

On the energetic and magnetic stability of potassium atomic clusters doped by yttrium

Henry Nicole González-Ramírez,^{*a} Zeferino Gómez-Sandoval,^a

Supplementary information

^a Facultad de Ciencias Químicas, Universidad de Colima, Km. 9 Carretera Colima-Coquimatlán s/n, 28400, Coquimatlán, Colima, México. E-mail: henrygonzalezr@gmail.com

Table S1 Ground state supershell configurations* for K_{n+1} , $K_n Y$, $K_n Y^+$ and $K_n Y^-$ clusters, for $n = 12 - 24$

n	K_{n+1}	$K_n Y$	$K_n Y^+$	$K_n Y^-$
12	$1S^2 1P^6 1D^3 1D^2_{\alpha\beta}$	$1S^2 1P^6 2S^2 1D^5_{\alpha}$	$1S^2 1P^6 1D^5_{\alpha} 2S^1_{\alpha}$	$1S^2 1P^6 2S^2 1D^3_{\alpha} 1D^1_{\beta}$
13	$1S^2 1P^6 1D^6$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^1_{\beta}$	$1S^2 1P^6 1D^5_{\alpha} 1D^1_{\beta} 2S^1_{\alpha}$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^2_{\beta}$
14	$1S^2 1P^6 1D^4_{\alpha} 1D^3_{\beta}$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^2_{\beta}$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^1_{\beta}$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^3_{\beta}$
15	$1S^2 1P^6 1D^8$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^3_{\beta}$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^2_{\beta}$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^4_{\beta}$
16	$1S^2 1P^6 1D^5_{\alpha} 1D^4_{\beta}$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^4_{\beta}$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^3_{\beta}$	$1S^2 1P^6 2S^2 1D^{10}$
17	$1S^2 1P^6 1D^{10}$	$1S^2 1P^6 2S^2 1D^{10}$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^4_{\beta}$	$1S^2 1P^6 2S^2 1D^{10} 1F^1_{\alpha}$
18	$1S^2 1P^6 1D^{10} 2S^1_{\alpha}$	$1S^2 1P^6 2S^2 1D^{10} 1F^1_{\alpha}$	$1S^2 1P^6 2S^2 1D^{10}$	$1S^2 1P^6 2S^2 1D^{10} 1F^2$
19	$1S^2 1P^6 1D^{10} 2S^2$	$1S^2 1P^6 2S^2 1D^{10} 1F^2_{\alpha}$	$1S^2 1P^6 2S^2 1D^{10} 1F^1_{\alpha}$	$1S^2 1P^6 2S^2 1D^{10} 1F^2_{\alpha} 1F^1_{\beta}$
20	$1S^2 1P^6 1D^{10} 2S^2 1F^1_{\alpha}$	$1S^2 1P^6 1D^{10} 2S^2 1F^2_{\alpha} 1F^1_{\beta}$	$1S^2 1P^6 1D^{10} 2S^2 1F^2$	$1S^2 1P^6 1D^{10} 2S^2 1F^3_{\alpha} 1F^1_{\beta}$
21	$1S^2 1P^6 1D^{10} 2S^2 1F^2$	$1S^2 1P^6 1D^{10} 2S^2 1F^3_{\alpha} 1F^1_{\beta}$	$1S^2 1P^6 1D^{10} 2S^2 1F^2_{\alpha} 1F^1_{\beta}$	$1S^2 1P^6 1D^{10} 2S^2 1F^3_{\alpha} 1F^2_{\beta}$
22	$1S^2 1P^6 1D^{10} 2S^2 1F^2_{\alpha} 1F^1_{\beta}$	$1S^2 1P^6 1D^{10} 2S^2 1F^3_{\alpha} 1F^2_{\beta}$	$1S^2 1P^6 1D^{10} 2S^2 1F^3_{\alpha} 1F^1_{\beta}$	$1S^2 1P^6 1D^{10} 2S^2 1F^6$
23	$1S^2 1P^6 1D^{10} 2S^2 1F^4$	$1S^2 1P^6 1D^{10} 2S^2 1F^6$	$1S^2 1P^6 1D^{10} 2S^2 1F^3_{\alpha} 1F^2_{\beta}$	$1S^2 1P^6 1D^{10} 2S^2 1F^4_{\alpha} 1F^3_{\alpha}$
24	$1S^2 1P^6 1D^{10} 2S^2 1F^3_{\alpha} 1F^2_{\beta}$	$1S^2 1P^6 1D^{10} 2S^2 1F^5_{\alpha} 1F^2_{\beta}$	$1S^2 1P^6 1D^{10} 2S^2 1F^6$	$1S^2 1P^6 1D^{10} 2S^2 1F^8$

*In this Table the filling of the valence electron supershells of the clusters under study is shown. This information is included as it allows us to understand the evolution of shell filling as the cluster increases in size and as it acquires a different charge. Furthermore, it enables us to identify the number of unpaired electrons and, consequently, the spin magnetic moment in a given cluster. However, it is important to note that this notation differs slightly from that used in our previous work with yttrium-doped lithium clusters. In this configuration, we still consider the energy order of the shells and their corresponding electron population. However, this time, we indicate full shells if they appear in the energy order and contain all the corresponding electrons. Thus, a configuration like $1S^2 1P^6 1D^3_{\alpha} 1D^3_{\beta} 2S^2 1D^2_{\alpha} 1D^2_{\beta} 1F^1_{\alpha}$ appears as $1S^2 1P^6 1D^{10} 2S^2 1F^1_{\alpha}$. This notation aligns more with the usual superatom context and allows for a more compact configuration.

Table S2 Ground-state supershell configurations* for the neutral and charged clusters doped by two and three yttrium atoms

Neutral cluster	Supershells	Cation cluster	Supershells	Anion cluster	Supershells
$K_{11} Y_2$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^2_{\beta}$	$K_{11} Y_2^+$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^1_{\beta}$	$K_{11} Y_2^-$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^3_{\beta}$
$K_{10} Y_3$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^4_{\beta}$	$K_{10} Y_3^+$	$1S^2 1P^6 2S^2 1D^5_{\alpha} 1D^3_{\beta}$	$K_{10} Y_3^-$	$1S^2 1P^6 2S^2 1D^{10}$
$K_{20} Y_2$	$1S^2 1P^6 2S^2 1D^{10} 1F^6$	$K_{20} Y_2^+$	$1S^2 1P^6 1D^{10} 1F^5_{\alpha} 1F^2_{\beta}$	$K_{20} Y_2^-$	$1S^2 1P^6 1D^{10} 1F^5_{\alpha} 1F^4_{\beta}$
$K_{19} Y_3$	$1S^2 1P^6 2S^2 1D^{10} 1F^8$	$K_{19} Y_3^+$	$1S^2 1P^6 2S^2 1D^{10} 1F^4_{\alpha} 1F^3_{\beta}$	$K_{19} Y_3^-$	$1S^2 1P^6 2S^2 1D^{10} 1F^5_{\alpha} 1F^4_{\beta}$

*In this Table the filling of the valence electron supershells of the clusters under study is shown. This information is included as it allows us to understand the evolution of shell filling as the cluster increases in size and as it acquires a different charge. Furthermore, it enables us to identify the number of unpaired electrons and, consequently, the spin magnetic moment in a given cluster. However, it is important to note that this notation differs slightly from that used in our previous work with yttrium-doped lithium clusters. In this configuration, we still consider the energy order of the shells and their corresponding electron population. However, this time, we indicate full shells if they appear in the energy order and contain all the corresponding electrons. Thus, a configuration like $1S^2 1P^6 1D^3_{\alpha} 1D^3_{\beta} 2S^2 1D^2_{\alpha} 1D^2_{\beta} 1F^1_{\alpha}$ appears as $1S^2 1P^6 1D^{10} 2S^2 1F^1_{\alpha}$. This notation aligns more with the usual superatom context and allows for a more compact configuration.

Table S3 Cartesian coordinates of the K₁₃ cluster

Energy:-7800.744136848
Multiplicity:2

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.357258
K	4.208461	0.000000	1.980235
K	2.011159	3.702416	2.491600
K	-0.507908	3.657112	6.614716
K	-2.351590	3.717760	2.338152
K	-6.683408	2.589599	2.081130
K	-3.774279	-0.735610	2.166150
K	-4.361782	1.672260	5.897561
K	-0.043862	4.481558	-1.323883
K	-0.076235	1.213636	-4.301584
K	3.665167	2.050102	-1.854774
K	-3.853282	1.898788	-1.597702

Table S4 Cartesian coordinates of the K₁₄ cluster

Energy:-8400.809046290
Multiplicity:1

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.348173
K	4.114033	0.000000	-2.050695
K	2.854466	2.417195	2.260659
K	6.839092	1.198879	1.209790
K	3.535934	-2.286944	1.680251
K	4.714453	-0.605930	5.449435
K	2.018171	-4.008886	5.339552
K	2.715099	2.769929	7.222155
K	0.788153	-0.973789	8.589709
K	-2.279616	-3.435013	6.228512
K	-0.915693	-4.015913	1.898831
K	6.422820	3.649557	4.916062
K	1.353563	-3.654804	-2.068527

