

Electronic Supplementary Information for

Chemical Ordering in Pt-Au, Pt-Ag and Pt-Cu Nanoparticles from Density Functional Calculations Using a Topological Approach

Lorena Vega,¹ Hristiyan A. Aleksandrov,^{2,*} Riccardo Farris,¹ Albert Bruix,¹ Francesc Viñes,¹
and Konstantin M. Neyman,^{1,3,*}

¹ Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTC-UB), Universitat de Barcelona, 08028 Barcelona, Spain

² Faculty of Chemistry and Pharmacy, University of Sofia, 1126 Sofia, Bulgaria

³ ICREA (Institució Catalana de Recerca i Estudis Avançats), 08010 Barcelona, Spain

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* E-mail addresses of the corresponding authors:

haa@chem.uni-sofia.bg (H.A.A.); konstantin.neyman@icrea.cat (K.M.N.)

Table S1. DFT energies of homotops with selected low- and high-energy topologies T of Pt-X (X = Au, Cu) particles, $T \equiv N_{\text{BOND}}^{\text{Pt-X}} \cdot N_{\text{CORNER}}^{\text{X}} \cdot N_{\text{EDGE}}^{\text{X}} \cdot N_{\text{FACET}}^{\text{X}}$. $E_{\text{T}_{\min}}^{\text{DFT}}$ is the minimum energy and $E_{\text{T}_{\max}}^{\text{DFT}}$ is the maximum energy of 10 arbitrarily constructed homotops for a given topology, $\Delta E_{\text{T}}^{\text{DFT}} = E_{\text{T}_{\max}}^{\text{DFT}} - E_{\text{T}_{\min}}^{\text{DFT}}$. $E_{\text{T}}^{\text{TOP}}$ are the corresponding topological energies.

Particle	$N_{\text{BOND}}^{\text{Pt-X}}$	$N_{\text{CORNER}}^{\text{X}}$	$N_{\text{EDGE}}^{\text{X}}$	$N_{\text{FACET}}^{\text{X}}$	$E_{\text{T}}^{\text{TOP}}$ eV	$E_{\text{T}_{\min}}^{\text{DFT}}$ eV	$E_{\text{T}_{\max}}^{\text{DFT}}$ eV	$\Delta E_{\text{T}}^{\text{DFT}}$ meV
Pt ₇₀ Au ₇₀	196	24	24	22	-586.913	-588.108	-587.081	1027
	472	13	12	25	-571.135	-574.345	-574.096	249
Pt ₁₅₁ Au ₅₀	214	20	30	0	-978.519	-978.283	-978.258	25
	478	0	0	20	-955.212	-958.353	-958.233	120
Pt ₁₀₁ Au ₁₀₀	267	24	36	40	-859.281	-859.505	-859.321	184
	594	24	0	54	-839.236	-833.665	-832.164	1501
Pt ₅₁ Au ₁₅₀	210	24	36	62	-730.064	-729.869	-729.583	286
	312	0	36	35	-708.124	-705.958	-705.635	323
Pt ₇₀ Cu ₇₀	340	24	12	0	-625.537	-626.610	-625.042	1568
	340	0	12	48	-608.392	-610.331	-609.691	640
Pt ₁₅₁ Cu ₅₀	412	0	0	0	-1013.842	-1015.214	-1014.284	930
Pt ₁₀₁ Cu ₁₀₀	560	24	8	8	-912.794	-913.767	-913.137	630
	295	13	27	60	-880.816	-891.388	-891.214	174
Pt ₅₁ Cu ₁₅₀	418	24	36	18	-799.020	-799.627	-799.474	153

