.541963	1.97987
Y	-0.454418	-3.360085	0.534359	2.15627
O	-2.383934	-1.193004	3.724944	-0.64562

$YO(Y_2O_3)_5^+$ [(11,16)]

	x	y	z	charge
Y	-6.447370	-0.131839	0.149572	2.12569
Y	-5.748196	3.030304	-0.950844	2.00577
Y	-1.641689	1.502700	-1.510211	1.92769
Y	-3.315108	-1.216976	-0.025563	2.15834
Y	-4.158517	1.310976	2.153534	2.09181
Y	-4.674611	0.327881	-2.752861	2.04642
O	-2.497390	0.699642	0.858811	-1.35894
O	-5.821715	1.838910	0.991613	-1.36606
O	-4.790625	-0.691414	1.581246	-1.40654
O	-4.298495	1.566655	-4.393621	-1.33759
O	-6.526312	1.067990	-1.617651	-1.36463
O	-2.673917	-0.388356	-1.887415	-1.36377
O	-5.152679	-1.280446	-1.063431	-1.35647
Y	-4.376467	6.090451	-1.623562	2.12579
Y	-1.248627	4.991824	-1.793250	2.15824
Y	-3.000756	4.791800	1.162305	2.09208
Y	-3.651139	3.400575	-3.628188	2.04643
O	-4.834607	4.808370	0.146048	-1.36612
O	-5.391431	4.475760	-2.588425	-1.36464
O	-1.510784	3.660918	0.017907	-1.35893
O	-2.488077	6.228547	-0.389848	-1.40650
O	-2.873412	5.565390	-3.014049	-1.35655
O	-1.485271	3.181599	-2.903289	-1.36380
O	-3.884902	2.198563	-1.692445	-1.32937
O	-2.762667	3.019611	2.501786	-1.43370
Y	-0.897938	2.094053	1.430491	2.07209
O	0.040464	1.322103	-0.182292	-1.31675

$YO_2(Y_2O_3)_5^+$ [(11,17)]

	x	y	z	charge
Y	-6.467395	-0.103932	0.198125	2.12566
Y	-5.762382	3.045345	-0.922688	2.01000
Y	-1.666409	1.490186	-1.593738	1.94755
Y	-3.334222	-1.213217	-0.016120	2.15998
Y	-4.143906	1.307894	2.178146	2.09264
Y	-4.724524	0.327479	-2.723134	2.01798
O	-2.508879	0.686066	0.861288	-1.35771
O	-5.809497	1.854517	1.030002	-1.36461
O	-4.802586	-0.691418	1.601073	-1.40779
O	-3.608943	1.332416	-4.434667	-0.65870
O	-6.565422	1.092907	-1.556724	-1.35851
O	-2.709392	-0.405043	-1.877247	-1.36094
O	-5.181721	-1.227683	-1.063363	-1.35687
Y	-4.398833	6.111358	-1.564715	2.12564
Y	-1.262455	5.011489	-1.780215	2.16003
Y	-2.981628	4.799028	1.189684	2.09298
Y	-3.683318	3.452979	-3.609004	2.01790
O	-4.824349	4.809647	0.191654	-1.36462
O	-5.425263	4.517537	-2.527552	-1.35851
O	-1.508629	3.682601	0.016220	-1.35768
O	-2.493493	6.249080	-0.366899	-1.40779
O	-2.923774	5.554892	-2.987036	-1.35694
O	-1.500668	3.226321	-2.905012	-1.36103
O	-3.913491	2.204675	-1.715632	-1.32628
O	-2.735936	3.009084	2.500527	-1.43363
Y	-0.899118	2.078825	1.374813	2.07341
O	0.004644	1.312446	-0.263848	-1.32285
O	-5.036731	1.818959	-4.396022	-0.66930

7. Spin multiplicities, atomic coordinates (Å), and natural charge and spin distributions for assigned structures of $(Y_2O_3)_x^+$ and O $(Y_2O_3)_x^+$ (x = 2–5).