Table S5 Cartesian coordinates of the K₁₅ cluster

Energy:-9000.865491446
Multiplicity:2

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.289090
K	3.974219	0.000000	2.655345
K	0.472162	4.945227	3.685281
K	1.889681	8.770443	1.407487
K	3.654418	7.734477	5.244294
K	-0.493344	9.513799	5.037468
K	-2.295450	7.627618	1.393486
K	3.225476	2.646454	6.182519
K	0.453831	6.129331	7.946442
K	-3.487870	6.071499	5.434337
K	-2.952004	2.682718	2.142105
K	0.461092	4.493224	-0.780095
K	3.814803	1.581475	-1.467915
K	4.566191	4.474327	1.883491

Table S6 Cartesian coordinates of the K₁₆ cluster

Energy:-9600.927430292
 Multiplicity:1

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.589603
K	4.654246	0.000000	1.172147
K	-2.393524	-3.451535	1.542029
K	3.878705	2.200717	4.998922
K	-4.074522	-0.478828	-2.091211
K	-2.006027	3.385352	-1.878355
K	3.999893	-2.274798	4.982149
K	-0.043140	-4.415742	5.154403
K	-0.954665	-3.454120	-2.890056
K	3.011551	-1.496138	-3.064091
K	-0.278923	0.475144	-4.915673
K	0.931841	3.560457	2.132110
K	5.374737	4.379078	1.089114
K	2.230660	-3.557779	1.199770
K	2.675931	3.064450	-2.238757

Table S7 Cartesian coordinates of the K₁₇ cluster

Energy:-10200.993130733
 Multiplicity:2

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.365348
K	4.382579	0.000000	0.168995
K	-3.626127	1.793339	-1.467392
K	-0.836775	-2.149391	-3.657453
K	-4.082220	-2.749256	-0.611074
K	-0.735199	-5.562618	-0.637880
K	3.257829	-3.904054	-2.020292
K	3.511107	-0.174727	-4.313171
K	-0.212427	2.325455	-4.293637
K	-0.593269	5.297713	-1.161287
K	-2.344856	3.744318	2.552508
K	-4.539822	0.026145	2.851257
K	-2.122900	-3.758995	3.341322
K	2.090440	-3.478079	2.292230
K	3.630362	3.771222	-2.172397
K	2.213925	3.455550	2.000051

Table S8 Cartesian coordinates of the K₁₈ cluster

Energy:-10801.056980247
Multiplicity:1

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.891029
K	2.488356	0.000000	-4.220811
K	2.900158	-3.298782	3.420370
K	3.966659	-2.679698	-0.982581
K	0.833978	-5.772406	0.224155
K	0.741676	-4.088986	-3.830108
K	-1.374156	-4.246307	3.615018
K	-2.178953	-1.044865	-4.715268
K	2.621258	3.514344	-1.393489
K	-0.831879	2.970856	-4.212501
K	-1.561598	5.033061	-0.408990
K	-3.108426	3.088528	3.125822
K	-4.015807	-1.018759	2.657984
K	-2.908078	-3.505375	-0.946545
K	-4.082705	1.262565	-1.244085
K	1.230479	4.028858	2.987721
K	3.908815	0.687364	1.981320

Table S9 Cartesian coordinates of the K₁₉ cluster

Energy:-11401.117200302
Multiplicity:2

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.278299
K	3.173984	0.000000	-2.873296
K	-2.584311	-3.209979	-1.139601
K	-2.543671	3.138438	1.554210
K	-0.532760	3.129605	-2.941425
K	3.306089	-2.252106	1.491742
K	-1.627351	-5.492457	-4.826033
K	-4.728624	-5.471707	2.017342
K	1.876221	-4.178439	-2.442148
K	2.784886	-6.599998	1.262401
K	-0.582541	-4.180110	3.060377
K	-4.300521	0.890999	-1.932117
K	-4.148647	-0.936151	2.541991
K	-0.866051	-0.955934	-4.785852
K	-5.102820	-2.599928	-4.813723
K	-6.997099	-2.581796	-0.627648
K	-1.201389	-7.282849	-0.508424
K	-5.386661	-6.576291	-2.400646

Table S10 Cartesian coordinates of the K₂₀ cluster

Energy:1
 Multiplicity:-12001.184141251

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.502302
K	4.503072	0.000000	0.572315
K	2.471405	3.674687	-0.835680
K	3.329630	3.239596	3.538115
K	4.084948	2.555387	7.847675
K	1.898446	-1.321502	8.784288
K	2.805671	-4.889506	6.294889
K	-0.223834	-6.883741	3.776483
K	-1.544075	-3.641129	6.667359
K	-2.348636	0.508759	8.397554
K	2.189920	-3.499676	2.042227
K	0.888273	2.532458	10.853507
K	-2.401736	-3.229383	2.209559
K	-4.285537	0.820743	1.401942
K	-4.267829	3.080516	5.186870
K	-0.998136	3.845741	2.140142
K	-0.042631	4.007984	6.643591
K	4.582485	-0.933049	5.015311
K	-5.129470	-1.245438	5.210257

Table S11 Cartesian coordinates of the K₂₁ cluster

Energy:-12601.239363908
 Multiplicity:2

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.002076
K	3.945873	0.000000	-1.593183
K	3.957499	-0.074887	5.500978
K	0.980410	3.878825	5.547522
K	0.979060	3.842746	-1.480082
K	1.115853	-3.755415	-1.996884
K	-3.386610	2.063390	-2.007661
K	1.162740	-3.825740	5.950599
K	-3.363107	2.120093	5.955563
K	-3.173084	-2.444108	6.048651
K	0.073275	0.006362	8.447934
K	-3.196554	-2.421847	-2.002449
K	0.041978	0.144930	-4.516731
K	3.721070	2.831143	2.023443
K	1.415452	6.624244	2.066540
K	6.666862	-0.505089	1.934128
K	3.199833	-3.222155	1.981617
K	-2.190318	3.956335	1.986961
K	-4.113637	-0.254121	2.019648
K	-1.361911	-3.890791	2.037188

Table S12 Cartesian coordinates of the K₂₂ cluster

Energy:-13201.296215462
 Multiplicity:1

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.086940
K	3.893388	0.000000	-1.904382
K	-3.349161	1.953404	6.146329
K	-3.461444	2.090581	-1.920383
K	0.943793	3.815068	-1.938600
K	3.268776	2.464279	2.321303
K	6.599273	-0.252811	1.728248
K	5.224344	4.337062	-1.335369
K	0.839270	-3.758208	6.168016
K	1.925016	6.498801	1.802657
K	-1.931500	3.986107	1.907261
K	3.272987	-3.197537	1.983844
K	-4.086047	-0.169521	2.004070
K	4.116496	-0.487037	5.603464
K	1.073094	-3.899231	-1.789246
K	0.678080	4.326034	5.506682
K	-1.315674	-3.934824	2.065635
K	-3.272436	-2.455917	-1.888182
K	-0.177068	-0.209024	-4.457620
K	0.620795	0.650006	8.360048
K	-3.496147	-2.739524	5.971041

Table S13 Cartesian coordinates of the K₂₃ cluster

Energy:-13801.357260583
 Multiplicity:2

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.090033
K	4.068917	0.000000	-1.472584
K	1.350618	-3.639740	6.024974
K	1.067741	-3.891143	-1.467094
K	3.888406	0.899586	6.041013
K	0.597827	3.985949	5.926783
K	6.013998	-2.890970	5.939635
K	-0.057295	-0.019608	8.559844
K	1.208405	3.818579	-1.883933
K	3.117839	3.065496	2.129559
K	3.993878	-1.683326	9.713637
K	-3.252093	-2.318442	5.830946
K	3.367748	-2.420785	2.230089
K	6.722382	0.366111	2.475573
K	1.570514	-6.440211	2.468587
K	-2.041176	-4.091338	1.923286
K	-3.216267	-2.095982	-2.136018
K	0.066725	0.018231	-4.474530
K	-4.149883	0.036331	1.884740
K	-3.295250	2.265026	-2.355846
K	-1.567888	3.820561	1.825571
K	-3.513492	2.302278	5.839299

Table S14 Cartesian coordinates of the K₂₄ cluster

Energy:-14401.418615069
 Multiplicity:1

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.174566
K	0.000000	0.305870	-4.317862
K	0.739778	3.714016	1.916245
K	0.239734	0.742925	8.424409
K	4.762961	5.303844	1.828603
K	1.831340	-3.574073	2.128453
K	-2.422462	6.626833	1.835231
K	-3.862800	-0.245156	-1.861215
K	2.994006	2.946300	-1.860621
K	1.539639	7.538600	4.093270
K	-3.844673	-0.057526	6.126638
K	-1.561897	4.074440	5.651484
K	3.429338	-1.758492	-1.888508
K	3.675329	-1.485462	5.922871
K	-1.061776	-4.225419	-1.421101
K	-3.133674	-2.551187	2.191604
K	-1.666328	3.902271	-1.890487
K	-0.742620	-4.159438	5.732595
K	1.447774	7.281576	-0.643965
K	3.078968	3.167801	5.571199
K	-1.665985	-6.840229	2.102864
K	4.627017	0.549358	1.921670
K	-3.989379	2.210772	2.069655