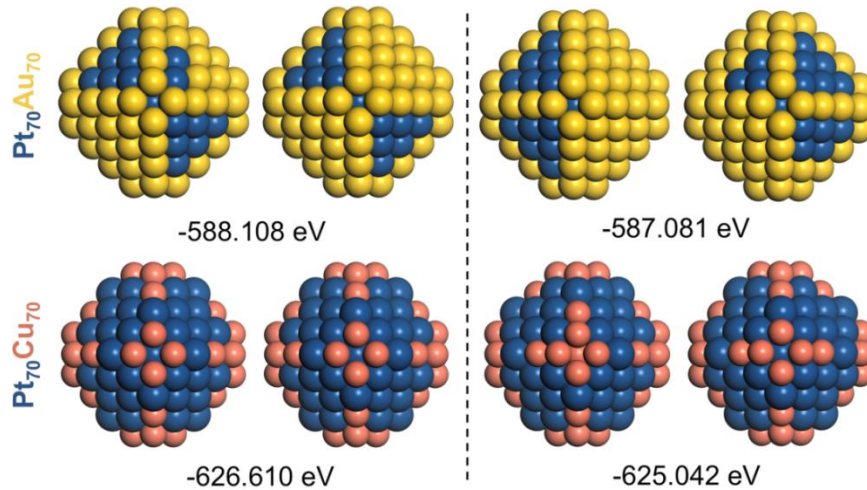


Figure S1. $E_{\text{min}}^{\text{T}}$ and $E_{\text{max}}^{\text{T}}$ homotops of the low-energy topologies 196.24.24.22 of the Pt₇₀Au₇₀ nanoparticle and 340.24.12.0 of the Pt₇₀Cu₇₀ nanoparticle. In each panel left image – front view and right image – back view. Pt – blue, Au – yellow, Cu – red-brown.

Optimized by DFT Cartesian coordinates of atoms (in Å) in selected homotops of 140- and 201-atomic PtX (X = Au, Ag, Cu) nanoparticles

Herein, each homotop is labelled as $Pt_mX_n \cdot N_{BOND}^{Pt-X} \cdot N_{CORNER}^X \cdot N_{EDGE}^X \cdot N_{FACET}^X$ -eV, with its stoichiometry Pt_mX_n , topology $N_{BOND}^{Pt-X} \cdot N_{CORNER}^X \cdot N_{EDGE}^X \cdot N_{FACET}^X$ and total DFT energy E-eV (in eV).

