Electronic supplementary materials *Mendeleev Commun.*, 2027, **37**, just accepted

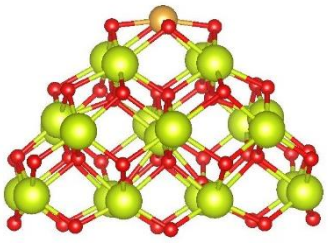
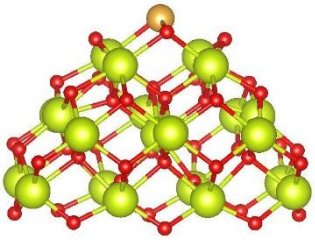
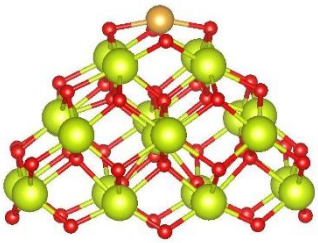
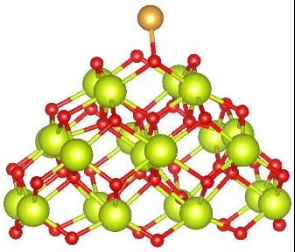
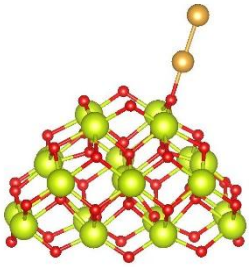
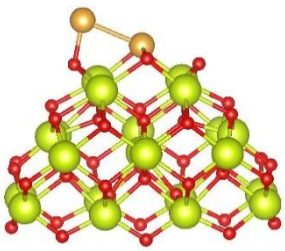
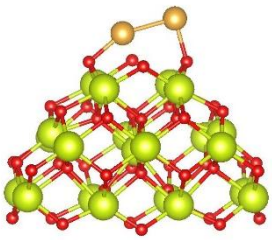
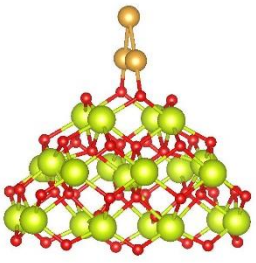
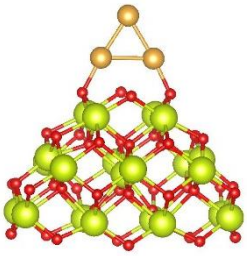
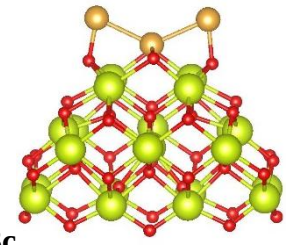
Bonding of Au_n (n=1-4) gold species at ceria nanoparticle $Ce_{21}O_{42}$

Elena A. Ivanova-Shor, Aleksey M. Shor, Svetlana S. Laletina and Vladimir A. Nasluzov

Table S1. Absolute energies (in a.u.) of unsupported gold Au_n (n=1-4) species and metal-free $Ce_{21}O_{42}$ nanoparticle.

Au_1	Au_2	Au_3	Au_4	$Ce_{21}O_{42}$
-0,15970618	-2,64245897	-4,1288864	-6,80256701	-494,87089263

Table S2. Optimized structures and absolute energies (in a.u.) of supported $Au_n/Ce_{21}O_{42}$ (n=1-4) models.

 1a	 1b	 1c	 1d
-497,33186954	-497,24827103	-497,13382966	-496,04825311
 2a	 2b	 2c	
-498,85936207	-498,60622093	-498,43624053	
 3a	 3b	 3c	
-502,11537817	-502,06394952	-499,78959935	

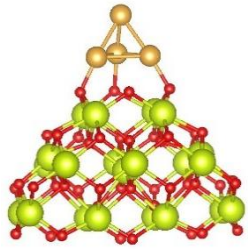
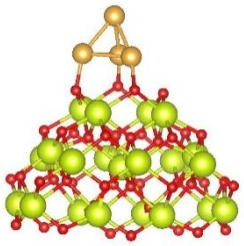
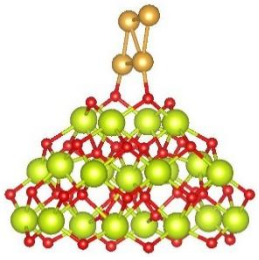
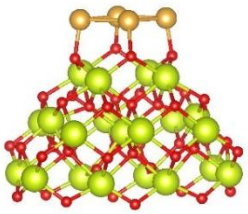
4a 	**4b** 	**4c** 	**4d** 
-504,32366819	**-504,31806858**	**-503,71917863**	**-503,19977532**

Table S3. XYZ-coordinates of ~~the lowest-energy~~ $Au_n/Ce_{21}O_{42}$ structures (n=1,2,3,4).