Table S15 Cartesian coordinates of the K₂₅ cluster

Energy:-15001.479415547
 Multiplicity:2

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.064060
K	0.000000	0.118164	-4.177919
K	-0.671502	0.117799	8.248462
K	-0.493459	-3.973334	5.786323
K	-3.503778	1.572187	2.026128
K	3.729178	-1.391644	5.901480
K	4.114658	-5.698752	5.012621
K	1.760612	-3.723303	1.917160
K	-6.886136	3.021254	-0.475338
K	-4.222616	5.933155	1.712119
K	-7.111141	-0.870266	1.856478
K	2.345516	3.326680	-1.743337
K	-6.944955	3.168358	4.214546
K	-0.831231	-3.925638	-1.860874
K	-2.442698	3.666739	5.783994
K	2.209583	3.123664	6.017014
K	3.973153	-1.447413	-1.402913
K	-2.375778	3.607709	-1.761281
K	-4.178847	-0.736926	-1.721440
K	0.308685	4.534619	2.095976
K	4.083176	1.219624	2.219880
K	6.206553	-2.850696	2.188406
K	-4.237809	-0.823747	5.665229
K	-3.153326	-3.463166	2.000840

Table S16 Cartesian coordinates of the K₁₂Y cluster

Energy: -7239.048452584
 Multiplicity: 6

Atom	x	y	z
Y	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.159079
K	3.719164	0.000000	1.866938
K	3.009819	-2.231953	-1.851276
K	-0.002150	-0.003633	-4.155076
K	-3.725317	0.002108	-1.865238
K	-3.010017	2.231669	1.858049
K	1.192072	3.783847	1.791709
K	-1.063145	3.784337	-1.873808
K	3.038284	2.376317	-1.876884
K	-1.192584	-3.778036	-1.786981
K	1.063725	-3.787515	1.878872
K	-3.038139	-2.375861	1.881058

Table S17 Cartesian coordinates of the K₁₃Y cluster

Energy: -7839.107477857
 Multiplicity: 5

Atom	x	y	z
K	-2.145358	-0.554745	3.248438
K	1.631812	-3.400872	-2.228221
K	-0.427024	3.612898	2.265710
K	1.649706	-3.457729	2.142277
K	2.387095	0.560547	3.607134
K	-2.101788	-3.552801	-0.024147
K	-3.765280	2.434858	0.016746
K	4.551762	-1.170432	-0.016477
K	3.459494	2.931523	0.037253
K	2.397150	0.655228	-3.586714
K	-5.621657	-1.311965	-0.019048
K	-2.134184	-0.490448	-3.254142
K	-0.419890	3.664493	-2.184972
Y	0.250958	0.047957	-0.004723

Table S18 Cartesian coordinates of the K₁₄Y cluster

Energy: -8439.171690913
 Multiplicity: 4

Atom	x	y	z
K	0.011860	-0.298590	4.029766
K	-0.012794	0.299402	-4.029527
K	0.465583	4.020063	2.136203
K	4.164329	-0.326285	-1.893391
K	3.853438	1.554034	1.957900
K	-2.488937	-3.241477	-2.078212
K	-3.380831	2.349778	2.034100
K	2.478177	3.507837	-1.619278
K	3.381827	-2.605429	1.664025
K	-4.174717	0.590077	-1.804969
K	-3.829682	-1.810810	1.739663
K	1.680816	-3.698735	-2.120113
K	-0.456701	-4.303433	1.561005
K	-1.693913	3.969692	-1.574858
Y	-0.000116	0.000324	-0.000462

Table S19 Cartesian coordinates of the K₁₅Y cluster

Energy: -9039.233640059
 Multiplicity: 3

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.672798
K	3.614996	0.000000	2.005747
K	0.223119	-3.579278	7.286721
K	3.677817	-2.302955	5.453757
K	-3.408370	-2.794806	5.488383
K	-3.490182	-1.444335	1.587663
K	-4.192054	-5.489503	2.040549
K	5.049983	-4.173444	1.937937
K	2.472185	-6.681467	4.391413
K	-1.751755	-6.840837	5.421811
K	-0.964100	-8.020817	1.437137
K	2.821886	-2.622321	-1.495430
K	2.442004	-6.591799	-0.380668
K	-1.289443	-4.461866	-1.222276
Y	0.321645	-3.662975	2.580660

Table S20 Cartesian coordinates of the K₁₆Y cluster

Energy: -9639.299396071
 Multiplicity: 2

Atom	x	y	z
Y	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.319703
K	4.009886	0.000000	-1.304873
K	-3.548057	1.939892	2.714453
K	-0.023545	4.158144	2.768205
K	-5.850751	1.601958	-0.970513
K	-2.976443	-0.493898	-3.328728
K	3.630085	2.021049	2.655947
K	3.409180	-2.113668	2.784459
K	2.649469	-4.071235	-0.881096
K	1.074425	-1.890749	-4.155239
K	-2.068052	3.774760	-1.071889
K	-0.349326	-3.918542	2.309924
K	-3.831970	-1.890363	0.798636
K	-1.526268	-4.305789	-1.829509
K	0.221361	2.181888	-4.078159
K	2.271051	3.962654	-0.851389

Table S21 Cartesian coordinates of the K₁₇Y cluster

Energy: -10239.366269603
 Multiplicity: 1

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.344930
K	3.892428	0.000000	-1.952486
K	4.267237	-3.464980	-4.389113
K	4.826786	-6.939638	-2.191624
K	-1.760479	-3.519457	2.446626
K	0.304649	-7.329063	3.161229
K	1.598276	-8.939564	-0.550163
K	-2.441715	-3.079402	-1.711393
K	0.621598	-5.932919	-3.668853
K	0.523287	-1.496819	-4.113165
K	-2.133057	-6.961091	-0.304308
K	2.207134	-3.824103	4.422135
K	6.539513	-3.562806	3.988482
K	3.819078	-0.577924	2.186614
K	4.505918	-6.870535	2.053838
K	6.215029	-3.347975	-0.365617
Y	1.851258	-4.020681	-0.077151

Table S22 Cartesian coordinates of the K₁₈Y cluster

Energy: -10839.420562405
 Multiplicity: 2

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	7.203831
K	2.519111	0.000000	3.568095
K	0.310679	4.514345	0.112832
K	0.321139	4.524403	7.101516
K	6.522107	0.985508	3.637083
K	7.359715	4.598966	5.721744
K	4.198365	6.230736	7.814492
K	1.454241	8.527494	5.715583
K	1.501220	8.519758	1.522684
K	4.169749	6.239073	-0.682334
K	7.261847	4.617606	1.539304
K	-1.072606	2.337612	3.593451
K	-1.623521	6.512002	3.616337
K	4.072821	2.001240	0.024852
K	4.062786	1.996106	7.156062
K	5.346383	8.001654	3.648503
K	-1.607358	-2.287614	3.571090
Y	3.022398	4.488775	3.603474

Table S23 Cartesian coordinates of the K₁₉Y cluster

Energy: -11439.474837194
 Multiplicity: 3

Atom	x	y	z
Y	0.007439	-0.403058	0.009162
K	-0.055125	-0.292214	4.385944
K	3.827952	-0.282140	2.142220
K	-3.283480	2.432286	-1.125322
K	0.657747	2.441552	-3.405370
K	-0.835016	-4.249489	-1.462495
K	1.479202	-3.985322	2.542421
K	-2.581838	-3.472067	2.576888
K	3.536194	-3.457449	-0.956337
K	-2.360023	-0.493108	-4.089420
K	1.582496	-1.798135	-4.291085
K	-4.502037	-1.811271	-0.776967
K	2.561732	3.511640	0.237052
K	-1.088711	3.505518	2.348672
K	2.666779	3.306070	4.629447
K	-4.020818	0.535698	2.754203
K	4.392717	0.554953	-2.107293
K	-0.829145	6.416329	-1.406557
K	-2.859766	4.812977	-4.927061
K	1.331039	7.410751	2.333327

Table S24 Cartesian coordinates of the K₂₀Y cluster

Energy: -12039.534254032
 Multiplicity: 2

Atom	x	y	z
K	4.754483	-2.364583	-2.108768
K	3.433903	4.509048	-2.008578
K	8.326965	-2.090623	0.559110
K	-0.611832	4.168121	0.613394
K	6.738814	1.739904	-0.589297
K	-3.946755	2.681096	2.858447
K	2.048329	0.690782	-0.682137
K	-4.536821	3.291448	-1.234321
K	-2.808761	-3.938167	-2.994856
K	-6.046874	-0.523375	0.261296
K	3.987384	-1.470231	2.469758
K	-0.796780	2.848292	-3.452047
K	-3.454264	-4.121764	1.046535
K	3.691785	3.335395	2.368221
K	0.782170	-3.694658	-0.552445
K	-3.762982	-1.217838	4.118199
K	0.007464	-3.168224	3.530218
K	0.074996	1.100247	3.716531
K	0.334548	-1.261885	-4.153714
K	-3.995620	-0.029973	-3.805906
Y	-1.845187	-0.188605	0.009719

Table S25 Cartesian coordinates of the K₂₁Y cluster

Energy: -12639.597552527
 Multiplicity: 3

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.373311
K	3.951551	0.000000	1.865703
K	2.597508	-3.881924	3.119933
K	4.080917	-7.885915	2.097860
K	0.386751	-6.926722	-0.204549
K	-3.486057	-7.304033	1.290539
K	-5.731418	-3.780012	1.976168
K	-3.746913	-0.096795	1.713642
K	-0.001115	-7.570170	4.109955
K	-3.807050	-5.987811	5.419330
K	-3.813892	-1.732722	5.677916
K	-0.149711	-3.894780	6.713662
K	7.557221	-1.717757	4.065445
K	7.596101	-3.885186	7.901797
K	7.737036	-6.198021	4.151494
K	6.168004	-4.021948	0.509774
K	3.856319	-6.258651	6.616145
K	3.825460	-1.528204	6.651644
K	1.973904	-3.292465	-1.366617
K	-2.638177	-3.560851	-1.357899
Y	-1.360637	-3.687289	2.538191