Atomic coordinates of homotops presented in Table 2 and in Figures 1 and 2

Pt₇₀Au₇₀_196.24.24.22-588.108

Au	13.15432219297798	20.95707249612691	11.10394030524896
Au	13.13110636956944	17.09571439528438	19.00055820472905
Au	19.06906191673500	13.14328731563428	9.05632951434813
Au	5.25092170213722	11.11687202244214	13.04808104317859
Au	13.06895933338910	7.16232974237563	9.08093018490514
Au	13.10278160801859	19.04790069986846	17.09399028463356
Au	7.13393876533343	9.08793647862316	13.05292149020946
Au	15.29289313549744	19.16502364005002	15.28812909735388
Au	15.09270871650923	13.14836747032315	5.23685731416294
Au	13.06035784508380	11.11218494790499	5.23901853950431
Au	9.07437119532363	13.07646583569939	7.12744573970884
Au	11.10830744996797	13.18047423489049	20.95028866309735
Au	5.25374810539711	13.15275954123246	15.07498214502809
Au	7.14087437048777	13.15013841751335	17.10544196525144
Au	15.28273312398120	7.00640288111141	10.91388317002753
Au	10.87951495899548	17.34252771578401	8.86722115862292
Au	13.08334660603214	20.95478391153936	15.08968152999759
Au	19.06592081561406	9.08545248375874	13.11993109179318
Au	13.15817929790580	11.15038109027344	20.92811261101994
Au	13.09993190333746	15.12098880863294	20.90938772483084
Au	10.92712963219546	15.28506894647181	6.99323999918882
Au	13.06720268902960	9.09930316604718	7.13771942067293
Au	17.12916612187527	19.04856565668102	13.06131991205245
Au	6.98609282414351	15.30468380419300	10.90562086030607
Au	11.10162072176131	5.26268883647897	13.04884646123869
Au	19.07935958184182	17.11733651102661	13.07045659425559
Au	15.11675070916461	20.94398435678659	13.07997438006567
Au	17.33035358992820	10.89278800411988	8.86027455437194
Au	13.14757267074543	19.07149108927903	9.07466180964469
Au	20.96542344741402	15.09166380815270	13.04971504781946
Au	19.24756277820057	15.30070996455698	15.29613303180021
Au	20.96019527476393	11.10661541290323	13.11413518832175
Au	8.86811250756603	17.35518685083535	10.86384699640096
Au	17.14464152828360	13.09379002465881	19.02855911570406
Au	13.13351288472261	15.10117817375992	5.24560334671208
Au	13.13705615658104	17.12803423287642	7.13450417257538
Au	9.07060230586941	7.14398349189151	13.05026843304201
Au	10.91869029743395	7.01040939288241	15.26498136244687
Au	15.09525068447399	5.26371994782240	13.12653305851615
Au	8.86405321559234	8.88366747252840	15.31485002372147
Au	17.12601191925060	13.14649396447677	7.11747808191466
Au	10.93944631922129	10.96779448933644	19.18645968355918
Au	6.98668914176191	10.93218213008518	15.27140060817544
Au	15.13036585893006	13.13626672328768	20.89956364133948
Au	15.32843445495677	8.89108382476618	8.86996586111392
Au	13.06590341655892	5.26073364486895	11.09221243018701
Au	17.37877414071496	17.35524717510235	15.35054713166498
Au	13.12995195224020	7.16767511241381	17.10317399168402
Au	7.13881977383216	13.08203886431978	9.07029278959183
Au	8.86422588735283	10.89038147465553	17.32762039636081
Au	5.25233016115334	15.11477042885639	13.12194203410803
Au	20.95970389030235	13.14085848633431	11.08071742083327
Au	15.27422863376273	10.94231328590186	6.99087866399492
Au	9.07720048612130	19.09126718774649	13.12804126252930

Au	8.86801489740058	15.34346764316924	8.86189142652822
Au	10.87037031381021	8.89247653303813	17.32076312491077
Au	10.93420665670573	19.21862572086916	10.92406458725861
Au	7.14252710247387	17.14025413535181	13.12096876767598
Au	20.97320133656915	13.06287992636042	15.07465827264749
Au	11.09928388076554	13.07020406767374	5.24268259940968
Au	17.39833123207212	15.37883868507651	17.36852583253976
Au	17.11600521355783	7.15408871266546	13.12420539755803
Au	13.13415370005847	5.27173721111685	15.08097780237385
Au	19.10216422880839	13.08445152809948	17.11362076149566
Au	9.07142685982234	13.16684930649202	19.06142028513877
Au	5.24999722458295	13.08004538911737	11.09356950276116
Au	17.32762908265189	8.88743816579906	10.87049081528343
Au	11.11597326992186	20.97221524425228	13.13099258866243
Au	13.14544716405219	9.10319726744363	19.05406290736955
Au	19.20172249087508	10.93960254567492	10.91499981105280
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Pt	13.11326599577636	15.06955212262329	16.95287843205652
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Pt₇₀Ag₇₀_196.24.24.22-561.294