$Au_1/Ce_{21}O_{42}$ (**1a**)				$Au_1/Ce_{21}O_{42}$ (**1b**)			
64				64			
Ce	13.610024	8.402024	10.168877	Ce	13.706610	8.162898	9.964582
Ce	12.346869	14.953667	7.377388	Ce	12.532481	14.721455	7.227159
Ce	13.984596	14.601770	10.510760	Ce	14.177953	14.354059	10.359181
Ce	10.786264	6.288419	11.441547	Ce	10.800878	6.189973	11.267371
Ce	5.679260	8.043405	8.015682	Ce	5.784204	8.036818	7.930071
Ce	8.974365	7.396524	14.397397	Ce	9.084259	7.248154	14.285544
Ce	9.300856	13.235720	8.321494	Ce	9.479787	13.129387	8.279731
Ce	9.994160	10.028906	10.074421	Ce	10.143572	9.898996	10.034026
Ce	7.228267	7.206293	11.225920	Ce	7.296663	7.097859	11.119123
Ce	5.705607	8.787116	14.155645	Ce	5.848277	8.695058	14.079355
Ce	11.356670	12.104633	5.489076	Ce	11.446048	11.863513	5.402923
Ce	6.540310	11.280592	9.524099	Ce	6.699872	11.247679	9.523664
Ce	11.289804	12.824756	12.148973	Ce	11.490978	12.675363	12.087158
Ce	9.034481	6.747331	8.069797	Ce	9.128382	6.553719	8.059706
Ce	14.662222	11.380643	11.886220	Ce	14.813619	11.136022	11.727351
Ce	13.452616	11.632944	8.450228	Ce	13.603420	11.380220	8.305190
Ce	11.961615	9.292400	13.399397	Ce	12.129521	9.084541	13.244676
Ce	4.087541	9.086687	11.022753	Ce	4.206965	9.071645	10.948942
Ce	11.887854	8.792614	6.778501	Ce	12.027918	8.516314	6.767855
Ce	8.518674	10.897339	13.367599	Ce	8.698312	10.781027	13.335993
Ce	8.396653	10.052892	6.455634	Ce	8.586697	9.898354	6.528010
O	14.113374	13.696031	8.328871	O	14.275930	13.441647	8.163360
O	7.002600	6.438146	9.055367	O	6.983725	6.428565	8.937825
O	13.061571	15.972284	9.124145	O	13.236359	15.725131	8.971526
O	9.556339	12.799019	13.401910	O	9.777433	12.643901	13.392905
O	4.572820	11.041398	10.386228	O	4.701609	11.023463	10.314417
O	11.041947	7.084769	13.654512	O	11.153421	6.860275	13.398972
O	7.710853	8.625792	12.966823	O	7.826262	8.510121	12.883883
O	13.013335	6.177636	10.322524	O	12.956529	5.953629	10.346809
O	7.574862	7.765889	6.735620	O	7.700775	7.785861	6.658423
O	9.303340	12.314700	6.150989	O	9.352541	12.046494	6.130896
O	13.017879	10.729905	6.385329	O	13.051052	10.533684	6.232304
O	11.061863	6.596927	6.774988	O	11.076532	6.373798	6.765498
O	14.138802	9.186059	12.193104	O	14.232117	8.947045	12.022661
O	7.043735	7.480525	15.320779	O	7.163936	7.329048	15.212388
O	13.139437	12.417016	10.578028	O	13.284721	12.212658	10.445036
O	12.163937	9.825659	8.904449	O	12.192255	9.726808	8.866402
O	10.347439	12.365974	10.127510	O	10.473736	12.304146	10.099406