Table S26 Cartesian coordinates of the K₂₂Y cluster

Energy: -13239.656920576
 Multiplicity: 2

Atom	x	y	z
K	-2.044466	-4.002616	-1.616958
K	-3.028667	-0.050410	-4.281908
K	2.193463	-4.852547	-0.981170
K	4.577053	-3.314677	2.196559
K	1.342206	-1.964007	-3.873469
K	5.446110	-2.177731	-2.071029
K	-4.621972	-2.571961	2.115679
K	-1.695735	-0.013804	-0.162422
K	0.198660	-3.149359	2.397130
K	2.743485	0.038912	4.341384
K	0.109263	3.093578	2.305262
K	-2.378572	4.054548	-1.505790
K	1.030291	2.079843	-3.659468
K	5.193507	2.252876	-2.163425
K	-8.315165	-0.180222	1.390382
K	-1.775756	-0.028107	4.677489
K	1.969810	5.142371	-0.994999
K	6.748039	0.115746	1.296365
K	4.408134	3.427708	2.080797
K	-6.325112	-2.365749	-1.915286
K	-6.470158	2.196422	-1.922603
K	-4.775268	2.407344	2.114556
Y	2.391642	-0.065622	0.097869

Table S27 Cartesian coordinates of the K₂₃Y cluster

Energy: -13839.716957632
 Multiplicity: 1

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.522807
K	3.753062	0.000000	2.339384
Y	-0.017725	3.856397	2.411049
K	-3.553693	2.444979	4.635077
K	3.829297	-2.747832	-1.221415
K	7.630083	-1.004959	0.210934
K	7.546072	-1.117243	4.601141
K	5.653637	-4.626785	2.293671
K	1.237235	-3.976126	2.269267
K	3.814624	2.106065	6.085224
K	3.712356	-2.879269	5.839413
K	-0.117967	3.108240	7.324158
K	-2.065663	6.543419	5.962106
K	2.232820	6.200996	5.334721
K	4.671579	4.381540	2.478487
K	2.317346	6.411381	-0.304878
K	3.893514	2.315747	-1.274814
K	-2.015786	6.732459	-0.991829
K	-0.334441	8.308828	2.543823
K	-3.553242	2.541376	0.152500
K	-0.058487	3.373167	-2.434826
K	-4.280361	6.074364	2.452449
K	-3.445274	-1.459112	2.273963

Table S28 Cartesian coordinates of the K₂₄Y cluster

Energy: -14439.777775034
 Multiplicity: 4

Atom	x	y	z
K	4.354581	4.882939	1.270274
K	4.764859	-3.997850	2.309022
K	-4.421903	4.299721	1.544692
K	-2.449760	-3.225314	-1.741863
K	2.846275	3.979597	-2.843562
K	4.891752	-5.359373	-1.792956
K	-3.366130	3.929334	-2.741285
K	-3.031035	-2.760560	2.626631
K	2.058167	2.554899	4.289244
K	0.847605	-5.223251	0.818401
K	-0.111328	3.619921	0.412990
K	1.079292	-2.118892	4.508940
K	-7.066019	2.113236	-1.097516
K	0.866676	-0.731562	0.484643
K	-0.376177	0.760490	-3.439599
K	-6.462859	-2.202383	-0.441132
K	7.096244	2.667137	-1.470786
K	1.368169	-3.652233	-3.619294
K	-6.271753	0.470155	2.851873
K	7.623017	-1.945209	-0.781158
K	5.096296	0.467359	1.970127
K	-2.066960	1.278299	4.020775
Y	-3.143742	0.575907	-0.069645
K	4.100814	-0.355410	-2.827613
K	-4.660228	-0.133206	-4.009548

Table S29 Cartesian coordinates of the $K_{11}Y_2$ cluster

Energy:-6677.350428115
Multiplicity: 4

Atom	x	y	z
K	4.593093	-0.453518	0.123560
K	2.625252	2.340768	-2.683763
K	2.411792	3.070486	1.733836
K	1.916607	-0.891354	3.700865
K	2.200416	-1.916862	-3.306658
K	1.909160	-3.950691	0.488564
K	-1.712455	-3.277509	-1.701057
K	-2.023132	-2.354623	2.786026
K	-1.218109	0.787046	-3.787306
K	-1.579783	1.894036	3.325392
K	-1.232886	3.951443	-0.433766
Y	0.062533	0.000814	0.003129
Y	-3.346418	0.315936	-0.158804

Table S30 Cartesian coordinates of the $K_{10}Y_3$ cluster

Energy: -6115.680781263
Multiplicity: 2

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.388774
K	3.758502	0.000000	2.255347
K	3.374125	-2.493744	-1.362155
K	5.539749	-4.044532	2.263490
K	-2.885843	-2.501310	2.197767
K	-0.877663	-4.064595	5.904730
K	-0.746797	-4.076372	-1.314043
K	2.576103	-6.553611	0.143082
K	-1.168097	-6.570510	2.274071
Y	1.472997	-3.416617	2.589488
Y	3.116233	-2.832307	5.477605
Y	2.543967	-6.020345	4.451321

Table S31 Cartesian coordinates of the K₂₀Y₂ cluster

Energy: -12077.926271957
 Multiplicity: 1

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	3.978257
K	3.648729	0.000000	-1.923433
K	7.086220	-0.709367	-0.064520
K	7.105080	0.072389	3.705608
K	5.435121	-4.027748	-2.102716
K	3.091572	-6.859161	0.090401
K	3.368660	-6.632634	4.192038
K	5.821823	-3.434967	5.694999
K	1.175391	-3.563006	-1.809908
K	3.700105	0.287853	5.992364
K	1.452523	-3.354749	6.092470
K	-0.082395	-4.296491	2.192302
K	6.812106	-4.860207	1.858441
K	-0.293048	4.057725	1.600017
K	1.742491	4.185705	5.215376
K	3.500889	6.507540	1.928998
K	5.953880	4.201702	4.558679
K	2.636433	4.134899	-1.440084
K	6.615501	3.655477	0.353516
Y	3.428253	1.460934	2.032113
Y	3.489268	-2.032138	2.006131

Table S32 Cartesian coordinates of the K₁₉Y₃ cluster

Energy: -11516.267650544
 Multiplicity: 1

Atom	x	y	z
K	0.000000	0.000000	0.000000
K	0.000000	0.000000	4.400196
K	4.233634	0.000000	-1.520217
K	1.881727	3.803123	5.704573
K	4.162578	0.035672	5.897874
K	6.240318	3.613759	-0.039760
K	2.011764	-3.902335	-1.412400
K	6.260236	-3.596559	-0.018847
K	6.277699	-3.617670	4.350072
K	9.968645	2.110453	1.858123
K	9.989157	-2.053307	1.892545
K	-0.603543	-3.951596	2.105064
K	3.144263	-6.083031	2.181024
K	1.889386	-3.856694	5.693687
K	3.088590	6.102924	2.182553
K	-0.606164	3.958252	2.100887
Y	6.108424	0.006609	2.223642
Y	3.169416	1.704710	2.153771
Y	3.172901	-1.694928	2.168680
K	8.790139	0.036222	5.588466
K	6.287293	3.658664	4.306879
K	1.998366	3.900203	-1.444342

Table S33 Intensity and frequency values for the ground state vibrational modes of the K₁₃ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	17.2	0.0	2	17.8	0.1
3	19.7	0.1	4	23.1	0.1
5	24.0	0.1	6	26.2	0.1
7	27.5	0.5	8	28.6	0.3
9	28.7	0.2	10	30.3	0.2
11	31.8	0.1	12	32.3	0.1
13	35.5	0.1	14	35.7	0.5
15	37.1	0.1	16	37.4	0.1
17	40.7	0.0	18	41.0	0.0
19	42.1	0.0	20	44.3	0.0
21	47.7	0.0	22	48.6	0.3
23	50.8	0.0	24	53.7	0.2
25	59.2	0.0	26	60.9	0.1
27	61.7	0.0	28	63.5	0.0
29	67.2	0.1	30	68.0	0.1
31	68.6	0.1	32	74.1	0.1
33	75.3	0.2			

Table S34 Intensity and frequency values for the ground state vibrational modes of the K₁₄ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	17.5	0.0	2	18.6	0.0
3	20.6	0.2	4	22.8	0.2
5	23.3	0.1	6	25.0	0.3
7	26.7	0.2	8	27.0	0.1
9	27.9	0.1	10	29.4	0.5
11	30.3	0.4	12	32.5	0.0
13	33.9	0.4	14	34.9	0.1
15	37.9	0.1	16	38.1	0.2
17	39.2	0.0	18	39.6	0.0
19	40.4	0.3	20	41.5	0.2
21	42.1	0.2	22	43.7	0.0
23	47.8	0.0	24	53.0	0.3
25	55.1	0.1	26	55.4	0.1
27	58.0	0.0	28	59.6	0.0
29	61.2	0.0	30	62.2	0.0
31	66.1	0.0	32	67.5	0.0
33	69.8	0.1	34	70.1	0.2
35	81.1	0.5	36	83.0	0.0

