

File 1. The xyz-coordinates for Au<sub>n</sub>(n=3-8)

Au <sub>n</sub> (n=3-8) xyz-Coordinates (Å)											
symbol	x	y	z	symbol	x	y	z	symbol	x	y	z
1Au	0.000000	2.486815	-0.295798	1Au	2.701672	1.559811	0.000000	1Au	0.000000	2.029930	0.000000
2Au	0.000000	-2.486815	-0.295798	2Au	0.000000	1.675263	0.000000	2Au	2.029930	0.000000	0.000000
3Au	0.000000	0.000000	0.591597	3Au	1.450820	-0.837631	0.000000	3Au	0.000000	-2.029930	0.000000
				4Au	-2.701672	1.559811	0.000000	4Au	-2.029930	0.000000	0.000000
1Au	0.000000	1.339303	0.000000	5Au	-1.450820	-0.837631	0.000000	5Au	-2.629397	2.629397	0.000000
2Au	0.000000	0.000000	2.424185	6Au	0.000000	-3.119622	0.000000	6Au	-2.629397	-2.629397	0.000000
3Au	0.000000	0.000000	-2.424185					7Au	2.629397	2.629397	0.000000
4Au	0.000000	-1.339303	0.000000	1Au	0.965598	-1.716463	0.000019	8Au	2.629397	-2.629397	0.000000
				2Au	-1.029214	0.659154	0.000026				
1Au	0.000000	2.696540	0.948870	3Au	-3.687530	-0.068564	0.000002				
2Au	0.000000	-1.388560	-1.470507	4Au	1.792025	1.029530	-0.000018				
3Au	0.000000	-2.696540	0.948870	5Au	3.593771	-0.998878	0.000001				
4Au	0.000000	0.000000	1.043274	6Au	0.098706	3.125549	-0.000005				
5Au	0.000000	1.388560	-1.470507	7Au	-1.733355	-2.030328	-0.000025				

File 2. The xyz-coordinates for  $Au_nM_2$  ( $n=1\sim6$ ,  $M=Ni, Pd,$  and  $Pt$ ) clusters.

Is	symbol	$Au_nNi_2(n=1-6)$ Coordinates (Å)			symbol	$Au_nPd_2(n=1-6)$ Coordinates (Å)			symbol	$Au_nPt_2(n=1-6)$ Coordinates (Å)		
		x	y	z		x	y	z		x	y	z
3a	1Au	0.000000	0.000000	0.000000	1Au	0.000000	0.000000	1.260859	1Au	0.000000	0.000000	0.000000
	2Ni	0.000000	0.000000	2.556590	2Pd	0.000000	1.285671	-1.082694	2Pt	0.000000	0.000000	2.590713
	3Ni	0.000000	0.000000	-2.556590	3Pd	0.000000	-1.285671	-1.082694	3Pt	0.000000	0.000000	-2.590713
3b	1Au	0.000000	0.000000	0.958962	1Pd	0.000000	0.000000	2.619942	1Pt	0.000000	1.272389	-0.787826
	2Ni	0.000000	1.166559	-1.352822	2Pd	0.000000	0.000000	-2.619942	2Pt	0.000000	-1.272389	-0.787826
	3Ni	0.000000	-1.166559	-1.352822	3Au	0.000000	0.000000	0.000000	3Au	0.000000	0.000000	1.555706
4a	1Ni	0.000000	1.199915	0.000000	1Pd	0.000000	1.417790	1.149037	1Au	-2.871332	-0.014993	-0.000595
	2Ni	0.000000	-1.199915	0.000000	2Pd	0.000000	-1.417790	1.149037	2Au	2.446206	-0.617079	-0.000618
	3Au	0.000000	0.000000	2.281693	3Au	-1.447767	0.000000	-0.669060	3Pt	-0.415592	-0.747808	0.000983
	4Au	0.000000	0.000000	-2.281693	4Au	1.447767	0.000000	-0.669060	4Pt	0.846169	1.387983	0.000245