Ag	7.342220	15.701578	13.561019
Ag	9.422015	17.630610	13.515107
Ag	9.436231	5.433492	9.476412
Ag	7.369398	7.361077	9.441253
Ag	13.564488	5.479233	9.457906
Ag	5.432839	9.419754	9.436034
Ag	9.418153	7.376729	7.399923
Ag	7.390073	9.407131	7.380506
Ag	9.424510	13.557671	5.404522
Ag	9.451320	9.432847	5.428116
Ag	13.597177	13.574374	5.380956
Ag	9.391458	15.687382	15.610578
Ag	5.421171	13.608479	13.575923
Ag	13.487548	11.537617	19.515123
Ag	11.444741	9.515897	19.471272
Ag	11.485947	13.533895	19.495550
Ag	9.475410	11.483646	19.456804
Ag	11.423417	7.493599	17.558077
Ag	15.551082	11.625613	17.538355
Ag	7.450448	11.459182	17.532917
Ag	11.542477	15.588964	17.486109
Ag	11.431142	5.530997	15.586124
Ag	17.549484	11.685372	15.565401
Ag	5.476481	11.458982	15.556201
Ag	11.579228	17.590582	15.506457
Ag	11.454752	3.601268	13.577057
Ag	19.437685	11.644968	13.488525
Ag	3.563654	11.478152	13.518203
Ag	11.562241	19.473738	13.397936
Ag	13.491773	3.521835	11.546050
Ag	15.553849	5.502416	11.465140
Ag	17.536684	7.482320	11.422623
Ag	17.431602	15.528288	11.461048
Ag	9.469474	3.588044	11.635051
Ag	5.471216	7.464767	11.637764
Ag	19.425024	9.558687	11.433135
Ag	3.563986	9.502583	11.553897
Ag	7.443413	5.507717	11.664064

Ag	15.499282	17.448145	11.453551
Ag	19.368801	13.565804	11.441910
Ag	3.578495	13.514810	11.447119
Ag	5.466950	15.578940	11.354114
Ag	7.447134	17.558823	11.320292
Ag	13.532078	19.380463	11.390206
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Ag	11.480309	3.502470	9.560820
Ag	3.572404	11.534509	9.477593
Ag	19.363813	11.535525	9.433232
Ag	11.539339	19.360308	9.343232
Ag	11.549861	5.473702	7.491884
Ag	5.488333	11.570172	7.437714
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Ag	11.504930	17.376560	7.431109
Ag	7.466094	11.536285	5.449198
Ag	11.592639	7.439505	5.507782
Ag	15.514516	11.454450	5.504751
Ag	11.503609	15.485949	5.446114
Ag	9.525132	11.458055	3.461531
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Ag	13.532470	11.413397	3.536957
Ag	11.523502	13.463788	3.444659
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Ag	9.435898	13.611032	17.567450
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Pt	13.473641	17.283947	9.470241
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Pt	13.489413	15.359988	7.532405
Pt	13.464765	9.527959	5.665613
Pt	11.525287	11.564701	17.473915
Pt	11.601033	9.526071	15.498714
Pt	13.531813	11.482376	15.520246
Pt	9.490642	11.624703	15.492638
Pt	11.442062	13.549298	15.480991
Pt	11.609908	7.559065	13.542506
Pt	13.593758	9.437018	13.617071
Pt	15.484491	11.414413	13.576514
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Pt	11.472722	11.487945	13.545268
Pt	7.534545	11.617767	13.538258
Pt	13.408769	13.432781	13.481307
Pt	9.392614	13.611680	13.586185
Pt	11.371823	15.500383	13.537786
Pt	11.523895	5.561893	11.508006
Pt	13.538665	7.509569	11.590587
Pt	9.491814	7.528809	11.433725
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Pt	11.487530	9.490665	11.547890
Pt	7.535260	9.473584	11.419275

Pt	15.383410	13.478317	11.520312
Pt	9.475061	11.488733	11.538496
Pt	13.436444	11.456478	11.591715
Pt	7.501365	13.548764	11.601797
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Pt	11.434301	13.437913	11.585739
Pt	9.441465	15.486761	11.588255
Pt	11.456960	7.536619	9.504551
Pt	9.433498	9.433244	9.447268
Pt	9.530069	13.402121	9.590388
Pt	13.402079	9.552736	9.606714
Pt	7.541871	11.410281	9.483600
Pt	11.449662	11.465405	9.554250
Pt	13.412251	13.404726	9.570178
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Pt	9.478838	11.446376	7.502456
Pt	13.435576	11.540705	7.543635
Pt	11.476472	13.463906	7.495507
Pt	11.490513	11.524714	5.504764
Pt	9.534933	9.574892	17.348112
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Cu	12.595736	16.392361	14.433095
Cu	5.241938	10.842258	12.552402
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Cu	12.601018	18.218418	16.258963
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Cu	14.394217	12.660321	5.178509
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Cu	6.987063	10.689990	12.592189
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Cu	12.528306	7.016801	7.043816
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Cu	5.191658	12.590111	16.270683
Cu	12.528749	14.497103	18.143963
Cu	14.421050	12.596037	7.047335
Cu	8.852506	19.959728	12.619493