Table S35 Intensity and frequency values for the ground state vibrational modes of the K₁₅ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	14.1	0.1	2	14.9	0.0
3	15.3	0.0	4	19.6	0.3
5	22.8	0.1	6	24.3	0.2
7	25.2	0.0	8	26.3	0.1
9	27.1	1.1	10	28.0	0.0
11	28.6	0.1	12	29.0	0.2
13	32.2	0.3	14	34.8	0.3
15	35.3	0.3	16	36.3	0.2
17	37.4	0.3	18	37.8	0.4
19	38.8	0.1	20	40.2	0.1
21	42.3	0.0	22	44.6	0.0
23	45.2	0.0	24	46.9	0.0
25	47.4	0.2	26	48.7	0.0
27	51.8	0.0	28	55.3	0.0
29	55.4	0.0	30	58.8	0.2
31	59.3	0.1	32	62.0	0.4
33	62.5	1.1	34	65.3	0.3
35	66.6	0.0	36	69.2	0.0
37	71.0	0.3	38	72.9	0.1
39	76.2	0.3			

Table S36 Intensity and frequency values for the ground state vibrational modes of the K₁₆ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	13.3	0.0	2	16.4	0.3
3	17.7	0.3	4	20.6	0.0
5	20.9	0.1	6	22.1	0.7
7	24.6	0.1	8	24.9	0.1
9	26.5	0.3	10	28.0	0.0
11	29.5	0.1	12	30.1	0.1
13	31.7	0.1	14	33.2	0.4
15	34.8	0.1	16	34.9	0.1
17	35.8	0.1	18	36.4	0.0
19	36.9	0.2	20	37.4	0.1
21	39.6	0.0	22	40.5	0.0
23	43.0	0.1	24	43.3	0.1
25	43.5	0.5	26	45.2	0.0
27	50.1	0.0	28	51.3	0.1
29	52.0	0.0	30	54.6	0.0
31	56.3	0.0	32	58.4	0.1
33	59.8	0.1	34	60.8	0.6
35	61.4	0.1	36	63.6	0.2
37	66.4	0.2	38	69.0	0.0
39	71.2	0.2	40	73.8	0.2
41	75.4	0.0	42	78.8	0.0

Table S37 Intensity and frequency values for the ground state vibrational modes of the K₁₇ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	4.5	0.4	2	14.3	0.2
3	14.5	0.1	4	17.2	0.4
5	20.9	0.2	6	22.5	0.2
7	25.0	0.1	8	26.4	0.2
9	27.3	0.2	10	28.1	0.1
11	30.2	0.0	12	30.7	0.0
13	31.0	0.1	14	32.1	0.3
15	32.6	0.3	16	32.9	0.0
17	33.8	0.1	18	34.5	0.2
19	35.5	0.0	20	36.0	0.1
21	37.1	0.1	22	39.3	0.0
23	40.8	0.0	24	41.9	0.1
25	43.1	0.5	26	44.4	0.1
27	46.7	0.1	28	50.2	0.0
29	51.1	0.0	30	53.2	0.0
31	53.5	0.0	32	56.9	0.1
33	57.3	0.0	34	58.5	0.0
35	59.3	0.2	36	60.2	0.1
37	61.0	0.1	38	63.0	0.1
39	63.3	0.0	40	64.6	0.0
41	66.9	0.0	42	67.6	0.0
43	68.0	0.0	44	70.5	0.0
45	75.0	0.1			

Table S38 Intensity and frequency values for the ground state vibrational modes of the K₁₈ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	5.5	0.5	2	12.5	0.0
3	15.2	0.3	4	17.2	0.1
5	18.5	0.2	6	19.1	0.1
7	22.4	0.1	8	23.1	0.1
9	24.2	0.0	10	25.7	0.2
11	26.4	0.1	12	27.0	0.1
13	29.1	0.0	14	30.0	0.1
15	31.3	0.1	16	32.2	0.0
17	32.5	0.1	18	33.3	0.2
19	34.1	0.2	20	34.5	0.2
21	37.4	0.5	22	38.4	0.2
23	39.1	0.3	24	40.3	0.1
25	41.5	0.1	26	42.6	0.2
27	43.7	0.4	28	44.5	0.1
29	46.6	0.1	30	51.6	0.1
31	52.6	0.0	32	55.4	0.0
33	56.6	0.0	34	56.9	0.0
35	58.2	0.2	36	58.9	0.1
37	60.0	0.0	38	60.8	0.0
39	60.9	0.1	40	61.8	0.0
41	64.8	0.0	42	66.0	0.0
43	66.6	0.1	44	67.9	0.0
45	69.4	0.0	46	70.3	0.1
47	71.7	0.0	48	77.3	0.1

Table S39 Intensity and frequency values for the ground state vibrational modes of the K₁₉ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	15.4	0.0	2	17.8	0.2
3	19.7	0.0	4	20.9	0.1
5	22.1	0.0	6	22.9	0.0
7	23.7	0.0	8	24.6	0.0
9	25.1	0.2	10	27.9	0.0
11	28.8	0.0	12	29.6	0.4
13	30.3	0.0	14	31.5	0.1
15	31.8	0.3	16	32.8	0.1
17	33.6	0.2	18	34.5	0.0
19	36.9	0.3	20	37.3	0.3
21	37.8	0.0	22	38.8	0.0
23	39.5	0.2	24	40.9	0.0
25	41.7	0.0	26	41.9	0.0
27	43.2	0.0	28	43.8	0.0
29	45.0	0.0	30	46.3	0.0
31	46.7	0.0	32	48.3	0.1
33	50.1	0.0	34	51.9	0.2
35	53.0	0.1	36	54.1	0.0
37	56.9	0.0	38	57.4	0.0
39	57.8	0.0	40	59.1	0.1
41	61.4	0.1	42	62.8	0.2
43	64.5	0.0	44	64.8	0.1
45	66.4	0.0	46	67.8	0.0
47	72.9	0.3	48	73.3	0.1
49	76.1	0.1	50	76.8	0.2
51	79.6	0.0			

Table S40 Intensity and frequency values for the ground state vibrational modes of the K₂₀ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	18.1	0.2	2	19.3	0.3
3	19.8	0.3	4	23.5	0.0
5	23.8	0.0	6	24.5	0.0
7	25.1	0.1	8	25.4	0.1
9	26.9	0.0	10	27.6	0.1
11	28.1	0.1	12	28.4	0.1
13	30.5	0.1	14	30.8	0.1
15	31.5	0.2	16	32.8	0.4
17	33.0	0.1	18	33.4	0.1
19	33.9	0.2	20	34.0	0.1
21	35.0	0.1	22	35.9	0.1
23	36.5	0.1	24	38.3	0.0
25	38.7	0.0	26	39.4	0.0
27	40.3	0.1	28	41.5	0.0
29	41.8	0.2	30	42.1	0.2
31	45.3	0.2	32	46.2	0.2
33	46.5	0.2	34	51.3	0.0
35	51.5	0.0	36	52.0	0.0
37	54.9	0.0	38	55.4	0.0
39	55.7	0.0	40	57.5	0.1
41	60.7	0.0	42	61.8	0.0
43	62.3	0.1	44	63.4	0.1
45	63.5	0.1	46	64.7	0.1
47	65.0	0.0	48	65.7	0.0
49	67.6	0.1	50	68.7	0.2
51	69.1	0.3	52	71.4	0.1
53	71.6	0.2	54	72.6	0.1

Table S41. Intensity and frequency values for the ground state vibrational modes of the K₂₁ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	14.3	0.1	2	19.1	0.3
3	19.5	0.3	4	21.4	0.0
5	22.0	0.2	6	22.8	0.3
7	23.8	0.2	8	25.6	0.2
9	26.2	0.3	10	26.8	0.1
11	27.2	0.3	12	28.0	0.2
13	28.5	0.2	14	30.1	0.1
15	30.7	0.0	16	31.0	0.2
17	32.9	0.1	18	33.9	0.2
19	34.2	0.0	20	34.8	0.3
21	35.3	0.1	22	35.5	0.3
23	36.6	0.1	24	37.3	0.4
25	37.9	0.2	26	38.3	0.1
27	38.7	0.1	28	40.2	0.3
29	41.0	0.4	30	41.5	0.4
31	42.5	0.2	32	43.8	0.1
33	44.2	0.0	34	46.0	0.1
35	47.6	0.1	36	48.2	0.3
37	50.3	0.0	38	51.7	0.1
39	52.3	0.0	40	53.6	0.2
41	54.3	0.2	42	55.1	0.1
43	55.8	0.2	44	57.8	0.0
45	58.5	0.8	46	59.2	0.4
47	59.7	0.2	48	60.0	0.2
49	62.9	0.1	50	65.6	0.1
51	68.7	0.2	52	72.3	0.1
53	73.7	0.0	54	75.5	0.1
55	76.5	0.1	56	77.4	0.2
57	94.3	0.0			

Table S42 Intensity and frequency values for the ground state vibrational modes of the K₂₂ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	8.0	0.1	2	15.0	0.1
3	17.6	0.0	4	19.2	0.1
5	19.6	0.1	6	21.7	0.0
7	22.2	0.1	8	22.4	0.2
9	24.9	0.1	10	25.6	0.3
11	26.0	0.1	12	26.7	0.2
13	27.9	0.1	14	28.9	0.0
15	29.4	0.1	16	30.5	0.1
17	30.7	0.1	18	31.2	0.2
19	32.3	0.0	20	33.0	0.0
21	34.1	0.1	22	35.2	0.0
23	35.7	0.3	24	36.3	0.1
25	37.2	0.0	26	37.7	0.2
27	38.7	0.2	28	39.1	0.1
29	39.6	0.0	30	40.4	0.1
31	41.3	0.2	32	42.2	0.2
33	42.9	0.1	34	43.7	0.0
35	44.6	0.1	36	45.2	0.1
37	45.6	0.1	38	47.7	0.0
39	48.9	0.1	40	49.7	0.1
41	50.5	0.1	42	50.9	0.2
43	52.5	0.3	44	52.9	0.1
45	53.4	0.2	46	55.4	0.3
47	56.8	0.3	48	59.0	0.0
49	59.7	0.0	50	61.8	0.0
51	63.3	0.1	52	64.7	0.2
53	67.1	0.2	54	69.3	0.3
55	72.6	0.1	56	73.8	0.3
57	74.6	0.1	58	76.5	0.1
59	77.4	0.1	60	91.2	0.1