Doublet was used for odd number of Y atoms as spin multiplicity. Atoms with high spin density are highlighted. Calculation level: B3LYP / Y: SDD, O: aug-cc pVTZ

$(Y_2O_3)_2^+$ [(4,6)]

	x	y	z	charge	spin
Y	-3.841670	2.689968	0.205446	2.16331	-0.00253
Y	-3.315233	-0.729539	1.354899	2.16330	-0.00250
Y	-1.397148	0.551707	-1.493984	2.13668	-0.03440
Y	-5.325454	-0.104118	-1.646443	2.13666	-0.03450
O	-4.811861	-1.183667	-0.027294	-1.35785	0.04099
O	-3.270425	-0.092021	-2.554888	-0.79119	0.90931
O	-3.661522	1.263918	1.662017	-1.37735	0.00091
O	-2.112993	2.340187	-0.910907	-1.35775	0.04108
O	-5.274306	1.812265	-1.033160	-1.35774	0.04112
O	-1.651279	-0.654511	0.097225	-1.35806	0.04052

$O(Y_2O_3)_2^+$ [(4,7)]

	x	y	z	charge	spin
Y	-2.453399	-0.113372	0.730780	2.14403	-0.00877
Y	0.439937	0.037511	-2.205666	2.10534	-0.01682
Y	-2.161130	2.605769	-1.753973	2.16449	-0.00042
Y	0.425112	2.202622	0.772587	2.16442	-0.00042
O	-3.185945	1.204568	-0.571455	-1.37032	0.00911
O	-0.821418	3.335424	-0.389897	-1.37866	-0.00012
O	1.312456	0.978433	-0.647126	-1.37702	0.00253
O	-1.063669	-1.115322	-0.849959	-0.47359	0.40379
O	-0.961973	1.330677	-2.866761	-1.37701	0.00256
O	-0.951345	0.855790	1.610715	-1.37031	0.00911
O	-0.522614	-2.093750	-1.562025	-0.23137	0.59945

$(Y_2O_3)_3^+$ [(6,9)]

	x	y	z	charge	spin
Y	-5.728703	-0.804246	0.497172	2.04083	-0.00433
Y	-5.977462	2.576068	-0.058707	2.14576	-0.00013
Y	-2.706218	2.760529	-0.945442	2.14014	0.00001
Y	-2.422786	-0.578001	-0.405835	2.14575	-0.00013
Y	-3.612537	1.419472	2.037728	2.14562	-0.00013
Y	-4.787468	0.579081	-2.502555	2.14575	-0.00013
O	-1.985660	1.358927	0.551363	-1.39343	0.00003
O	-3.640831	-0.627711	1.369725	-1.37785	0.00387
O	-4.009410	3.161675	0.745693	-1.39324	0.00004
O	-5.697146	1.212269	1.573915	-1.37715	-0.00031
O	-4.684310	2.679503	-1.841739	-1.39343	0.00003
O	-6.380995	0.712734	-1.060112	-1.37778	0.00387
O	-2.653104	0.884970	-2.040283	-1.39324	0.00004
O	-4.312779	-1.111414	-1.269583	-1.37703	-0.00031
O	-7.058722	-2.376668	1.123145	-0.68070	0.99757

$O(Y_2O_3)_3^+$ [(6,10)]

	x	y	z	charge	spin
Y	-5.474445	-0.747184	1.056422	2.14639	-0.00021
Y	-6.001783	2.375184	-0.066355	2.14629	-0.00020
Y	-2.863021	2.459085	-1.307403	2.14626	-0.00020
Y	-2.335521	-0.662915	-0.184351	2.14624	-0.00020
Y	-3.363523	1.746776	1.972147	2.13653	-0.00002
Y	-4.997327	-0.060291	-2.283057	1.97265	-0.02140
O	-1.910054	1.423381	0.390527	-1.39196	-0.00002
O	-5.106744	-0.848202	-4.424789	-0.32283	0.51101
O	-4.004575	3.154923	0.446043	-1.39259	0.00001
O	-5.488514	1.327620	1.805262	-1.39198	-0.00001
O	-4.910769	2.169403	-1.914007	-1.37216	-0.00006
O	-6.429245	0.329331	-0.528015	-1.36772	0.00010
O	-2.771477	0.426977	-1.974229	-1.36771	0.00011
O	-4.302910	-1.427550	-0.620633	-1.37208	-0.00006
O	-6.348572	-0.889836	-3.928077	-0.32271	0.51114
O	-3.402169	-0.412295	1.728615	-1.39261	0.00000