O 12.952431 11.551919 13.206673	O 13.130919 11.332533 13.089264
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O 11.662819 8.442145 11.193386	O 11.711315 8.260229 11.050252
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O 6.198819 8.899882 10.020934	O 6.308767 8.871346 9.954775
O 15.450898 13.327564 11.603007	O 15.635966 13.079759 11.423365
O 7.261043 13.244600 8.986984	O 7.444228 13.182146 8.961448
O 12.413336 14.673828 11.897257	O 12.652055 14.483495 11.805248
O 6.640826 10.658758 14.416503	O 6.830332 10.528331 14.410604
O 3.990300 9.587496 13.100385	O 4.164743 9.564569 13.025389
O 14.770615 10.346650 9.796309	O 14.904708 10.152720 9.680929
O 12.203457 14.032930 5.343765	O 12.319566 13.764124 5.204763
O 8.033035 10.747686 11.139256	O 8.144579 10.730818 11.141685
O 3.836576 8.065806 9.043399	O 3.941815 8.096234 8.941918
O 10.533022 10.600619 12.173615	O 10.688869 10.456875 12.109823
O 10.607391 9.935266 5.372865	O 10.567817 9.721864 5.380602
O 8.652523 10.981300 8.517794	O 8.800892 10.869320 8.495836
O 9.822135 9.422551 14.581106	O 10.000706 9.208702 14.489125
O 13.518507 7.572725 7.921504	O 13.852066 7.988214 7.773432
O 10.313026 15.108339 7.877613	O 10.491947 14.949250 7.714301
O 11.615710 12.743817 7.627728	O 9.725066 5.201591 9.615892
O 5.304792 7.484540 12.221031	O 11.734867 12.547794 7.529312
O 6.199306 10.098717 7.515312	O 5.395668 7.413665 12.125627
O 8.649405 6.087867 12.525778	O 6.454844 10.090305 7.425003
O 10.409868 5.296733 9.192134	O 8.772014 5.994678 12.420930
Au 12.093783 6.222819 8.500952	Au 12.165592 5.871796 8.448366
$Au_1/Ce_{21}O_{42}$ (**1c**)	$Au_1/Ce_{21}O_{42}$ (**1d**)
64	64
Ce 13.562862 8.213838 10.037011	Ce 13.496795 8.248268 9.842696
Ce 12.388450 14.875053 7.384835	Ce 12.322330 14.990538 7.448143
Ce 14.049931 14.456491 10.481152	Ce 14.022261 14.499718 10.522247
Ce 10.845573 6.301021 11.223718	Ce 10.781973 6.303321 11.035320
Ce 5.653337 8.101433 7.966407	Ce 5.592396 8.156089 7.969265
Ce 9.064445 7.277183 14.258414	Ce 9.081808 7.228457 14.172815
Ce 9.282118 13.270094 8.311991	Ce 9.236842 13.328186 8.342293
Ce 9.969576 10.008674 9.949948	Ce 9.937613 10.042153 9.925977
Ce 7.268087 7.163495 11.082697	Ce 7.201629 7.163800 11.074512
Ce 5.781972 8.637062 14.111597	Ce 5.797589 8.616123 14.133487
Ce 11.324251 12.085013 5.475793	Ce 11.266520 12.224556 5.484425
Ce 6.514152 11.328439 9.529325	Ce 6.483759 11.347811 9.556319
Ce 11.291275 12.773295 12.097099	Ce 11.284953 12.767230 12.107333
Ce 9.029573 6.771208 7.849972	Ce 8.933869 6.764555 7.909526
Ce 14.651128 11.217370 11.808705	Ce 14.633180 11.202057 11.733197
Ce 13.434795 11.498514 8.377892	Ce 13.417954 11.616086 8.347415
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Ce 4.122722 9.059816 11.019492	Ce 4.092829 9.090788 11.055942
Ce 11.759791 8.685933 6.657792	Ce 11.823339 8.837202 6.641742
Ce 8.536388 10.831934 13.310700	Ce 8.545137 10.804943 13.316961
Ce 8.329334 10.129710 6.410493	Ce 8.319448 10.152611 6.415834
O 14.137239 13.566131 8.311852	O 14.101252 13.687391 8.324488
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O 7.457908 7.876655 6.656313	O 7.422626 7.903850 6.662367
O 9.263725 12.384444 6.157482	O 9.212132 12.450819 6.178579
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O 10.000430 9.306323 14.443544	O 10.023849 9.241989 14.379700
O 13.447115 7.504240 7.831643	O 13.365391 7.840595 7.706457
O 10.362364 15.105077 7.900861	O 10.288513 15.187615 7.960098
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O 11.606163 12.691404 7.628145	O 11.558931 12.801770 7.643220
O 5.379624 7.405272 12.159781	O 5.333515 7.406136 12.173253
O 6.139017 10.190248 7.528544	O 6.110357 10.226698 7.537975
O 8.835712 6.027450 12.358628	O 8.787280 6.023275 12.280997
Au 12.035219 6.096640 8.368847	Au 11.717671 5.149711 6.124877
$Au_2/Ce_{21}O_{42}$ (**2a**)	$Au_2/Ce_{21}O_{42}$ (**2b**)
65	65
Ce 13.506690 8.154336 10.078547	Ce 13.754892 8.235984 9.945560
Ce 12.335320 14.802023 7.362051	Ce 12.493505 14.798516 7.250342
Ce 13.984112 14.408392 10.480451	Ce 14.142866 14.434111 10.379310
Ce 10.726709 6.261912 11.236735	Ce 10.894240 6.208170 11.261878
Ce 5.629611 8.084475 7.966967	Ce 5.810151 8.040596 7.896276
Ce 8.951401 7.292950 14.291624	Ce 9.138185 7.211277 14.244936
Ce 9.236620 13.246237 8.361424	Ce 9.468030 13.152370 8.304112
Ce 9.933231 9.980514 10.033146	Ce 10.159729 9.887682 10.005908
Ce 7.174056 7.159929 11.123886	Ce 7.353630 7.064300 11.047228
Ce 5.682154 8.679982 14.117249	Ce 5.893197 8.619215 14.043589