Table S43 Intensity and frequency values for the ground state vibrational modes of the K₂₃ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	6.2	0.6	2	8.5	2.3
3	11.1	0.5	4	14.1	0.9
5	19.1	0.9	6	19.4	0.1
7	22.1	0.1	8	22.6	0.1
9	23.4	0.2	10	24.5	0.2
11	25.6	0.1	12	26.3	0.1
13	27.5	0.1	14	28.8	0.2
15	29.2	0.2	16	29.4	0.2
17	30.0	0.2	18	30.4	0.0
19	31.4	0.3	20	31.6	0.1
21	32.4	0.1	22	33.5	0.2
23	33.7	0.2	24	34.7	0.1
25	35.8	0.5	26	36.1	0.1
27	36.9	0.0	28	38.3	0.3
29	39.2	0.5	30	40.2	0.2
31	40.3	0.2	32	40.9	0.0
33	41.5	0.1	34	41.8	0.0
35	42.6	0.3	36	43.6	0.2
37	45.4	0.5	38	46.2	0.2
39	47.0	0.1	40	47.9	0.2
41	48.2	0.6	42	49.3	0.2
43	51.5	0.0	44	51.7	0.6
45	52.1	0.2	46	53.6	0.2
47	55.0	0.2	48	55.8	0.2
49	56.8	0.1	50	58.1	0.7
51	60.4	0.2	52	60.6	0.1
53	62.2	0.0	54	64.8	0.2
55	66.4	0.1	56	67.4	0.1
57	70.7	0.2	58	72.4	0.1
59	73.7	0.2	60	75.0	0.4
61	75.4	0.1	62	76.4	0.1
63	89.3	0.3			

Table S44 Intensity and frequency values for the ground state vibrational modes of the K_{24} cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	14.1	0.0	2	16.8	0.0
3	17.3	0.0	4	20.0	0.1
5	20.3	0.2	6	22.3	0.1
7	22.5	0.1	8	23.4	0.0
9	24.0	0.1	10	24.7	0.1
11	26.0	0.0	12	26.5	0.1
13	26.7	0.1	14	27.6	0.1
15	28.4	0.0	16	29.3	0.3
17	30.3	0.1	18	30.9	0.1
19	32.0	0.2	20	32.4	0.1
21	33.6	0.0	22	34.2	0.0
23	34.5	0.1	24	35.6	0.1
25	36.1	0.1	26	36.4	0.2
27	37.0	0.2	28	37.7	0.0
29	38.8	0.1	30	38.9	0.1
31	39.2	0.1	32	40.1	0.2
33	40.9	0.1	34	41.4	0.2
35	42.3	0.1	36	42.6	0.1
37	43.2	0.5	38	44.6	0.0
39	46.0	0.1	40	47.0	0.0
41	47.1	0.1	42	47.9	0.1
43	48.3	0.2	44	50.2	0.1
45	51.4	0.2	46	51.7	0.0
47	52.1	0.1	48	52.5	0.3
49	53.8	0.3	50	53.9	0.2
51	55.0	0.2	52	55.0	0.1
53	55.9	0.1	54	59.0	0.1
55	60.8	0.2	56	62.4	0.1
57	66.5	0.3	58	67.1	0.1
59	69.9	0.0	60	70.5	0.0
61	73.1	0.1	62	74.6	0.1
63	75.7	0.1	64	82.1	0.2
65	82.8	0.3	66	91.8	0.0

Table S45 Intensity and frequency values for the ground state vibrational modes of the K₂₅ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	7.5	0.2	2	11.6	0.0
3	17.3	0.0	4	18.4	0.1
5	20.1	0.0	6	20.6	0.0
7	22.4	0.0	8	23.8	0.1
9	23.9	0.1	10	24.9	0.1
11	25.3	0.0	12	26.0	0.0
13	26.9	0.1	14	27.4	0.1
15	27.7	0.5	16	28.2	0.0
17	28.8	0.2	18	28.9	0.2
19	30.0	0.1	20	30.6	0.1
21	30.7	0.0	22	32.4	0.3
23	32.8	0.0	24	33.1	0.1
25	33.9	0.2	26	34.4	0.2
27	35.0	0.4	28	35.3	0.1
29	37.1	0.2	30	37.5	0.1
31	38.3	0.1	32	38.7	0.0
33	39.2	0.0	34	40.4	1.3
35	41.1	0.0	36	41.3	0.0
37	42.4	0.9	38	42.8	0.0
39	43.5	0.3	40	44.2	0.1
41	45.1	0.1	42	46.0	0.4
43	46.8	0.0	44	47.5	0.0
45	48.6	0.0	46	50.1	0.1
47	50.8	0.0	48	51.2	0.5
49	51.3	0.1	50	52.2	0.1
51	53.5	0.0	52	53.9	0.1
53	55.1	0.1	54	56.3	0.1
55	56.8	0.1	56	58.5	0.1
57	59.4	0.1	58	60.8	0.1
59	64.3	0.1	60	65.8	0.0
61	67.9	0.2	62	68.4	0.1
63	71.8	0.0	64	72.3	0.0
65	73.6	0.1	66	74.0	0.4
67	80.6	0.1	68	81.4	0.5
69	96.6	0.0			

Table S46 Intensity and frequency values for the ground state vibrational modes of the K₁₂Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	8.9	0.0	2	23.5	0.0
3	30.9	0.0	4	31.6	0.0
5	35.0	0.0	6	37.2	0.0
7	37.6	0.1	8	45.0	0.0
9	45.5	0.0	10	47.0	0.0
11	48.1	0.0	12	51.1	0.0
13	51.7	0.5	14	52.2	0.9
15	52.4	1.0	16	55.6	0.0
17	56.3	0.0	18	56.4	0.0
19	56.7	0.0	20	60.4	0.0
21	61.0	0.0	22	61.9	0.0
23	63.0	0.1	24	67.7	0.0
25	68.3	0.0	26	68.5	0.9
27	76.0	0.0	28	76.5	0.0
29	77.6	0.0	30	80.1	0.0
31	91.1	0.7	32	97.5	1.1
33	97.9	1.1			

Table S47 Intensity and frequency values for the ground state vibrational modes of the K₁₃Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	12.3	0.0	2	14.2	0.1
3	25.4	0.0	4	30.6	0.2
5	31.3	0.0	6	33.1	0.0
7	35.2	0.3	8	38.0	0.0
9	39.0	0.0	10	40.4	0.0
11	41.7	0.3	12	44.2	0.1
13	47.0	0.0	14	49.0	0.1
15	50.7	0.3	16	51.1	0.5
17	53.1	0.0	18	54.0	0.0
19	56.4	0.2	20	57.3	0.0
21	58.4	0.1	22	60.2	0.0
23	60.7	0.0	24	63.2	0.2
25	65.8	0.0	26	68.0	0.1
27	70.0	0.0	28	70.5	0.0
29	74.4	0.3	30	76.4	0.0
31	78.3	0.1	32	80.1	0.3
33	84.8	0.3	34	90.0	0.5
35	95.5	1.0	36	101.3	1.6

Table S48 Intensity and frequency values for the ground state vibrational modes of the K₁₄Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	23.4	0.0	2	23.7	0.0
3	26.8	0.0	4	27.2	0.0
5	27.3	0.0	6	27.8	0.0
7	36.2	0.0	8	37.7	0.0
9	37.9	0.0	10	38.2	0.0
11	38.6	0.0	12	40.3	0.0
13	40.4	0.0	14	42.6	0.4
15	45.0	0.0	16	45.3	0.0
17	46.0	0.0	18	46.1	0.0
19	51.4	0.2	20	52.2	0.2
21	54.5	0.0	22	54.6	0.0
23	56.3	0.6	24	57.5	0.0
25	62.1	0.6	26	63.1	0.6
27	64.0	0.0	28	64.1	0.0
29	74.9	0.0	30	76.4	0.0
31	76.4	0.0	32	76.8	0.5
33	77.1	0.5	34	79.0	0.0
35	79.8	0.0	36	79.9	0.0
37	81.8	0.0	38	81.8	0.0
39	97.7	1.1			

Table S49 Intensity and frequency values for the ground state vibrational modes of the K₁₅Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	12.4	0.0	2	23.7	0.1
3	24.4	0.0	4	25.4	0.0
5	26.5	0.0	6	27.7	0.0
7	28.8	0.0	8	30.1	0.0
9	30.9	0.0	10	31.8	0.0
11	33.3	0.1	12	34.2	0.0
13	34.8	0.0	14	35.2	0.0
15	40.6	0.0	16	41.2	0.0
17	42.0	0.0	18	43.2	0.0
19	47.6	0.1	20	48.8	0.0
21	49.6	0.1	22	53.7	0.5
23	54.0	0.1	24	57.0	0.5
25	60.4	0.1	26	60.5	0.2
27	62.7	0.0	28	64.9	0.0
29	67.9	0.1	30	69.5	0.2
31	69.8	0.1	32	70.9	0.1
33	71.4	0.0	34	73.2	0.1
35	76.1	0.0	36	79.3	0.3
37	80.5	0.0	38	84.2	0.0
39	84.6	0.1	40	87.2	0.0
41	87.8	0.3	42	91.4	0.1