$(Y_2O_3)_4^+$ [(8,12)]

	x	y	z	charge	spin
Y	-6.344063	-0.136925	0.891498	2.03329	-0.02171
Y	-5.171576	2.861567	-0.286676	2.04642	-0.00006
Y	-1.985228	2.042167	-0.792627	2.15173	-0.00007
Y	-3.275806	-1.008222	-0.373758	2.07951	-0.00213
Y	-3.569226	1.212975	2.096458	2.14294	-0.00011
Y	-4.262566	0.714349	-2.845220	2.04714	0.00000
O	-3.194825	2.910555	0.791189	-1.38217	0.00031
O	-2.058295	0.477155	0.731010	-1.37702	0.00028
O	-5.648755	1.774267	1.652865	-1.37624	0.00229
O	-4.388411	-0.781030	1.563811	-1.36703	0.01241
O	-3.727638	2.654788	-1.995700	-1.36762	0.00036
O	-7.046332	2.912747	-1.340225	-1.32741	0.00043
O	-2.341716	0.256955	-1.961177	-1.36889	0.00057
O	-4.989549	0.580551	-0.739997	-1.34295	0.00002
Y	-6.516161	-1.601489	-2.170423	2.08081	-0.02814
Y	-7.942974	1.387749	-2.250337	2.13149	0.00441
O	-6.481152	0.280557	-3.352776	-1.39505	0.00040
O	-4.465329	-1.596574	-2.212308	-1.34544	0.01750
O	-6.609824	-2.241874	-0.046138	-0.73301	0.90721
O	-7.817643	-0.232556	-0.904199	-1.33050	0.10604

$O(Y_2O_3)_4^+$ [(8,13)] #1 (The leftmost structure in Fig. S1)

	x	y	z	charge	spin
Y	-0.247990	1.125885	-1.058896	2.09994	-0.00012
Y	-0.737756	-0.348537	2.061888	2.04637	-0.00005
Y	-3.918013	-1.567097	1.985260	2.12086	-0.00012
Y	1.939885	-0.945352	0.298461	2.14803	0.00000
Y	-2.659167	-0.883764	-1.531637	2.05568	-0.00020
Y	0.338508	-1.760147	-2.571386	2.14929	-0.00001
O	0.715447	0.847288	0.971105	-1.37466	0.00000
O	1.480292	-0.121100	-1.642872	-1.38222	0.00000
O	-2.410914	1.431659	-0.798460	-1.36528	0.00029
O	-2.946971	0.270245	2.378972	-1.38027	0.00010
O	-1.499669	-2.762025	-1.734884	-1.37541	0.00001
O	1.240518	-2.695401	-0.822382	-1.38270	0.00000
O	0.699863	-1.908680	1.794167	-1.36968	0.00000
O	-1.032460	-0.815416	-0.051828	-1.35384	-0.00002
O	-1.047940	-0.135257	-2.764432	-1.36919	0.00007
O	-4.275808	-0.723464	0.098177	-1.37780	0.00042
O	-5.060439	3.288270	1.272175	-0.33049	0.51385
Y	-3.855087	1.430251	0.694899	2.02544	-0.02170
Y	-0.618023	-3.036957	0.302548	2.08546	0.00000
O	-2.165476	-2.543435	1.822338	-1.33749	0.00006
O	-5.901250	2.438457	0.673917	-0.33203	0.50743

$O(Y_2O_3)_4^+$ [(8,13)] #2 (The structure in the middle in Fig. S2)

	x	y	z	charge	spin
Y	-0.819787	1.210350	-1.439746	2.09191	0.00015
Y	-0.484205	0.349539	1.904562	2.01814	-0.00333
Y	-3.548668	-1.795200	2.189447	2.14671	-0.00003
Y	2.156301	-0.819928	0.034079	2.04900	-0.01600
Y	-2.878388	-1.153638	-1.544443	2.08294	-0.00002
Y	0.252834	-1.755161	-2.600103	2.13814	-0.00013
O	3.082967	0.872273	1.447244	-0.26253	0.56431
O	1.102863	0.097171	-1.587070	-1.37401	0.00161
O	-3.052329	1.093558	-1.371618	-1.35634	0.00006
O	-2.547334	0.057861	2.570966	-1.38775	0.00211
O	-2.146889	-3.138615	1.717950	-1.33574	0.00002
O	-1.396758	-2.798633	-1.637730	-1.36831	0.00021
O	1.389739	-2.580904	-0.937719	-1.38806	-0.00055
O	0.772249	-1.389911	1.564893	-1.36124	0.00368
O	-1.325352	-0.606283	0.007164	-1.34491	0.00012
O	-1.323590	-0.348315	-2.913815	-1.37247	0.00011
O	-4.156419	-0.901388	0.379002	-1.38160	0.00002
O	-1.244986	1.949100	0.659057	-1.36514	0.00086
Y	-3.304975	1.166666	0.686836	2.08231	-0.00005
Y	-0.505116	-2.800118	0.394091	2.05157	-0.00009
O	1.801159	1.199547	1.321265	-0.36262	0.44694