Ce	11.230378	11.981792	5.502861	Ce	11.422878	11.941024	5.407048
Ce	6.467856	11.326750	9.578718	Ce	6.710838	11.230093	9.526983
Ce	11.235246	12.770597	12.149669	Ce	11.482701	12.681778	12.086068
Ce	9.029978	6.670534	7.998636	Ce	9.159568	6.534385	7.895566
Ce	14.571500	11.183506	11.842308	Ce	14.829401	11.211791	11.723127
Ce	13.368572	11.431671	8.407148	Ce	13.592663	11.467594	8.310489
Ce	11.853603	9.203074	13.229897	Ce	12.172052	9.107098	13.234285
Ce	4.042000	9.067451	10.993300	Ce	4.244500	9.016834	10.930340
Ce	11.756587	8.577177	6.741154	Ce	12.049171	8.595363	6.724613
Ce	8.460626	10.853559	13.365046	Ce	8.721777	10.738932	13.321583
Ce	8.348005	10.041092	6.568269	Ce	8.581749	9.935370	6.506699
O	14.063892	13.494791	8.304539	O	14.249028	13.533552	8.182173
O	6.871812	6.482104	8.960542	O	6.957316	6.429373	8.900794
O	13.058543	15.787498	9.124264	O	13.206232	15.809798	8.997353
O	9.513395	12.728835	13.435707	O	9.769876	12.620504	13.389093
O	4.487517	11.039850	10.388465	O	4.729138	10.989941	10.343279
O	11.058281	7.077525	13.456539	O	11.239046	6.849004	13.364573
O	7.681496	8.554143	12.925217	O	7.881411	8.465148	12.849740
O	12.806491	6.228294	10.649239	O	13.006600	5.988103	10.298651
O	7.495337	7.929811	6.671312	O	7.661185	7.860272	6.558329
O	9.127892	12.200360	6.220108	O	9.339711	12.108284	6.144969
O	12.835621	10.623400	6.322536	O	13.061486	10.624237	6.234337
O	10.693611	6.738655	6.620746	O	11.293730	6.463213	6.631451
O	13.907136	9.035277	12.231812	O	14.273180	9.008789	12.004396
O	7.064595	7.329920	15.234121	O	7.221761	7.258097	15.173409
O	13.060045	12.264460	10.569710	O	13.285871	12.272541	10.455178
O	12.021955	9.752752	8.905664	O	12.215115	9.772219	8.859165
O	10.249674	12.393509	10.171766	O	10.481081	12.297811	10.101006
O	12.806693	11.321288	13.205427	O	13.143818	11.363549	13.089262
O	9.777452	8.840831	7.873478	O	10.020185	8.696190	7.745509
O	11.482812	8.431686	11.119666	O	11.760000	8.276564	11.038762
O	9.085756	7.794590	10.201975	O	9.340772	7.599407	10.124430
O	6.144435	8.920990	9.998144	O	6.351504	8.856045	9.934517
O	15.411184	13.097923	11.581544	O	15.619747	13.167449	11.440988
O	7.205250	13.279291	9.055830	O	7.443914	13.185555	9.004177
O	12.450336	14.539304	11.925810	O	12.607871	14.521206	11.814528
O	6.636979	10.526761	14.477135	O	6.855186	10.467285	14.382273
O	4.004770	9.541132	13.090449	O	4.187141	9.465530	13.026443
O	14.678043	10.182459	9.824327	O	14.921423	10.236965	9.664697
O	12.116142	13.888157	5.342063	O	12.272560	13.860500	5.224748
O	7.918560	10.800352	11.197658	O	8.191345	10.667539	11.119938
O	3.791206	8.107094	8.997566	O	3.958234	8.095675	8.929782
O	10.455912	10.544462	12.152538	O	10.718630	10.449042	12.091771
O	10.317974	9.894612	5.409423	O	10.580006	9.812146	5.341227
O	8.563352	10.995544	8.558590	O	8.815279	10.883663	8.491762
O	9.902035	9.309341	14.477710	O	10.043718	9.178115	14.469266
O	13.478817	7.761391	7.892294	O	13.869529	7.993915	7.789406
O	10.298615	15.053860	7.853945	O	10.461353	15.000910	7.767922
O	9.983682	5.393565	9.426811	O	9.640941	4.940442	9.717489
O	11.516205	12.630730	7.641651	O	11.721657	12.615625	7.540157
O	5.270622	7.428174	12.159302	O	5.463739	7.355010	12.081890
O	6.229905	10.185907	7.493333	O	6.460648	10.128341	7.438824

O 8.689340 6.046917 12.426727 Au 16.370213 4.800609 5.902917 Au 14.769001 6.411972 6.999042	O 8.867476 5.978183 12.376561 Au 12.291609 5.893187 8.353648 Au 10.831453 3.495907 8.955735
$Au_2/Ce_{21}O_{42}$(**2c**) 65 Ce 13.556351 8.229388 10.086369 Ce 12.373907 14.868785 7.353786 Ce 14.011665 14.461872 10.470437 Ce 10.790153 6.316817 11.282516 Ce 5.672861 8.132049 7.919920 Ce 8.957602 7.276749 14.267043 Ce 9.305199 13.267032 8.380756 Ce 9.998127 10.009974 10.068326 Ce 7.212815 7.175334 11.083440 Ce 5.704469 8.683578 14.068466 Ce 11.282386 12.050520 5.484877 Ce 6.533463 11.343089 9.579214 Ce 11.315123 12.764364 12.177209 Ce 9.053534 6.740846 7.943070 Ce 14.651812 11.235144 11.799126 Ce 13.427390 11.497413 8.386275 Ce 11.970617 9.203382 13.325687 Ce 4.073648 9.083112 10.949716 Ce 11.798952 8.656726 6.729641 Ce 8.528645 10.831493 13.377239 Ce 8.403847 10.103537 6.556260 O 14.101838 13.566935 8.268862 O 6.936380 6.511430 8.887533 O 13.094557 15.860870 9.095112 O 9.582609 12.711569 13.462721 O 4.543355 11.058533 10.369030 O 11.032392 6.968402 13.438850 O 7.702465 8.544699 12.879055 O 12.911006 6.286654 10.753588 O 7.557215 7.977663 6.635895 O 9.181032 12.249700 6.212046 O 12.889461 10.664481 6.290953 O 10.674199 6.844263 6.489606 O 14.078810 9.083843 12.120739 O 7.030087 7.314579 15.181856 O 13.118923 12.308002 10.528694 O 12.110987 9.753746 8.854029 O 10.327970 12.380461 10.163839 O 12.961102 11.445341 13.171001 O 9.830963 8.882053 7.865564 O 11.529941 8.449295 11.087769 O 9.160546 7.733743 10.142300 O 6.188850 8.936872 9.948097 O 15.473989 13.182047 11.511645 O 7.269985 13.299781 9.081619 O 12.473855 14.575680 11.903825	