4b	1Ni	0.000000	1.478433	0.000000	1Pd	0.000000	1.424877	0.448872	1Au	0.000000	1.717015	-0.793717
	2Ni	0.000000	-1.478433	0.000000	2Pd	0.000000	-1.424877	0.448872	2Au	0.000000	-1.717015	-0.793717
	3Au	0.000000	0.000000	2.067357	3Au	-2.154073	0.000000	-0.261368	3Pt	-1.338917	0.000000	0.803892
	4Au	0.000000	0.000000	-2.067357	4Au	2.154073	0.000000	-0.261368	4Pt	1.338917	0.000000	0.803892
4c	1Au	0.000000	2.007199	-0.235093	1Au	0.000000	1.457389	0.000000	1Pt	0.000000	1.355752	0.516448
	2Au	0.000000	-2.007199	-0.235093	2Au	0.000000	-1.457389	0.000000	2Pt	0.000000	-1.355752	0.516448
	3Ni	1.231569	0.000000	0.663299	3Pd	0.000000	0.000000	2.260361	3Au	2.058693	0.000000	-0.509910
	4Ni	-1.231569	0.000000	0.663299	4Pd	0.000000	0.000000	-2.260361	4Au	-2.058693	0.000000	-0.509910
5a	1Au	0.000000	1.596821	-1.362326	1Au	0.000000	0.000000	1.468098	1Pt	0.000000	1.239945	-1.464219
	2Au	0.000000	-1.596821	-1.362326	2Au	0.000000	2.272350	-0.208684	2Pt	0.000000	-1.239945	-1.464219
	3Au	0.000000	0.000000	2.524397	3Au	0.000000	-2.272350	-0.208684	3Au	0.000000	2.665993	0.855188
	4Ni	-1.236070	0.000000	0.282502	4Pd	-1.446402	0.000000	-0.902257	4Au	0.000000	0.000000	1.180994
	5Ni	1.236070	0.000000	0.282502	5Pd	1.446402	0.000000	-0.902257	5Au	0.000000	-2.665993	0.855188
5b	1Au	0.000000	0.000000	2.083413	1Pd	0.204452	-0.237114	1.452609	1Pt	-0.000032	-0.046921	1.354886
	2Au	0.000000	2.211683	-0.960111	2Pd	0.204452	-0.237114	-1.452609	2Pt	-0.000032	-0.046921	-1.354886
	3Au	0.000000	-2.211683	-0.960111	3Au	-2.131947	0.060925	0.000000	3Au	2.138880	-1.095914	0.000000
	4Ni	1.125057	0.000000	-0.230215	4Au	1.689398	-1.901327	0.000000	4Au	-0.000032	2.284682	0.000000
	5Ni	-1.125057	0.000000	-0.230215	5Au	0.204452	2.116534	0.000000	5Au	-2.138785	-1.096114	0.000000
5c	1Au	0.000000	0.000000	0.618378	1Pd	0.000000	1.246249	-1.757657	1Pt	1.553602	0.000713	0.000000
	2Au	0.000000	2.695221	0.314512	2Pd	0.000000	-1.246249	-1.757657	2Pt	-1.553603	0.000713	0.000000
	3Au	0.000000	-2.695221	0.314512	3Au	0.000000	2.675153	0.612390	3Au	0.000000	-1.089484	1.885323
	4Ni	0.000000	1.126026	-1.759726	4Au	0.000000	-2.675153	0.612390	4Au	0.000000	-1.089484	-1.885323
	5Ni	0.000000	-1.126026	-1.759726	5Au	0.000000	0.000000	0.822111	5Au	0.000000	2.177560	0.000000

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6a	1Au	0.000000	0.000000	3.198167	1Au	0.000000	0.000000	-1.481222	1Au	0.000000	0.000000	3.141825
	2Au	0.000000	0.000000	-1.518163	2Au	0.000000	2.672648	-1.434244	2Pt	0.000000	1.265578	0.824019
	3Au	0.000000	2.644925	-1.172320	3Pd	0.000000	-1.451234	0.975229	3Pt	0.000000	-1.265578	0.824019