Cu	14.423908	12.604167	18.135075
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Cu	12.535903	7.032942	10.696991
Cu	6.978239	7.030087	12.611938
Cu	10.632764	7.040577	12.601420
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Cu	6.987466	12.588856	7.063850
Cu	14.425238	14.495346	12.631321
Cu	12.570601	14.494432	14.490843
Cu	16.365601	8.776535	16.437468
Cu	5.157628	16.276815	12.609859
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Cu	14.394349	10.687724	8.799234
Cu	14.450741	7.012782	12.595577
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Cu	18.068554	12.604933	14.488907
Cu	10.643552	18.130680	12.602218
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Cu	12.528193	16.288937	5.210777
Cu	12.518694	19.966135	16.296497
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 Pt 8.778445 10.707335 7.063974
 Pt 8.799158 10.737743 18.133781
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 Pt 12.536262 12.585174 8.942003
 Pt 6.953845 14.482802 8.940741
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 Pt 10.678641 8.854225 18.130239
 Pt 8.792373 14.473971 7.014712

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Cu	8.863083	12.591241	16.269735
Cu	12.544017	14.481029	14.485499
Cu	14.419945	12.598186	14.485354
Cu	10.664799	14.473845	12.601827
Cu	10.703589	18.108419	12.594440
Cu	10.696136	7.081821	12.599728
Cu	10.671304	16.291643	14.478186
Cu	12.545546	10.715584	10.723255
Cu	16.093035	19.869785	12.577733
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Cu	12.534064	8.920962	8.926018
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Cu	14.359108	7.082889	12.598927
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Cu	12.550574	18.122442	7.120861
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Cu	18.054178	12.584062	14.436502
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Cu	10.670068	10.733685	12.598017
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Cu	19.870972	14.399074	10.794079
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Cu	14.411884	10.715870	12.602069
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Atomic coordinates of some homotops presented in Table S1

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Pt	14.422006	5.050002	12.343962
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Pt	14.523600	12.399342	19.697445
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Pt	12.534414	8.507859	10.365259
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Pt	10.588324	12.407104	8.546474
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Pt	16.410389	6.771542	12.328018
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Cu	6.888453	8.616341	12.332170
Cu	14.559704	18.053099	14.315933
Cu	14.525625	16.216351	16.138885
Cu	8.718302	10.416798	8.529770