O 6.644492 10.533703 14.414825 O 3.993333 9.525575 13.034584 O 14.740027 10.235120 9.731994 O 12.159834 13.949269 5.316631 O 7.998415 10.769553 11.171107 O 3.829596 8.138851 8.926548 O 10.521070 10.560637 12.174172 O 10.375852 9.950356 5.400315 O 8.625208 11.024209 8.549006 O 9.823868 9.265151 14.529668 O 13.618921 7.747629 7.793114 O 10.335196 15.089408 7.860563 O 10.021467 5.258290 9.365511 O 11.568136 12.680454 7.617239 O 5.294674 7.437131 12.089674 O 6.284673 10.231071 7.463169 O 8.705803 6.043128 12.347016 Au 11.847354 4.974390 8.395264 Au 14.073037 5.723670 7.316455	
$Au_3/Ce_{21}O_{42}$ (**3a**) 66	$Au_3/Ce_{21}O_{42}$ (**3b**) 66
Ce 13.592874 8.251143 9.987585 Ce 12.341463 14.887982 7.357741 Ce 13.993954 14.488435 10.480421 Ce 10.808974 6.166160 11.232450 Ce 5.670496 8.095786 7.980673 Ce 9.037530 7.309196 14.279577 Ce 9.281834 13.256128 8.360475 Ce 9.983536 9.936532 10.016055 Ce 7.235523 7.150900 11.138460 Ce 5.758130 8.680594 14.127901 Ce 11.275732 12.052689 5.489688 Ce 6.518479 11.322062 9.575714 Ce 11.276482 12.782061 12.121945 Ce 9.031046 6.643848 7.983965 Ce 14.623405 11.246376 11.811818 Ce 13.419648 11.534300 8.385888 Ce 11.924818 9.193100 13.178440 Ce 4.102084 9.069171 11.012940 Ce 11.860796 8.667313 6.747918 Ce 8.519041 10.847726 13.345485 Ce 8.412403 10.045063 6.562922 O 14.093132 13.601695 8.287679 O 6.890799 6.486873 8.952429 O 13.057443 15.872687 9.122957 O 9.570485 12.727581 13.413548 O 4.543398 11.043825 10.399351 O 11.150933 7.110871 13.499060 O 7.743659 8.569155 12.915913 O 13.169776 6.174826 10.612434 O 7.546265 7.935370 6.667069 O 9.175612 12.219723 6.211737	Ce 13.567122 8.259474 10.067531 Ce 12.357951 14.893641 7.340923 Ce 13.999794 14.495657 10.454574 Ce 10.820137 6.328260 11.271357 Ce 5.686715 8.124865 7.925982 Ce 9.002610 7.283698 14.261346 Ce 9.296894 13.280935 8.376445 Ce 10.005599 10.026524 10.066353 Ce 7.239276 7.168307 11.087009 Ce 5.737731 8.667465 14.075363 Ce 11.271000 12.065361 5.479314 Ce 6.537217 11.341789 9.584622 Ce 11.316790 12.786762 12.169645 Ce 9.070821 6.745190 7.943168 Ce 14.657411 11.268978 11.781879 Ce 13.424325 11.529797 8.375212 Ce 11.993853 9.225956 13.317123 Ce 4.094489 9.066269 10.960511 Ce 11.812529 8.678123 6.739557 Ce 8.544842 10.836899 13.377323 Ce 8.404457 10.107979 6.556976 O 14.090871 13.602386 8.253942 O 6.953972 6.508054 8.891111 O 13.080902 15.894911 9.076960 O 9.587632 12.724710 13.458228 O 4.553416 11.045590 10.384007 O 11.075291 6.983320 13.433565 O 7.732776 8.542569 12.876415 O 12.892942 6.295076 10.649830 O 7.566909 7.976129 6.632860 O 9.171595 12.258488 6.207905