	4Au	0.000000	-2.644925	-1.172320	4Pd	0.000000	1.451234	0.975229	4Au	0.000000	2.653338	-1.466883
	5Ni	0.000000	1.133741	0.937610	5Au	0.000000	0.000000	3.214000	5Au	0.000000	-2.653338	-1.466883
	6Ni	0.000000	-1.133741	0.937610	6Au	0.000000	-2.672648	-1.434244	6Au	0.000000	0.000000	-1.835235
6b	1Au	0.000000	2.568196	-1.396297	1Au	0.000000	2.703817	-1.467238	1Pt	0.017618	1.242278	0.000000
	2Au	0.000000	-2.568196	-1.396297	2Au	0.000000	-2.703817	-1.467238	2Pt	-0.017618	-1.242278	0.000000
	3Au	0.000000	-1.406913	1.056441	3Au	0.000000	-1.488165	0.951315	3Au	2.542003	2.078191	0.000000
	4Au	0.000000	1.406913	1.056441	4Au	0.000000	1.488165	0.951315	4Au	2.542003	-0.690789	0.000000
	5Ni	0.000000	0.000000	3.188307	5Pd	0.000000	0.000000	3.199157	5Au	-2.542003	0.690789	0.000000
	6Ni	0.000000	0.000000	-1.270545	6Pd	0.000000	0.000000	-1.427076	6Au	-2.542003	-2.078191	0.000000
6c	1Au	0.000000	1.503864	0.378062	1Au	2.540167	0.331524	0.000000	1Au	0.000000	0.000000	3.121753
	2Au	0.000000	-1.503864	0.378062	2Au	-0.082984	1.352658	0.000000	2Au	0.000000	1.450521	0.838635
	3Au	0.000000	0.000000	2.658150	3Au	0.082984	-1.352658	0.000000	3Au	0.000000	-1.450521	0.838635
	4Au	0.000000	0.000000	-2.054684	4Au	-2.540167	-0.331524	0.000000	4Pt	0.000000	-2.667015	-1.545438
	5Ni	0.000000	2.567463	-1.917994	5Pd	-2.540167	2.337323	0.000000	5Pt	0.000000	2.667015	-1.545438
	6Ni	0.000000	-2.567463	-1.917994	6Pd	2.540167	-2.337323	0.000000	6Au	0.000000	0.000000	-1.747271
6d	1Au	1.125487	-3.334378	0.000000	1Au	0.000000	0.000000	-1.915572	1Pt	0.000000	0.000000	2.690495
	2Au	-1.310214	-1.697060	0.000000	2Au	0.000000	0.000000	2.890818	2Pt	0.000000	0.000000	-0.822852
	3Au	1.310214	1.697060	0.000000	3Au	0.000000	1.448540	0.581094	3Au	0.000000	1.900674	0.921442
	4Au	-1.125487	3.334378	0.000000	4Au	0.000000	-1.448540	0.581094	4Au	0.000000	-1.900674	0.921442
	5Ni	-1.125487	0.821444	0.000000	5Pd	0.000000	2.695233	-1.835406	5Au	0.000000	-2.425526	-1.843443
	6Ni	1.125487	-0.821444	0.000000	6Pd	0.000000	-2.695233	-1.835406	6Au	0.000000	2.425526	-1.843443
6e	1Au	0.000000	0.000000	0.000000	1Pd	0.000000	0.000000	2.878713	1Au	0.068064	1.377464	0.000000
	2Au	0.000000	0.000000	4.687155	2Pd	0.000000	0.000000	-0.693100	2Au	-0.068064	-1.377464	0.000000
	3Au	2.747242	0.000000	3.724507	3Au	0.000000	1.872653	1.062825	3Au	-2.613072	0.642901	0.000000
	4Au	2.747412	-0.000221	0.962537	4Au	0.000000	-1.872653	1.062825	4Au	2.613072	-0.642901	0.000000
	5Ni	0.856206	-1.019892	2.343556	5Au	0.000000	2.440823	-1.699142	5Pt	2.613072	1.947538	0.000000
