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Revisit the Structure of $Au_{20}(SCH_2CH_2Ph)_{16}$: A Cubic Nanocrystal like Gold Kernel

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Full version of reference [42]: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.;Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci,B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H.P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.;Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima,T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin,K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.;Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega,N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.;Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.;Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.;Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.;Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas; Foresman, J.B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision A.1;Wallingford, CT, **2009**.

Table S1. The lowest vibration frequencies of six $Au_{20}(SR)_{16}$ (R = CH_3) isomers calculated from the M06 functional and the LANL2DZ basis set for Au and 6-31G(d) basis set for S, C and H atoms.

	Au_{20}-Exp.	**Au_{20}-Iso1**	**Au_{20}-Iso2**	**Au_{20}-Iso3**	**Au_{20}-Iso4**	**Au_{20}-IsoP**
Frequencies (cm^{-1})	6.2634	10.3428	12.2992	8.6336	11.0471	12.1822

The model and details of the hybrid gene algorithm (GA) and molecular mechanics (MM) calculations

For the simple ligand $–SCH_3$, the steric effects of the substituent group is negligible. However, for the large ligand, such as R = C_2H_4Ph, Ph, Adm, Ph, Ph-^{t}Bu and -^{t}Bu, the steric effect of hydrocarbon substituent groups may greatly affect the total energy of nanoclusters. For the $Au_{20}(SR)_{16}$, there are 2^{16} configurations of R substituent, and the rotation along the C-C bond in some substituent groups such as C_2H_4Ph and Ph-^{t}Bu will also increase the conformational degrees of freedom.

In order to rapidly explore the landscape of ligand orientations, in this work, we used hybrid gene algorithm (GA) and molecular mechanics (MM) calculations to rapidly search the low-energy conformation of the ligands. Then, the obtained low-lying isomers from the conformational searches are re-optimized by the DFT-D calculations to find the lowest energy structure of any $Au_{20}(SR)_{16}$ isomer with ligand protections.

As shown in Figure S1 and Table S2, for each –RS–Au–SR– unit (as a monomeric motif or as a part of a long staple motif), each R group has two possible orientations (left or right of the S-Au-S plane), denoted as S_1-R_a and S_1-R_b. The total number of ligand configurations are therefore 2^{16}.

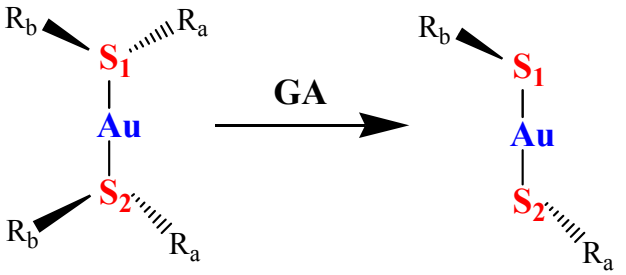


Figure S1. An illustration of ligand orientations in a –RS–Au–SR– unit .

Table S2. Each sulfur atom of the $Au_{20}(SR)_{16}$ cluster has two possible ways to link the R group, labeled as **a** and **b**.

S-R	S_1	S_2	S_3	…	S_{15}	S_{16}
R	a	a	a	a	a	a
	b	b	b	b	b	b

In order to search the energy landscape of the ligand orientations, the GA is combined with the MM calculations to search the optimal orientation of the S-R ligand. Each generated $Au_{20}(SR)_{16}$ cluster with specific ligand orientation is optimized using the universal force field (UFF).[1] During the UFF optimizations, we fixed the position of Au and S atoms, only allow the R groups to freely change their atomic positions and orientations. Geometry minimization was carried out using the conjugate-gradient method. Convergence criteria for the minimization are that all partial forces on each atom are less than 0.0001 eV/Å.

For example, Figure S2 shows the energy landscape of the **Au_{20}-Iso1** (the protection ligand is -SCH_2CH_2Ph) calculated from the hybrid GA and MM method. It is seen that in the first ~3000 step runs, several high energy ligand configurations were generated. After ~3000 step runs, the lowest-energy ligand configuration is determined.

Because the MM calculations only provided approximate estimations of the relative stabilities of different isomer configurations, after the GA/MM searches, the generated low-energy isomers were then re-optimized by the DFT-D method. After each structural search run by GA/MM calculations, we selected ten lowest-energy structures to re-optimize by the DFT-D method. This basically ensures to find the lowest energy ligand configuration.

In order to confirm the accuracy of energy calculations of MM method, here we randomly selected three high energy configurations **A**, **B** and **C** and the lowest energy one (**D**) determined from the GA/MM searches, which have different orientations of R ligand as shown in Table S3. These isomer structures were then re-optimized by the DFT-D method. The DFT-D calculations indicate that the **Au_{20}-Iso1-A, B and C** all possess higher DFT-D total energies, e.g. 0.85 eV, 1.03 eV and 0.64 eV, respectively, in agreement with the MM predictions (cf. Table S4).