$(Y_2O_3)_5^+$ [(10,15)]

	x	y	z	charge	spin
Y	-6.216482	-0.082357	0.579744	2.12152	-0.00014
Y	-5.653822	3.126040	-0.547777	2.04966	-0.00024
Y	-1.830263	1.762211	-1.081683	2.04955	-0.00023
Y	-3.132644	-1.182640	0.148909	2.12158	-0.00014
Y	-3.685003	1.359292	2.361180	2.13413	-0.00005
Y	-4.715322	0.334808	-2.395497	2.05348	-0.00972
O	-2.947320	3.260225	2.795039	-1.39636	0.00001
O	-2.293281	0.688367	0.838366	-1.36968	0.00000
O	-5.509085	1.835684	1.287599	-1.36965	0.00001
O	-4.507511	-0.727226	1.798493	-1.40443	0.00027
O	-4.524113	1.641150	-4.368194	-0.67286	0.98582
O	-6.433399	1.137553	-1.246261	-1.37762	0.00824
O	-2.657545	-0.208729	-1.773826	-1.37762	0.00828
O	-5.045936	-1.202682	-0.837633	-1.37072	-0.00073
Y	-4.239391	6.185169	-1.272302	2.12156	-0.00014
Y	-1.155420	5.085023	-1.702665	2.12158	-0.00014
Y	-2.618901	4.739703	1.363369	2.13423	-0.00005
Y	-3.678747	3.619804	-3.365863	2.05341	-0.00972
O	-4.557904	4.846317	0.396904	-1.36968	0.00000
O	-5.355581	4.554928	-2.256026	-1.37763	0.00826
O	-1.344637	3.700404	-0.051225	-1.36966	0.00000
O	-2.283125	6.325951	-0.285256	-1.40451	0.00027
O	-2.892143	5.624651	-2.854768	-1.37069	-0.00073
O	-1.578913	3.208081	-2.783284	-1.37760	0.00826
O	-3.907563	2.274409	-1.565579	-1.35198	0.00262

$O(Y_2O_3)_5^+$ [(10,16)]

	x	y	z	charge	spin
Y	-6.215363	-0.073814	0.566364	2.12405	0.00003
Y	-5.636856	3.121784	-0.595725	2.05196	0.00013
Y	-1.823900	1.768312	-1.082109	2.05189	0.00013
Y	-3.115805	-1.174665	0.170432	2.12416	0.00003
Y	-3.702123	1.372374	2.362136	2.13332	-0.00002
Y	-4.689144	0.301922	-2.390025	2.03161	-0.00165
O	-2.972330	3.268801	2.812472	-1.39596	-0.00001
O	-2.298962	0.700985	0.848631	-1.36807	0.00001
O	-5.511524	1.841882	1.259043	-1.36800	0.00002
O	-4.516867	-0.720439	1.796649	-1.40441	0.00005
O	-4.505050	1.549541	-4.413444	-0.38320	0.42776
O	-6.415390	1.120048	-1.276314	-1.37733	0.00292
O	-2.635647	-0.221163	-1.759125	-1.37734	0.00292
O	-5.023115	-1.194603	-0.844748	-1.36641	-0.00055
Y	-4.226169	6.183541	-1.277002	2.12520	-0.00003
Y	-1.132149	5.085106	-1.671413	2.12516	-0.00003
Y	-2.632606	4.742091	1.374363	2.13370	-0.00001
Y	-3.628263	3.652998	-3.401628	1.96183	-0.01563
O	-4.557438	4.832748	0.381067	-1.36842	0.00002
O	-5.326653	4.562552	-2.279001	-1.37490	0.00064
O	-1.352337	3.695300	-0.027360	-1.36840	0.00002
O	-2.279698	6.325494	-0.266009	-1.40510	0.00002
O	-2.855910	5.628709	-2.844156	-1.36226	-0.00031
O	-1.536958	3.217643	-2.762421	-1.37486	0.00063
O	-3.897045	2.253266	-1.611173	-1.34838	0.00054
O	-4.301908	2.452818	-5.360254	-0.21983	0.58235