	6Ni	-0.186671	0.895117	2.343577	6Au	0.000000	-2.440823	-1.699142	6Pt	-2.613072	-1.947538	0.000000
7a	1Au	2.484104	-0.368092	0.000000	1Au	0.397793	2.471557	-0.000190	1Au	-0.185585	0.000000	-0.132806
	2Au	2.280321	2.431421	0.000000	2Au	2.473270	0.385501	0.000181	2Au	-0.185585	0.000000	2.828698
	3Au	-2.601489	1.540981	0.000000	3Au	1.131436	-2.233094	-0.000125	3Au	2.632780	0.000000	3.747779
	4Au	0.000000	0.842188	0.000000	4Au	-1.774709	-1.765802	-0.000017	4Au	4.378322	0.000000	1.347946
	5Au	-1.602640	-3.449606	0.000000	5Au	-2.227745	1.141871	0.000071	5Au	2.632780	0.000000	-1.051887
	6Ni	-1.980191	-0.933709	0.000000	6Pd	-0.000108	-0.000022	1.290870	6Pt	1.857154	1.274118	1.347946
	7Ni	0.399359	-1.878950	0.000000	7Pd	0.000028	-0.000032	-1.290733	7Pt	1.857154	-1.274118	1.347946
7b	1Au	-0.092630	0.000000	-0.067323	1Au	0.000000	2.342864	1.409907	1Au	2.594358	0.306126	0.000000

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	2Au	-0.092630	0.000000	2.787323	2Au	0.000000	2.342864	-1.409907	2Au	2.127319	3.055558	0.000000
	3Au	2.622327	0.000000	3.669481	3Au	0.000000	-2.342864	-1.409907	3Au	-2.696679	1.508417	0.000000
	4Au	4.299846	0.000000	1.360000	4Au	0.000000	-2.342864	1.409907	4Au	0.000000	1.329295	0.000000
	5Au	2.622327	0.000000	-0.949481	5Au	0.000000	0.000000	0.000000	5Au	-1.079117	-3.611694	0.000000
	6Ni	1.871957	1.135626	1.360000	6Pd	0.000000	0.000000	-2.898738	6Pt	-1.694597	-0.984981	0.000000
	7Ni	1.871957	-1.135626	1.360000	7Pd	0.000000	0.000000	2.898738	7Pt	0.736589	-1.635898	0.000000
	1Au	1.577685	-1.204058	0.000000	1Au	-1.798199	-1.134939	0.000000	1Au	0.000000	1.362359	-1.915652
	2Au	-1.186083	-1.740266	0.000000	2Au	1.051575	-1.609467	0.000000	2Au	0.000000	-1.362359	-1.915652
	3Au	-2.668256	0.578865	0.000000	3Au	2.790376	0.531063	0.000000	3Au	0.000000	0.000000	3.173501
7c	4Au	2.704372	1.282996	0.000000	4Au	-2.694771	1.443921	0.000000	4Au	0.000000	3.682402	-0.478232
	5Au	0.000000	1.264179	0.000000	5Au	0.000000	1.095156	0.000000	5Au	0.000000	-3.682402	-0.478232
	6Ni	-1.850113	3.047295	0.000000	6Pd	1.817503	3.065091	0.000000	6Pt	0.000000	1.258193	0.817482
	7Ni	0.643335	-3.559994	0.000000	7Pd	-0.699448	-3.624502	0.000000	7Pt	0.000000	-1.258193	0.817482
	1Au	0.072798	0.000000	-0.155096	1Au	2.609749	0.053459	0.000000	1Au	-1.885474	-0.946402	0.000000
	2Au	0.072798	0.000000	2.929707	2Au	2.077399	2.814520	0.000000	2Au	0.926868	-1.721586	0.000000
	3Au	4.732970	0.000000	2.929707	3Au	-2.609812	1.545311	0.000000	3Au	2.686367	0.343264	0.000000