Table S50 Intensity and frequency values for the ground state vibrational modes of the K₁₆Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	15.0	0.1	2	18.9	0.1
3	21.7	0.1	4	23.5	0.0
5	24.8	0.1	6	26.5	0.3
7	28.8	0.1	8	29.1	0.0
9	30.2	0.0	10	31.0	0.0
11	33.5	0.1	12	34.1	0.0
13	35.5	0.0	14	38.1	0.0
15	38.6	0.0	16	39.3	0.0
17	41.9	0.0	18	44.0	0.0
19	45.4	0.0	20	46.2	0.0
21	48.5	0.1	22	49.9	0.0
23	52.1	0.0	24	54.1	0.0
25	54.8	0.2	26	58.0	0.0
27	60.6	0.2	28	63.5	0.1
29	64.4	0.1	30	65.0	0.1
31	68.6	0.3	32	69.3	0.0
33	70.5	0.1	34	72.3	0.1
35	72.9	0.1	36	74.6	0.0
37	75.6	0.0	38	76.3	0.0
39	78.8	0.1	40	79.9	0.1
41	80.8	0.0	42	82.2	0.0
43	83.9	0.0	44	86.0	0.0
45	88.2	0.0			

Table S51 Intensity and frequency values for the ground state vibrational modes of the K₁₇Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	22.0	0.0	2	22.9	0.1
3	23.5	0.2	4	24.1	0.0
5	24.8	0.0	6	26.9	0.0
7	29.1	0.0	8	29.3	0.0
9	29.5	0.0	10	30.2	0.1
11	30.8	0.2	12	32.6	0.3
13	32.9	0.1	14	34.8	0.1
15	36.3	0.0	16	36.8	0.0
17	38.9	0.1	18	40.8	0.0
19	41.2	0.0	20	44.3	0.1
21	45.6	0.1	22	45.8	0.1
23	48.1	0.1	24	49.7	0.0
25	51.5	0.0	26	54.1	0.0
27	56.4	0.1	28	56.8	0.1
29	59.2	0.0	30	60.8	0.0
31	61.6	0.2	32	64.1	0.0
33	69.9	0.0	34	70.0	0.0
35	70.7	0.0	36	71.1	0.3
37	71.8	0.0	38	72.5	0.2
39	73.3	0.0	40	73.7	0.0
41	74.9	0.1	42	78.3	0.2
43	79.6	0.0	44	79.7	0.1
45	80.8	0.1	46	85.0	0.0
47	86.0	0.0	48	90.2	0.0

Table S52 Intensity and frequency values for the ground state vibrational modes of the K₁₈Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	17.3	0.0	2	21.7	0.0
3	22.1	0.2	4	23.5	0.0
5	25.0	0.1	6	25.5	0.2
7	27.6	0.1	8	28.3	0.0
9	28.9	0.0	10	30.5	0.0
11	32.1	0.0	12	32.7	0.4
13	33.6	0.6	14	34.8	0.1
15	35.8	0.0	16	36.6	0.1
17	37.4	0.3	18	37.9	0.0
19	38.6	0.2	20	41.4	0.3
21	41.8	0.4	22	42.9	0.2
23	44.7	0.0	24	47.2	0.0
25	48.0	0.0	26	48.6	0.0
27	50.6	0.0	28	52.2	0.0
29	53.0	0.0	30	55.4	0.0
31	57.3	0.0	32	60.6	0.0
33	61.4	0.0	34	62.7	0.2
35	63.1	0.1	36	68.6	0.1
37	69.8	0.0	38	70.1	0.0
39	70.8	0.0	40	71.2	0.0
41	71.9	0.0	42	72.6	0.0
43	73.0	0.0	44	75.7	0.0
45	79.6	0.0	46	80.2	0.1
47	82.3	0.4	48	82.5	0.4
49	83.3	0.0	50	88.2	0.7
51	90.6	0.0			

Table S53 Intensity and frequency values for the ground state vibrational modes of the K₁₉Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	15.4	0.0	2	16.9	0.0
3	19.5	0.0	4	20.3	0.0
5	21.0	0.1	6	21.7	0.3
7	23.5	0.0	8	25.6	0.0
9	26.9	0.1	10	28.4	0.1
11	29.8	0.1	12	30.0	0.0
13	30.3	0.0	14	31.6	0.1
15	32.7	0.0	16	34.0	0.4
17	34.9	0.4	18	35.8	0.1
19	35.8	0.4	20	37.8	0.0
21	38.6	0.4	22	39.2	0.1
23	41.6	0.1	24	43.8	0.0
25	45.5	0.0	26	47.0	0.0
27	47.6	0.7	28	47.9	0.1
29	49.4	0.3	30	51.3	0.2
31	52.9	0.1	32	55.1	0.0
33	56.2	0.1	34	58.4	0.0
35	59.4	0.0	36	59.9	0.1
37	61.9	0.1	38	65.5	0.2
39	68.3	0.0	40	69.2	0.2
41	71.2	0.0	42	71.6	0.1
43	71.8	0.0	44	71.8	0.2
45	74.1	0.0	46	74.3	0.1
47	76.9	0.1	48	79.1	0.6
49	80.7	0.0	50	81.7	0.1
51	82.3	1.3	52	83.4	0.0
53	89.4	0.9	54	89.7	0.1

Table S54 Intensity and frequency values for the ground state vibrational modes of the K₂₀Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	3.1	0.0	2	10.7	0.0
3	12.7	0.0	4	16.9	0.2
5	18.3	0.0	6	20.1	0.1
7	21.7	0.1	8	22.1	0.1
9	25.4	0.1	10	27.9	0.0
11	29.3	0.1	12	30.0	0.3
13	31.2	0.0	14	32.5	0.1
15	34.4	0.5	16	35.1	0.0
17	35.9	0.1	18	37.0	0.1
19	37.8	0.0	20	39.1	0.1
21	40.7	0.2	22	41.3	0.1
23	42.1	0.1	24	42.5	0.1
25	44.5	0.1	26	44.6	0.1
27	46.0	0.3	28	46.8	0.4
29	47.2	0.2	30	48.2	0.0
31	49.1	0.1	32	50.8	0.2
33	52.0	0.0	34	54.8	0.1
35	56.0	0.2	36	57.0	0.0
37	57.4	0.2	38	59.6	0.1
39	60.8	0.0	40	63.9	0.2
41	65.6	0.1	42	66.5	0.2
43	68.9	0.2	44	70.3	0.2
45	72.1	0.2	46	73.2	0.3
47	74.0	0.4	48	75.2	0.2
49	76.2	0.1	50	77.1	0.2
51	78.5	0.1	52	79.3	0.1
53	80.7	0.1	54	81.4	0.0
55	83.2	0.1	56	87.2	0.0
57	97.3	0.1			

Table S55 Intensity and frequency values for the ground state vibrational modes of the K₂₁Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	7.6	0.0	2	12.8	0.0
3	15.8	0.0	4	18.3	0.0
5	19.1	0.1	6	22.6	0.2
7	24.1	0.1	8	25.3	0.0
9	27.2	0.0	10	27.6	0.1
11	28.8	0.1	12	31.1	0.0
13	31.4	0.0	14	32.7	0.1
15	33.3	0.0	16	35.2	0.0
17	35.9	0.1	18	37.6	0.1
19	38.0	0.0	20	39.2	0.0
21	40.3	0.1	22	40.5	0.2
23	41.0	0.1	24	42.2	0.0
25	42.6	0.1	26	43.7	0.0
27	44.3	0.0	28	45.1	0.2
29	46.8	0.1	30	47.7	0.0
31	48.6	0.0	32	49.5	0.1
33	50.9	0.0	34	51.5	0.1
35	52.3	0.1	36	53.6	0.0
37	55.0	0.1	38	55.7	0.0
39	57.0	0.0	40	58.2	0.0
41	58.9	0.1	42	60.8	0.3
43	61.6	0.1	44	63.6	0.1
45	64.8	0.1	46	65.8	0.6
47	68.0	0.0	48	68.2	0.1
49	69.3	0.1	50	71.9	0.1
51	72.2	0.2	52	74.9	0.1
53	75.2	0.0	54	76.7	0.4
55	77.6	0.1	56	80.2	0.1
57	81.2	0.6	58	85.6	0.5
59	86.3	0.0	60	98.3	0.7