Cu	8.680659	12.378963	6.726257
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Cu	10.581822	8.562135	8.514524
Cu	16.347885	8.590636	14.296463
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Cu	6.873168	14.393465	10.343341
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Cu	18.199223	14.372772	10.355410
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Cu	10.579330	8.561049	16.155745
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Pt	18.167891	18.229822	12.599838
Pt	6.861593	16.399950	14.519578
Pt	16.348730	18.287138	14.546263
Pt	14.465943	16.284058	10.685868
Pt	10.575493	14.520942	12.601420
Pt	18.203167	14.508973	8.784441
Pt	10.672809	10.755401	20.137999
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Pt	8.705774	10.669816	6.902517
Pt	14.370364	10.758878	20.102243
Pt	5.019581	14.445808	10.753081
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Pt	16.334028	10.665522	6.944108
Pt	8.701275	14.513463	18.291792
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Pt	10.598018	6.945871	16.385620
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Pt	6.568620	12.587462	14.551720
Pt	10.546112	14.547197	12.549311
Pt	8.575067	12.570420	8.633104
Pt	10.595549	10.602427	20.255705
Pt	14.549210	8.631945	14.590446
Pt	10.455398	10.571414	16.511475
Pt	12.533363	18.309399	10.581475
Pt	10.527232	14.563556	8.613689
Pt	14.475746	14.576164	20.209446
Pt	14.544323	8.601353	10.580816
Pt	14.484119	10.615099	20.246103
Pt	10.487453	8.644726	10.563151
Pt	12.544423	14.544326	6.661426
Pt	6.581254	14.563614	12.562677
Pt	12.533702	14.562509	10.587686
Pt	16.475769	14.577353	14.566022
Pt	12.534950	16.513124	8.567992
Pt	12.522888	18.280073	14.546263
Pt	12.520472	10.613200	18.315231
Pt	16.472288	10.550289	14.573013
Pt	14.551888	14.611637	16.497580
Pt	14.523047	18.303492	12.564490
Pt	14.576056	10.528410	16.520582
Pt	18.462900	10.562299	12.595855
Pt	14.511092	12.571573	10.602443
Pt	10.488400	8.707164	14.577882
Pt	8.550655	14.563632	14.564935
Pt	16.485950	8.611136	12.574476
Pt	12.533067	10.575897	6.686404
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Pt	10.523456	10.573967	8.629818
Pt	8.506834	16.521635	12.565777
Pt	8.513171	8.681915	12.558735
Pt	14.544884	14.558105	8.622811
Pt	10.556932	12.570314	6.664759
Pt	12.526390	10.591950	10.605901
Pt	10.560947	5.006670	14.618484
Pt	12.531890	6.839515	14.554127
Pt	14.486450	20.260681	10.637568
Pt	8.517536	10.576236	10.554438
Pt	12.533331	8.630096	8.662083
Pt	8.545444	14.571116	10.563713
Pt	16.510399	10.559176	10.586477
Pt	12.539705	12.586975	20.304216
Pt	8.553917	12.575949	12.557517
Pt	14.562389	16.487152	14.585094
Pt	10.548421	12.572443	10.600793
Cu	14.596889	14.629539	5.182622
Cu	12.546062	6.917597	18.379589
Cu	8.663723	10.598696	18.426640
Cu	10.529814	18.326525	16.485861
Cu	19.948439	14.559121	14.697257
Cu	12.538711	8.662127	5.164649
Cu	16.442450	12.571801	5.160503
Cu	19.980183	10.598185	14.676331
Cu	10.493977	14.650917	5.178838