O 12.909851 10.710264 6.299541 O 10.777056 6.710689 6.414534 O 13.993414 9.092435 12.156812 O 7.139907 7.360221 15.244350 O 13.107853 12.333591 10.543348 O 12.053060 9.865904 8.889490 O 10.287771 12.435627 10.159718 O 12.865625 11.345840 13.165255 O 9.866159 8.792878 7.828584 O 11.600438 8.380365 11.060343 O 9.120218 7.789963 10.174741 O 6.192389 8.924952 10.000643 O 15.437827 13.180391 11.571250 O 7.245893 13.272687 9.038403 O 12.461034 14.587880 11.913723 O 6.698803 10.542336 14.464618 O 4.060089 9.533169 13.104949 O 14.750419 10.273366 9.763461 O 12.133628 13.968543 5.325170 O 7.976828 10.800930 11.175786 O 3.829702 8.118320 9.008612 O 10.524243 10.528592 12.102776 O 10.399736 9.939700 5.413820 O 8.637175 10.979099 8.542435 O 9.970442 9.341343 14.441561 O 13.492631 7.863875 7.859594 O 10.307201 15.096594 7.849546 O 9.941503 5.342720 9.253922 O 11.561148 12.703576 7.621591 O 5.331381 7.427100 12.168900 O 6.291106 10.192033 7.486849 O 8.702788 6.046272 12.469784 Au 13.362597 4.784966 9.111307 Au 12.006777 5.087787 6.720867 Au 13.549215 3.038825 7.183333	O 12.888458 10.691691 6.286198 O 10.736158 6.819057 6.575502 O 14.098205 9.110685 12.106728 O 7.076967 7.313550 15.185908 O 13.115472 12.340146 10.516391 O 12.106697 9.787506 8.853287 O 10.322630 12.398659 10.160114 O 12.971861 11.473753 13.158692 O 9.833120 8.894359 7.859529 O 11.549948 8.468133 11.087036 O 9.185426 7.728947 10.135386 O 6.204698 8.929885 9.954628 O 15.470156 13.219324 11.492957 O 7.263625 13.301860 9.086090 O 12.465237 14.606223 11.889471 O 6.667572 10.524398 14.419755 O 4.022221 9.503939 13.047525 O 14.743038 10.274368 9.715484 O 12.137173 13.970173 5.306287 O 8.008426 10.772601 11.172533 O 3.845102 8.125371 8.938339 O 10.534545 10.579130 12.168422 O 10.376270 9.958080 5.398719 O 8.626514 11.033758 8.548729 O 9.853717 9.278134 14.523424 O 13.612567 7.783365 7.799352 O 10.320411 15.107036 7.857329 O 10.055839 5.271055 9.359720 O 11.558419 12.702438 7.609268 O 5.325589 7.418067 12.097291 O 6.287490 10.225403 7.470767 O 8.745962 6.046204 12.347441 Au 13.618278 3.155406 7.208661 Au 11.586096 4.249568 8.423866 Au 13.705399 5.745996 7.491145
$Au_3/Ce_{21}O_{42}$ (**3c**) 66 Ce 13.750542 8.220716 9.993884 Ce 12.491926 14.784386 7.253627 Ce 14.150411 14.413432 10.374623 Ce 10.881407 6.211221 11.260737 Ce 5.800874 8.029876 7.906163 Ce 9.122342 7.215297 14.251937 Ce 9.461506 13.143095 8.306397 Ce 10.157317 9.885719 10.004936 Ce 7.342794 7.077474 11.059361 Ce 5.878664 8.630899 14.050703 Ce 11.403342 11.947237 5.404990 Ce 6.700720 11.224971 9.533663 Ce 11.480236 12.674722 12.084333 Ce 9.160603 6.523684 7.920634	

Ce	14.827711	11.203238	11.734533
Ce	13.597051	11.440945	8.306774
Ce	12.156681	9.108401	13.253635
Ce	4.228067	9.018353	10.937285
Ce	12.005932	8.604604	6.687543
Ce	8.713863	10.742144	13.322421
Ce	8.557986	9.930523	6.510942
O	14.250613	13.503372	8.178806
O	6.959196	6.422233	8.915792
O	13.218970	15.791134	8.993073
O	9.766014	12.626503	13.379951
O	4.718796	10.990263	10.351610
O	11.218464	6.859951	13.373765
O	7.868977	8.473213	12.859965
O	13.024113	6.045343	10.322666
O	7.652748	7.860108	6.572264
O	9.326806	12.108754	6.150431
O	13.032267	10.623673	6.221584
O	11.287573	6.513921	6.630672
O	14.273032	8.989758	12.022438
O	7.207677	7.268569	15.180964
O	13.286132	12.253263	10.452511
O	12.259488	9.694304	8.825108
O	10.492971	12.265112	10.089777
O	13.140133	11.359921	13.093481
O	10.012568	8.717087	7.744608
O	11.760602	8.299620	11.050945
O	9.333767	7.619360	10.131331
O	6.336246	8.855522	9.940850
O	15.623132	13.154219	11.442685
O	7.442877	13.181800	9.018016
O	12.613255	14.507277	11.807217
O	6.843091	10.479976	14.378988
O	4.171415	9.472887	13.031849
O	14.913198	10.220984	9.692516
O	12.258668	13.863400	5.225890
O	8.189739	10.658924	11.118822
O	3.949820	8.088291	8.936938
O	10.709316	10.448765	12.099094
O	10.560129	9.806970	5.327234
O	8.798852	10.880697	8.495209
O	10.030100	9.185947	14.478456
O	14.088498	8.167955	7.671329
O	10.461372	14.987467	7.777296
O	9.768513	4.945530	9.709441
O	11.718593	12.599243	7.542108
O	5.449981	7.365158	12.092365
O	6.442764	10.122642	7.446462
O	8.847346	5.984261	12.376911
Au	12.318176	5.887867	8.350462
Au	14.898592	6.327424	7.141902
Au	10.891262	3.465141	8.828541