7d	4Au	4.732970	0.000000	-0.155096	4Au	0.000000	0.953330	0.000000	4Au	-2.686471	1.623233	0.000000
	5Au	2.402884	0.000000	1.387306	5Au	-1.296240	-3.644898	0.000000	5Au	0.000000	1.202397	0.000000
	6Ni	2.402884	0.000000	4.013296	6Pd	-2.046803	-1.084827	0.000000	6Pt	-1.082441	-3.511389	0.000000
	7Ni	2.402884	0.000000	-1.238685	7Pd	0.705355	-1.872044	0.000000	7Pt	2.053442	3.004061	0.000000
	1Au	0.000000	-1.346207	-1.695101	1Au	0.000000	1.355415	-1.776824	1Au	0.000000	2.432235	1.487901
	2Au	0.000000	1.346207	-1.695101	2Au	0.000000	-1.355415	-1.776824	2Au	0.000000	2.432235	-1.487901
	3Au	0.000000	0.000000	3.062359	3Au	0.000000	0.000000	3.315030	3Au	0.000000	-2.432235	-1.487901
7e	4Au	0.000000	-3.547481	-0.131170	4Au	0.000000	3.697378	-0.437201	4Au	0.000000	-2.432235	1.487901
	5Au	0.000000	3.547481	-0.131170	5Au	0.000000	-3.697378	-0.437201	5Au	0.000000	0.000000	0.000000
	6Ni	0.000000	-1.120674	0.832580	6Pd	0.000000	-1.261619	0.955747	6Pt	0.000000	0.000000	2.721737
	7Ni	0.000000	1.120674	0.832580	7Pd	0.000000	1.261619	0.955747	7Pt	0.000000	0.000000	-2.721737
	1Au	0.000000	2.190475	2.710022	1Au	0.000891	-0.005710	-0.003818	1Au	-2.727875	2.224728	0.000011
	2Au	0.000000	-2.190475	2.710022	2Au	-0.001573	-0.002517	2.785817	2Au	0.000000	2.499167	0.000000
	3Au	0.000000	-2.190475	-2.710022	3Au	2.481578	0.016291	4.057452	3Au	2.727875	2.224728	-0.000011
8a	4Au	0.000000	2.224654	0.000000	4Au	4.393043	1.074165	2.368922	4Au	2.727875	-2.224728	0.000011
	5Au	0.000000	2.190475	-2.710022	5Au	2.378554	1.033336	-0.951894	5Au	0.000000	-2.499167	0.000000
	6Au	0.000000	-2.224654	0.000000	6Au	3.884077	2.964731	0.383753	6Au	-2.727875	-2.224728	-0.000011
	7Ni	0.000000	0.000000	-1.376088	7Pd	1.697864	1.884924	1.725731	7Pt	-1.306997	0.000000	0.000000
	8Ni	0.000000	0.000000	1.376088	8Pd	2.454054	-0.672688	1.292316	8Pt	1.306997	0.000000	0.000000
8b	1Au	0.000000	1.359823	-2.760317	1Au	0.000000	2.709136	2.259514	1Au	2.445036	-2.691033	0.000000
	2Au	0.000000	0.000000	-0.329378	2Au	0.000000	0.000000	2.517984	2Au	2.351307	-0.009011	0.000000
	3Au	0.000000	-1.359823	-2.760317	3Au	0.000000	-2.709136	2.259514	3Au	2.407420	2.676708	0.000000
	4Au	0.000000	0.000000	4.365754	4Au	0.000000	-2.709136	-2.259514	4Au	-2.383968	0.086689	0.000000

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	5Ni	0.000000	-1.135705	2.099300	5Au	0.000000	0.000000	-2.517984	5Au	-2.609115	-2.603470	0.000000
	6Ni	0.000000	1.135705	2.099300	6Au	0.000000	2.709136	-2.259514	6Pt	-2.171322	2.721942	0.000000