Cu	10.533400	8.707055	18.367193
Cu	5.161849	14.691816	14.665209
Cu	14.527326	6.892674	16.559450
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Cu	6.841156	10.557124	16.558189
Cu	12.539515	6.869339	6.897145
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Cu	12.531252	5.149194	8.713369
Cu	6.832965	8.634336	14.572636
Cu	14.488931	6.829391	8.686213
Cu	8.619619	6.815688	10.601120
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Cu	5.380159	12.599474	16.701027
Cu	10.519423	16.528591	6.906370
Cu	18.273481	8.672466	14.551793
Cu	6.784557	14.543920	8.647518
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Cu	8.686816	18.392172	14.575510
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Cu	6.812143	12.572992	6.873795
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Cu	12.552842	12.552139	5.015615
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Cu	10.575015	8.654408	6.867336
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Cu	14.498678	8.660619	6.869823
Cu	18.068079	18.524567	12.595287
Cu	6.870533	16.554251	14.604441
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Cu	5.102003	14.651593	10.511203
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Cu	16.396265	18.396870	10.603437
Cu	5.076693	10.524516	10.524152
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Cu	19.998037	10.522430	10.558422
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Cu	4.910919	12.592879	12.560278
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Cu	8.630397	8.692387	8.685212
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Cu	20.126593	12.549116	12.624174
Cu	16.440987	16.452272	8.685690
Cu	19.949766	14.639338	10.523802
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Cu	6.858148	14.625661	16.550318
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Cu	16.401186	10.598021	18.398432
Cu	8.613159	14.538617	6.852993
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Cu	14.529191	8.699292	18.396940
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Cu	8.625213	12.566959	5.168093
Cu	16.385353	14.573596	18.371775
Cu	10.500525	10.520751	5.145564
Cu	10.545251	18.397913	8.721618
Cu	8.643588	16.491192	16.490391
Cu	12.541164	18.497887	7.047002
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Pt	8.838314	18.124548	14.510463
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Pt	8.785300	10.711190	18.204889
Pt	12.526319	5.170454	12.602597
Pt	12.534957	12.595174	8.948691
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Pt	12.518162	12.617681	20.035660
Pt	18.119534	8.865969	10.735729
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Pt	8.798754	14.499937	18.180016
Pt	10.636648	8.848860	18.197441
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Pt	16.251478	18.212328	14.469502
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Cu	12.533237	14.466837	14.470442
Cu	14.408298	12.579586	14.475222
Cu	10.664109	14.465968	12.602918
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Cu	10.689611	7.084986	12.616488
Cu	10.679028	16.280252	14.490957
Cu	12.546124	10.708259	10.716137
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Cu	12.538711	8.897814	8.934639
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Cu	14.370024	7.080747	12.584146
Cu	16.309204	8.812120	16.379683
Cu	12.538263	18.099438	7.116678
Cu	14.400405	10.707532	16.291676
Cu	18.033829	12.581271	14.425288
Cu	10.641964	18.165026	16.332247
Cu	8.850515	12.593192	8.929264
Cu	16.256495	14.479775	18.163847
Cu	18.023962	12.621868	7.112136
Cu	19.797499	12.621215	9.043862
Cu	12.521698	5.321739	16.150688
Cu	16.306124	16.372032	16.368540
Cu	18.032427	7.108934	12.607702
Cu	10.669537	16.275707	10.719520
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Cu	14.323948	10.809166	19.951729
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Cu	6.974012	16.326311	14.497643
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Cu	14.402643	8.893730	14.473081
Cu	8.846955	14.474681	14.465531
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Cu	14.313973	14.421715	5.279707
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Cu	7.024986	12.588790	14.430449
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Cu	16.226799	10.689734	14.450404
Cu	7.016148	10.751467	12.594541
Cu	12.539566	16.269585	16.272911
Cu	12.527579	7.089458	14.437940
Cu	18.010807	18.072950	12.545556
Cu	18.043179	12.602888	10.765550
Cu	14.410048	12.582692	10.715542
Cu	18.041029	10.749343	12.612250
Cu	8.956604	12.610563	19.862333
Cu	12.546967	16.167059	19.850504
Cu	5.267129	12.601575	9.022367
Cu	10.660792	10.718858	8.911560
Cu	5.203980	10.753843	14.396451
Cu	14.404325	16.286669	14.474684
Cu	7.008180	12.597695	10.771343
Cu	18.001507	12.601159	18.090479
Cu	12.521657	18.103462	14.447789
Cu	10.655755	10.711918	12.602862
Cu	16.211891	12.599778	8.916550
Cu	19.834175	14.431648	10.806165
Cu	12.528509	18.101200	18.078909
Cu	14.410086	10.702339	12.595099
Cu	14.315192	5.281621	10.766301
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Cu	19.843023	14.414827	14.406560
Cu	12.537615	5.367774	9.026728
Cu	7.021750	14.434557	12.630087
Cu	8.991930	12.601240	5.330163
Cu	8.969197	5.353115	12.620968
Cu	14.330769	19.889225	10.767890
Cu	10.660106	12.577924	14.483808
Cu	14.408686	14.466847	12.591529
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Cu	10.683045	8.900383	10.708436
Cu	14.419058	18.160967	8.874465
Cu	12.534334	10.749578	7.092625
Cu	16.200403	12.580532	16.270382
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Cu	10.646914	8.894174	14.463313
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Cu	12.559371	18.104170	10.751212
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Cu	16.117277	5.337961	12.590445
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Cu	5.218100	14.430806	14.395799
Cu	16.228342	14.476420	10.735977
Cu	18.095434	16.333082	10.701697
Cu	12.531273	7.075047	10.743007
Cu	14.374499	12.594445	7.087408
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Cu	18.028250	14.439228	12.580090
Cu	5.306148	16.190718	12.663741
Cu	14.363305	14.384762	19.913158
Cu	10.664992	14.467072	8.910719
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Cu	19.749937	16.179104	12.553409
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Cu	16.215706	8.914013	12.592849
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Cu	19.775204	12.591147	16.172394
Cu	10.750891	10.746914	5.279607
Cu	14.393947	8.883758	10.702138
Cu	14.417732	10.721727	8.901902
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Atomic coordinates of selected homotops discussed in Section 3.1