$Au_4/Ce_{21}O_{42}$ (**4a**)				$Au_4/Ce_{21}O_{42}$ (**4b**)			
67				67			
Ce	13.694311	8.233618	10.028295	Ce	13.592892	8.282087	9.983245
Ce	12.356120	14.909481	7.345685	Ce	12.365143	14.897264	7.354035
Ce	13.995332	14.513737	10.454081	Ce	14.007816	14.502339	10.481041
Ce	10.782694	6.299448	11.322197	Ce	10.802852	6.168931	11.291313
Ce	5.666926	8.154408	7.909935	Ce	5.672833	8.131912	7.952430
Ce	8.974677	7.301792	14.281271	Ce	9.040233	7.336963	14.284304
Ce	9.303354	13.286325	8.379621	Ce	9.286095	13.301016	8.362187
Ce	10.038198	10.004074	10.031396	Ce	9.990728	9.945129	10.016897
Ce	7.225538	7.191216	11.074074	Ce	7.248511	7.137422	11.124358
Ce	5.716529	8.691112	14.065743	Ce	5.776449	8.702069	14.102712
Ce	11.269345	12.092791	5.472136	Ce	11.303295	12.063256	5.489752
Ce	6.548859	11.347504	9.588929	Ce	6.532493	11.368465	9.568211
Ce	11.334141	12.773833	12.149020	Ce	11.280656	12.816148	12.138200
Ce	9.043246	6.779002	7.921545	Ce	8.986226	6.675081	7.961113
Ce	14.670460	11.286016	11.774094	Ce	14.636917	11.261293	11.811333
Ce	13.431963	11.541021	8.376119	Ce	13.456171	11.554451	8.379520
Ce	12.032854	9.205594	13.268019	Ce	11.930614	9.221869	13.179478
Ce	4.078823	9.088888	10.949903	Ce	4.125388	9.084430	10.989350
Ce	11.798632	8.707738	6.708000	Ce	11.884737	8.695589	6.765294
Ce	8.559417	10.821666	13.352798	Ce	8.531478	10.898298	13.351501
Ce	8.387080	10.144080	6.540355	Ce	8.434365	10.080714	6.558487
O	14.081474	13.626457	8.248997	O	14.123709	13.618807	8.283386
O	6.937685	6.532797	8.872853	O	6.910463	6.495922	8.905166
O	13.084557	15.925225	9.068581	O	13.079578	15.892408	9.116056
O	9.593237	12.693816	13.438017	O	9.590619	12.769009	13.456820
O	4.554844	11.062032	10.389132	O	4.535667	11.045286	10.358202
O	11.037822	6.969953	13.435053	O	11.143781	7.097216	13.488205
O	7.718427	8.538416	12.877279	O	7.770702	8.583356	12.876604
O	13.039959	6.062811	11.110416	O	13.206718	6.153345	10.613249
O	7.543831	8.003980	6.610781	O	7.567136	7.912800	6.659093
O	9.158813	12.282657	6.202937	O	9.207249	12.237728	6.174817
O	12.875916	10.717855	6.261332	O	12.950956	10.705421	6.299295
O	10.728721	6.796650	6.595563	O	10.762652	6.679961	6.421829
O	14.148083	9.178664	12.140738	O	14.007845	9.104540	12.136893
O	7.052114	7.336484	15.197087	O	7.133675	7.375599	15.228444
O	13.113712	12.355996	10.510849	O	13.114642	12.336911	10.534306
O	12.115166	9.779573	8.815644	O	12.136450	9.827040	8.842658
O	10.332752	12.374677	10.143427	O	10.266088	12.611704	10.195080
O	12.949600	11.481008	13.148930	O	12.910610	11.361858	13.177275
O	9.814834	8.904045	7.834143	O	9.858313	8.769213	7.791658
O	11.597975	8.342222	11.048851	O	11.630092	8.354773	11.088973
O	9.176304	7.728793	10.131802	O	9.178552	7.599353	10.104889
O	6.190598	8.942336	9.942981	O	6.234929	8.929395	9.976806
O	15.456981	13.269499	11.504953	O	15.462145	13.185635	11.551769
O	7.268539	13.306237	9.098681	O	7.236033	13.319926	9.008583
O	12.440929	14.614525	11.875343	O	12.510829	14.609657	11.935309
O	6.659865	10.533219	14.391665	O	6.711901	10.544783	14.479484
O	3.990417	9.511528	13.040868	O	4.067002	9.537184	13.081279
O	14.798347	10.362358	9.684716	O	14.772982	10.270772	9.746174
O	12.128740	13.999387	5.300736	O	12.181913	13.966822	5.322347