	7Au	0.000000	-2.698958	-0.001926	7Pd	0.000000	1.302794	0.000000	7Pt	0.000000	1.516488	0.000000
	8Au	0.000000	2.698958	-0.001926	8Pd	0.000000	-1.302794	0.000000	8Au	-0.066844	-1.644661	0.000000
	1Au	0.000000	2.654968	2.133713	1Au	0.000000	0.000000	-0.984264	1Au	1.444990	0.935748	0.000000
	2Au	0.000000	0.000000	2.362635	2Au	0.000000	0.000000	3.702564	2Au	-3.507743	0.201177	0.000000
	3Au	0.000000	-2.654968	2.133713	3Au	0.000000	2.846938	-0.902925	3Au	-1.227409	0.354893	1.449374
8c	4Au	0.000000	-2.654968	-2.133713	4Au	0.000000	-2.846938	-0.902925	4Au	-1.227409	0.354893	-1.449374
	5Au	0.000000	0.000000	-2.362635	5Au	-0.009240	1.491757	1.445856	5Au	1.136586	-1.638490	1.545296
	6Au	0.000000	2.654968	-2.133713	6Au	0.009240	-1.491757	1.445856	6Au	1.136586	-1.638490	-1.545296
	7Ni	-0.000005	1.183285	0.000000	7Pd	-0.108614	1.497735	-3.266617	7Pt	1.136586	0.724302	2.659580
	8Ni	0.000005	-1.183285	0.000000	8Pd	0.108614	-1.497735	-3.266617	8Pt	1.136586	0.724302	-2.659580
	1Au	0.000000	0.000000	-0.730257	1Au	0.000000	0.000000	-0.629637	1Au	0.167202	3.143892	1.363539
	2Au	0.000000	0.000000	4.042515	2Au	0.000000	0.000000	4.013583	2Au	0.042425	0.738690	0.000000
	3Au	0.000000	1.419876	1.660858	3Au	0.000000	1.475748	1.696083	3Au	0.167202	3.143892	-1.363539
8d	4Au	0.000000	-1.419876	1.660858	4Au	0.000000	-1.475748	1.696083	4Au	-0.079445	-4.191834	0.000000
	5Au	0.000000	1.447587	-3.075738	5Au	0.000000	1.387309	-3.020542	5Au	-0.074820	0.414918	-2.719340
	6Au	0.000000	-1.447587	-3.075738	6Au	0.000000	-1.387309	-3.020542	6Au	-0.074820	0.414918	2.719340
	7Ni	0.000000	-2.608202	-0.680666	7Pd	0.000000	2.861971	-0.631166	7Pt	-0.074820	-1.855729	1.256599
	8Ni	0.000000	2.608202	-0.680666	8Pd	0.000000	-2.861971	-0.631166	8Pt	-0.074820	-1.855729	-1.256599
	1Au	0.000000	2.395852	1.227934	1Au	-0.000059	2.952340	1.350024	1Au	0.000000	0.000000	-0.493137
	2Au	0.000000	1.702062	-1.567162	2Au	0.000004	0.485422	0.000000	2Au	0.000000	0.000000	4.030787
	3Au	1.474029	-0.851031	-1.567162	3Au	-0.000059	2.952340	-1.350024	3Au	0.000000	2.785055	-0.694064
8e	4Au	2.074869	-1.197926	1.227934	4Au	0.000028	-4.390688	0.000000	4Au	0.000000	-2.785055	-0.694064
	5Au	-2.074869	-1.197926	1.227934	5Au	0.000027	0.221477	-2.705080	5Au	-0.104545	1.549877	1.788863
	6Au	-1.474029	-0.851031	-1.567162	6Au	0.000027	0.221477	2.705080	6Au	0.104545	-1.549877	1.788863
	7Ni	0.000000	0.000000	2.500462	7Pd	0.000027	-2.097250	1.292790	7Pt	-0.594999	1.144393	-2.900337
	8Ni	0.000000	0.000000	0.370856	8Pd	0.000027	-2.097250	-1.292790	8Pt	0.594999	-1.144393	-2.900337