Table S56 Intensity and frequency values for the ground state vibrational modes of the K₂₂Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	5.5	0.0	2	13.5	0.1
3	16.4	0.0	4	18.0	0.1
5	19.1	0.0	6	20.7	0.0
7	21.8	0.1	8	22.6	0.1
9	24.5	0.2	10	25.2	0.0
11	27.3	0.1	12	29.0	0.1
13	30.0	0.0	14	30.7	0.0
15	31.9	0.0	16	33.3	0.1
17	33.4	0.0	18	33.7	0.1
19	34.5	0.0	20	37.7	0.0
21	38.5	0.1	22	39.1	0.0
23	40.2	0.0	24	41.1	0.0
25	42.1	0.1	26	43.1	0.0
27	43.5	0.1	28	44.1	0.1
29	44.5	0.0	30	45.1	0.0
31	47.0	0.1	32	47.3	0.2
33	48.2	0.1	34	49.8	0.2
35	50.4	0.3	36	51.1	0.0
37	52.5	0.1	38	53.9	0.1
39	54.2	0.1	40	55.1	0.1
41	57.6	0.1	42	59.1	0.1
43	59.8	0.0	44	60.2	0.0
45	61.3	0.0	46	64.6	0.0
47	65.6	0.7	48	68.2	0.1
49	69.3	0.1	50	69.9	0.0
51	70.6	0.3	52	71.6	0.0
53	72.8	0.1	54	74.3	0.0
55	75.9	0.0	56	76.8	0.0
57	77.8	0.0	58	79.0	0.0
59	80.1	0.1	60	82.6	0.2
61	85.0	0.1	62	88.2	0.0
63	91.4	1.3			

Table S57 Intensity and frequency values for the ground state vibrational modes of the K₂₃Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	10.9	0.0	2	13.1	0.0
3	13.2	0.0	4	15.9	0.0
5	17.5	0.0	6	20.1	0.1
7	20.4	0.2	8	22.3	0.2
9	23.4	0.1	10	24.0	0.1
11	26.0	0.1	12	26.4	0.3
13	26.9	0.1	14	28.6	0.2
15	29.7	0.1	16	31.0	0.3
17	31.2	0.6	18	31.6	0.1
19	34.1	0.0	20	34.9	0.1
21	35.3	0.0	22	36.0	0.0
23	36.6	0.4	24	38.4	0.0
25	38.9	0.1	26	40.3	0.1
27	40.6	0.1	28	41.3	0.4
29	41.6	0.0	30	43.7	0.3
31	43.8	0.3	32	45.0	0.1
33	46.3	0.1	34	47.3	0.0
35	48.5	0.0	36	49.7	0.0
37	50.3	0.1	38	51.6	0.1
39	51.6	0.3	40	54.3	0.0
41	55.3	0.0	42	56.0	0.1
43	58.6	0.1	44	59.5	0.1
45	61.3	0.0	46	63.0	0.3
47	64.3	0.0	48	65.1	0.1
49	67.1	0.0	50	67.8	0.1
51	68.1	0.1	52	69.2	0.2
53	71.3	0.2	54	71.9	0.0
55	72.7	0.0	56	74.2	0.0
57	75.4	0.0	58	76.7	0.0
59	76.9	0.0	60	78.3	0.1
61	78.6	0.1	62	80.8	0.0
63	82.3	0.0	64	84.1	0.0
65	85.0	0.0	66	86.4	0.0

Table S58 Intensity and frequency values for the ground state vibrational modes of the K₂₄Y cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	9.6	0.0	2	11.5	0.0
3	12.1	0.0	4	17.2	0.0
5	17.7	0.0	6	19.6	0.0
7	20.2	0.0	8	22.2	0.1
9	24.1	0.1	10	24.6	0.0
11	25.3	0.0	12	26.2	0.0
13	27.6	0.3	14	28.9	0.0
15	30.4	0.3	16	30.6	0.0
17	31.4	0.0	18	32.7	0.1
19	33.3	0.0	20	34.4	0.0
21	35.8	0.1	22	36.6	0.1
23	37.0	0.0	24	38.1	0.1
25	38.7	0.1	26	40.2	0.2
27	41.4	0.0	28	42.6	0.0
29	43.6	0.1	30	44.7	0.0
31	45.6	0.0	32	46.7	0.1
33	48.2	0.0	34	49.4	0.0
35	49.9	0.0	36	51.1	0.1
37	52.0	0.1	38	52.9	0.1
39	53.0	0.2	40	53.9	0.1
41	55.0	0.0	42	55.9	0.0
43	56.7	0.2	44	57.4	0.1
45	58.4	0.1	46	59.1	0.1
47	59.3	0.0	48	61.1	0.1
49	61.7	0.0	50	62.3	0.1
51	62.8	0.1	52	63.8	0.1
53	64.3	0.0	54	65.1	0.1
55	66.6	0.1	56	67.7	0.1
57	69.0	0.0	58	69.8	0.2
59	70.4	0.1	60	72.2	0.0
61	73.2	0.0	62	74.7	0.2
63	76.9	0.0	64	77.4	0.1
65	80.4	0.1	66	81.3	0.1
67	91.4	0.5	68	93.7	1.1
69	95.1	0.4			

Table S59 Intensity and frequency values for the ground state vibrational modes of the K₁₁Y₂ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	28.0	0.1	2	32.4	0.0
3	34.0	0.1	4	35.8	0.3
5	36.3	0.1	6	37.9	0.1
7	40.6	0.2	8	41.2	0.3
9	42.4	0.1	10	44.2	0.4
11	46.7	0.1	12	49.6	0.0
13	51.5	0.0	14	54.1	0.1
15	54.5	0.9	16	55.8	0.1
17	59.3	0.3	18	62.3	0.2
19	64.0	0.4	20	65.6	0.1
21	65.8	0.2	22	66.9	0.2
23	69.9	0.1	24	73.7	0.1
25	74.4	0.1	26	75.2	0.4
27	75.5	0.4	28	79.4	0.2
29	80.2	0.3	30	84.6	0.3
31	100.7	2.1	32	103.2	3.0
33	121.5	0.0			

Table S60 Intensity and frequency values for the ground state vibrational modes of the $K_{10}Y_3$ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	23.5	0.0	2	31.9	0.0
3	35.5	0.0	4	37.9	0.0
5	39.2	0.0	6	40.3	0.0
7	41.3	0.0	8	42.8	0.4
9	45.9	0.0	10	47.6	0.1
11	49.1	0.1	12	49.4	0.1
13	52.5	0.8	14	57.4	0.0
15	59.9	0.0	16	60.4	0.1
17	66.3	0.2	18	67.3	0.0
19	67.5	0.1	20	69.2	0.0
21	69.6	0.0	22	69.6	0.1
23	70.4	0.6	24	71.3	0.0
25	75.4	0.0	26	83.9	0.4
27	84.5	0.4	28	86.7	2.0
29	87.1	0.2	30	104.1	2.4
31	105.7	0.2	32	126.3	0.9
33	143.7	0.1			

Table S61 Intensity and frequency values for the ground state vibrational modes of the $K_{20}Y_2$ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	9.6	0.1	2	14.3	0.0
3	18.2	0.0	4	23.8	0.1
5	23.9	0.2	6	25.0	0.1
7	26.6	0.2	8	27.2	0.1
9	28.7	0.0	10	29.6	0.4
11	32.8	0.3	12	33.7	0.2
13	34.3	0.1	14	36.0	0.0
15	37.4	0.0	16	38.1	0.1
17	39.5	0.2	18	40.5	0.2
19	42.3	0.0	20	42.8	0.1
21	43.6	0.0	22	45.2	0.1
23	46.6	0.0	24	48.1	0.0
25	49.4	0.2	26	50.0	0.1
27	52.1	0.1	28	52.7	0.1
29	54.9	0.3	30	56.0	0.4
31	56.3	0.2	32	58.0	0.4
33	59.5	0.2	34	61.4	0.7
35	62.7	0.9	36	63.7	1.1
37	64.7	0.1	38	67.2	0.1
39	67.9	0.1	40	70.5	0.3
41	71.6	0.8	42	71.9	0.0
43	73.2	0.3	44	74.2	0.0
45	75.3	0.1	46	75.6	0.1
47	76.9	0.1	48	77.5	0.0
49	78.1	0.0	50	79.3	0.0
51	80.4	0.0	52	82.7	0.2
53	83.2	0.2	54	86.5	0.2
55	88.3	0.0	56	90.5	0.2
57	94.5	0.1	58	96.5	0.0
59	100.2	0.0	60	107.0	0.0

Table S62 Intensity and frequency values for the ground state vibrational modes of the $K_{19}Y_3$ cluster.

Mode	Frequency [1/cm]	Intensity [Km/mol]	Mode	Frequency [1/cm]	Intensity [Km/mol]
1	15.2	0.0	2	22.8	0.0
3	25.5	0.0	4	27.4	0.1
5	27.7	0.0	6	29.4	0.0
7	30.6	0.2	8	32.7	0.0
9	33.8	0.1	10	35.7	0.0
11	36.6	0.0	12	37.4	0.0
13	39.1	0.0	14	40.9	0.1
15	41.6	0.1	16	43.1	0.0
17	43.6	0.0	18	44.5	0.1
19	45.9	0.4	20	46.3	0.3
21	47.5	0.4	22	49.5	0.1
23	50.4	0.1	24	50.6	0.0
25	51.7	0.2	26	53.6	0.2
27	54.0	0.2	28	54.5	0.5
29	54.7	0.4	30	56.6	0.1
31	57.7	1.1	32	59.1	0.2
33	59.2	0.2	34	62.1	0.1
35	62.6	0.1	36	63.8	0.1
37	64.6	0.0	38	65.7	0.0
39	66.0	0.0	40	67.0	0.1
41	67.7	0.0	42	71.0	0.1
43	72.0	0.3	44	73.2	0.0
45	74.0	0.2	46	75.1	0.1
47	75.3	0.2	48	76.2	0.1
49	76.8	0.4	50	78.8	0.0
51	79.3	0.0	52	82.9	0.0
53	84.4	1.1	54	84.8	2.1
55	88.7	0.2	56	92.2	0.1
57	101.1	1.4	58	122.4	0.1
59	124.7	0.0	60	140.4	0.0