O 8.021162 10.751352 11.158071 O 3.825661 8.155746 8.920352 O 10.557812 10.527944 12.124390 O 10.356345 9.980638 5.380317 O 8.629412 11.036597 8.538401 O 9.854142 9.273157 14.512165 O 13.625607 7.760333 7.574098 O 10.315376 15.118830 7.875407 O 10.005070 5.262489 9.349282 O 11.553648 12.720499 7.599079 O 5.312614 7.439360 12.083406 O 6.273906 10.252751 7.465808 O 8.733173 6.045385 12.342930 Au 13.813685 3.063756 7.693300 Au 11.493715 4.216954 8.399230 Au 13.700327 5.727583 7.441258 Au 13.751987 4.529702 9.971090	O 7.895834 10.925041 11.231007 O 3.842466 8.129189 8.986168 O 10.550917 10.578899 12.163012 O 10.443588 9.942667 5.423776 O 8.618023 11.038136 8.498487 O 9.978568 9.341420 14.459791 O 13.442251 7.736021 7.866511 O 10.331372 15.127571 7.798977 O 9.633438 5.050151 9.398026 O 11.582115 12.705355 7.627461 O 5.353403 7.426348 12.141190 O 6.293585 10.194955 7.448563 O 8.708996 6.049845 12.478106 Au 13.316904 4.720699 9.175346 Au 10.825101 3.541970 8.685442 Au 11.982059 5.057032 6.678300 Au 13.073016 2.717533 7.415734
$Au_4/Ce_{21}O_{42}$ (**4c**) 67 Ce 13.521503 8.222082 10.039833 Ce 12.397437 14.853970 7.356205 Ce 14.031592 14.447821 10.494961 Ce 10.686861 6.181681 11.286377 Ce 5.616470 8.169861 7.993836 Ce 8.925861 7.376717 14.319727 Ce 9.314288 13.273667 8.354564 Ce 9.950524 9.955551 10.041384 Ce 7.135692 7.229943 11.174303 Ce 5.674567 8.817755 14.138251 Ce 11.301742 12.016459 5.504399 Ce 6.516520 11.390599 9.562822 Ce 11.279498 12.794972 12.133377 Ce 8.948203 6.657774 8.044592 Ce 14.600853 11.205914 11.852057 Ce 13.426681 11.495020 8.414943 Ce 11.855507 9.200901 13.218307 Ce 4.045457 9.212100 11.006106 Ce 11.839430 8.635353 6.801008 Ce 8.482865 10.917973 13.353945 Ce 8.408787 10.051826 6.576009 O 14.130979 13.548031 8.306192 O 6.792457 6.550676 8.994715 O 13.110735 15.830098 9.126696 O 9.567085 12.778084 13.418129 O 4.529582 11.169696 10.373671 O 11.039925 7.133885 13.546951 O 7.663812 8.653588 12.938022 O 13.015475 6.150073 10.591022 O 7.504043 7.956751 6.695165 O 9.202683 12.215473 6.211877 O 12.914010 10.660983 6.337280	$Au_4/Ce_{21}O_{42}$ (**4d**) 67 Ce 13.650414 8.275305 10.051058 Ce 12.354258 14.888199 7.354581 Ce 14.005857 14.492984 10.464860 Ce 10.817415 6.193123 11.280878 Ce 5.654991 8.143280 7.945745 Ce 9.032489 7.324850 14.289152 Ce 9.299983 13.261736 8.357401 Ce 10.024581 9.938291 9.979187 Ce 7.257128 7.167999 11.112829 Ce 5.762635 8.692993 14.107228 Ce 11.279182 12.069557 5.478427 Ce 6.539784 11.328751 9.566730 Ce 11.291771 12.780846 12.104840 Ce 8.978905 6.686774 7.920289 Ce 14.638960 11.279187 11.829685 Ce 13.421559 11.514015 8.363954 Ce 11.930352 9.212981 13.186247 Ce 4.108852 9.082996 10.995785 Ce 11.882348 8.631354 6.635922 Ce 8.531488 10.852436 13.319577 Ce 8.433737 10.074157 6.533631 O 14.097097 13.583856 8.286108 O 6.890825 6.527190 8.909075 O 13.099525 15.885284 9.110382 O 9.572300 12.734068 13.384123 O 4.563696 11.055094 10.409070 O 11.149296 7.111167 13.494576 O 7.757499 8.573271 12.904638 O 13.206156 6.217725 10.670462 O 7.520527 7.951591 6.633677 O 9.172384 12.255062 6.222493 O 12.923367 10.789762 6.261311

O 10.782782 6.644429 6.571404	O 10.565668 6.560126 6.409397
O 13.928142 9.059021 12.204795	O 14.012113 9.103305 12.186716
O 7.026705 7.478409 15.272816	O 7.136024 7.380831 15.245770
O 13.111049 12.309047 10.565800	O 13.124061 12.332975 10.546137
O 12.027327 9.841646 8.925496	O 12.113089 9.785887 8.871140
O 10.296618 12.448769 10.165918	O 10.323484 12.384973 10.137581
O 12.836559 11.339997 13.193574	O 12.866521 11.359137 13.175588
O 9.829396 8.789604 7.857058	O 9.844060 8.794312 7.797366
O 11.523160 8.384591 11.107077	O 11.617455 8.394574 11.076306
O 9.044879 7.817206 10.208256	O 9.175759 7.733262 10.136405
O 6.138496 9.012407 10.012201	O 6.200592 8.934072 9.977849
O 15.450552 13.119783 11.599761	O 15.451717 13.206844 11.582789
O 7.277761 13.326948 9.020155	O 7.266255 13.280092 9.058877
O 12.499295 14.577619 11.925336	O 12.460743 14.592073 11.893221
O 6.653037 10.659437 14.469113	O 6.697018 10.556114 14.427022
O 4.008127 9.703516 13.092694	O 4.049546 9.520462 13.095448
O 14.722500 10.219809 9.810246	O 14.767660 10.290306 9.814028
O 12.191624 13.917022 5.332566	O 12.130848 14.009041 5.333831
O 7.957350 10.858667 11.177968	O 8.004082 10.776034 11.151926
O 3.769526 8.246014 9.008638	O 3.817378 8.160854 8.984272
O 10.489202 10.557803 12.126740	O 10.536432 10.526706 12.092304
O 10.401454 9.908916 5.440794	O 10.359057 9.994392 5.347090
O 8.634375 11.004543 8.548052	O 8.651503 10.983263 8.530760
O 9.899261 9.392694 14.468251	O 9.975816 9.351753 14.442487
O 13.462179 7.829371 7.904502	O 13.929232 8.057015 7.824671
O 10.362539 15.094443 7.824865	O 10.323624 15.104851 7.881674
O 9.805861 5.335913 9.323071	O 9.631825 5.149351 9.428947
O 11.586813 12.681957 7.634428	O 11.563814 12.704517 7.624988
O 5.231696 7.554556 12.189660	O 5.356656 7.435183 12.140995
O 6.282929 10.245027 7.483663	O 6.289346 10.222236 7.475883
O 8.572213 6.108666 12.519626	O 8.713901 6.069995 12.477657
Au 13.160446 4.785474 9.048685	Au 13.330421 4.744807 9.114359
Au 13.507117 2.885937 7.304640	Au 10.891477 3.598522 8.808577
Au 11.883684 4.907375 6.512653	Au 14.430798 6.173818 7.068443
Au 12.446031 2.886892 4.849691	Au 12.005745 5.004914 6.753417