Pt₅₁Au₁₅₀_212.24.36.62-729.864

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Au	8.30148947638757	16.70094299043643	8.29577152724205
Au	12.53970329103677	16.53030471036682	8.45619259001793
Au	6.33924437253858	14.66267304630555	8.32652918570977
Au	10.46751679864857	14.51912871902108	8.44856799950983
Au	8.47839170287316	12.42645316644717	8.46399593902774
Au	18.61672222304985	10.38319587326814	8.41106719830551
Au	6.32173704705177	10.32887011018413	8.33682006365169
Au	16.64359800276664	8.36972333833039	8.36471086723854
Au	8.40575991622507	8.44001302274212	8.38369824758773
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Au	12.50305116261818	20.80706654126566	12.50892758212981
Au	10.54213546687903	18.53473964761828	12.50397013020219
Au	14.54440985770279	18.52201180754009	12.50712376940657
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Au 6.48904094810896 14.45822892372755 12.50280269959800
 Au 18.50225385083926 14.47434983844113 12.50597237102880
 Au 4.20378269581230 12.48185334454677 12.50008429669590
 Au 20.70538244577034 12.47501686262050 12.50372075980860
 Au 6.49765160745094 10.43558841554138 12.50526407087776
 Au 18.51204605575360 10.44919666360006 12.50311431442486
 Au 12.51093017036418 4.41772970539892 12.50522775479049
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 Au 10.30758728685852 18.70932708668771 16.70542305858686
 Au 12.54432297160347 16.54555221295736 16.54108583555995
 Au 16.56741197203855 16.59439893249132 16.58795326219262
 Au 8.30230718204447 16.70845735648120 16.70696446982698
 Au 10.47270173688677 14.52632428541880 16.55146375296527
 Au 18.57621218565047 14.58747612778499 16.56096721302433
 Au 6.33717876839459 14.66129396006237 16.67234191787641
 Au 4.50264241326016 12.49010511341870 16.50584559247527
 Au 8.47678624130422 12.42902157440268 16.53858767712939
 Au 6.30507678131948 10.32320773485580 16.66571510189153
 Au 18.64048648481515 10.37513788690465 16.59802563316543
 Au 8.38561192725625 8.42725036209436 16.61592051986790
 Au 16.65645155047284 8.36578382385668 16.63004677468409
 Au 10.41131944708037 6.44402429814480 16.59020054936282
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Pt	16.46529169739415	10.45107113187598	14.52657444641796
Pt	10.50219941330112	8.50089036025229	14.50264182067811
Pt	14.53416320098819	8.47672379823103	14.52116181040940
Pt	12.51822087246266	6.54662304229113	14.47648902697417
Pt	14.51313790385326	12.45823614656110	18.49810605725752
Pt	12.53373896685586	10.51047604677231	18.48228632915895

***** End of data *****