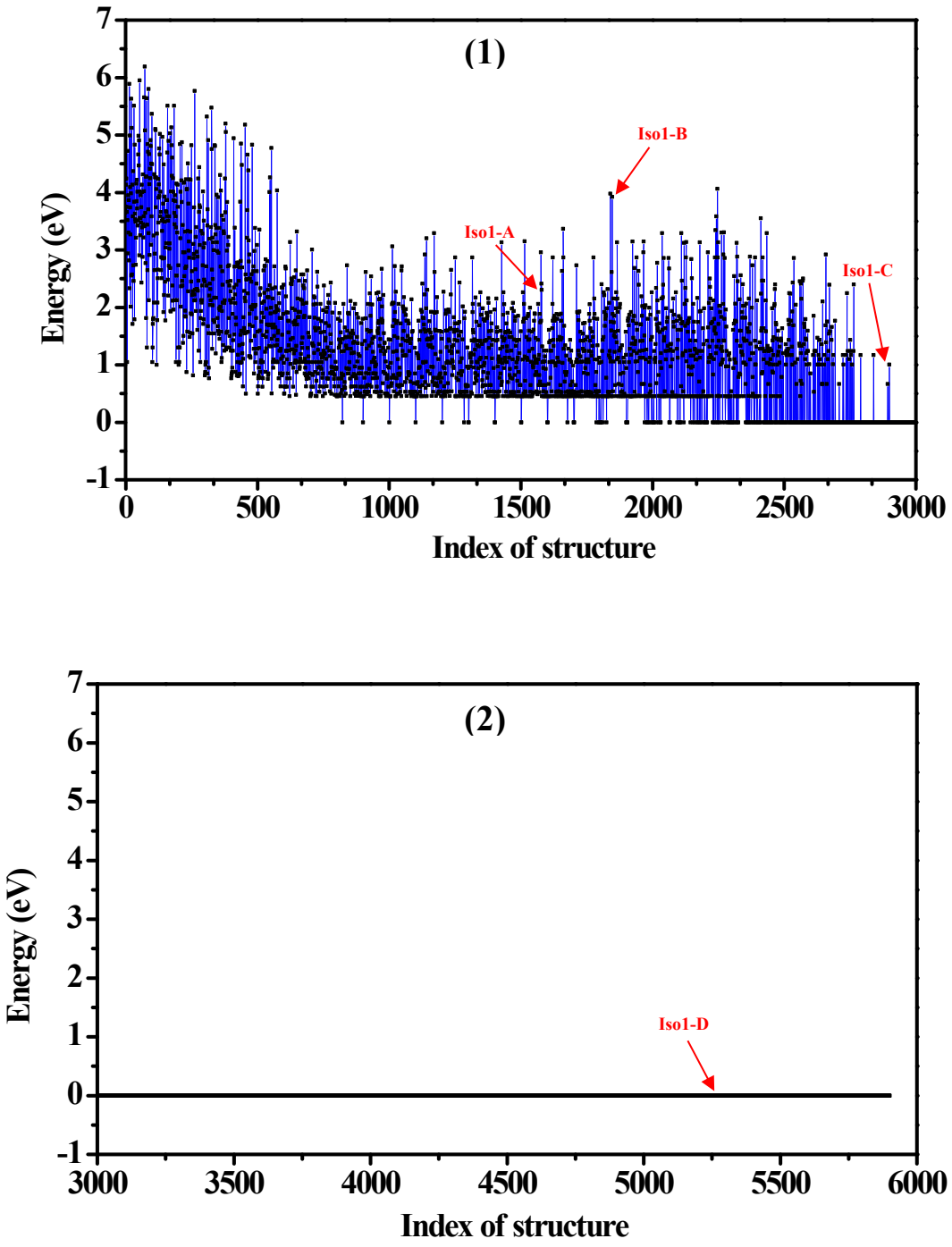


Figure S2. The energy landscape of the $Au_{20}(SCH_2CH_2Ph)_{16}$ by changing the orientation of the S-R ligand based on the GA/MM calculations. (1) The first 3000 conformations; (2) The last several thousand conformations have the same ligand orientations, indicating the structural search converges to a lowest-energy configuration.

Table S3. The orientation of the R groups in the isomers A, B, C and D.

Au_{20}-Forcite	S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8	S_9	S_{10}	S_{11}	S_{12}	S_{13}	S_{14}	S_{15}	S_{16}
Iso1-A	a	a	a	b	a	a	a	b	a	b	b	a	a	b	b	b
Iso1-B	a	a	b	a	a	a	a	b	b	b	a	b	a	b	b	b
Iso1-C	b	a	b	a	b	a	a	b	b	b	a	a	a	b	b	b
Iso1-D	b	a	b	a	a	a	a	b	b	b	a	a	a	b	a	a

Table S4. Relative energies of the isomers isomers A, B, C and D basing on the DFT-D calculation.

$Au_{20}(SCH_2CH_2Ph)_{16}$	**ΔE (eV)**
Iso1-A	0.85
Iso1-B	1.03
Iso1-C	0.64
Iso1-D	0.00

Reference

[1] Rappe, A. K.; Casewit, C. J.; Colwell, K. S.; Goddard III, W. A.; Skiff, W. M. *J. Am. Chem. Soc.***1992**, *114*, 10024–10035.

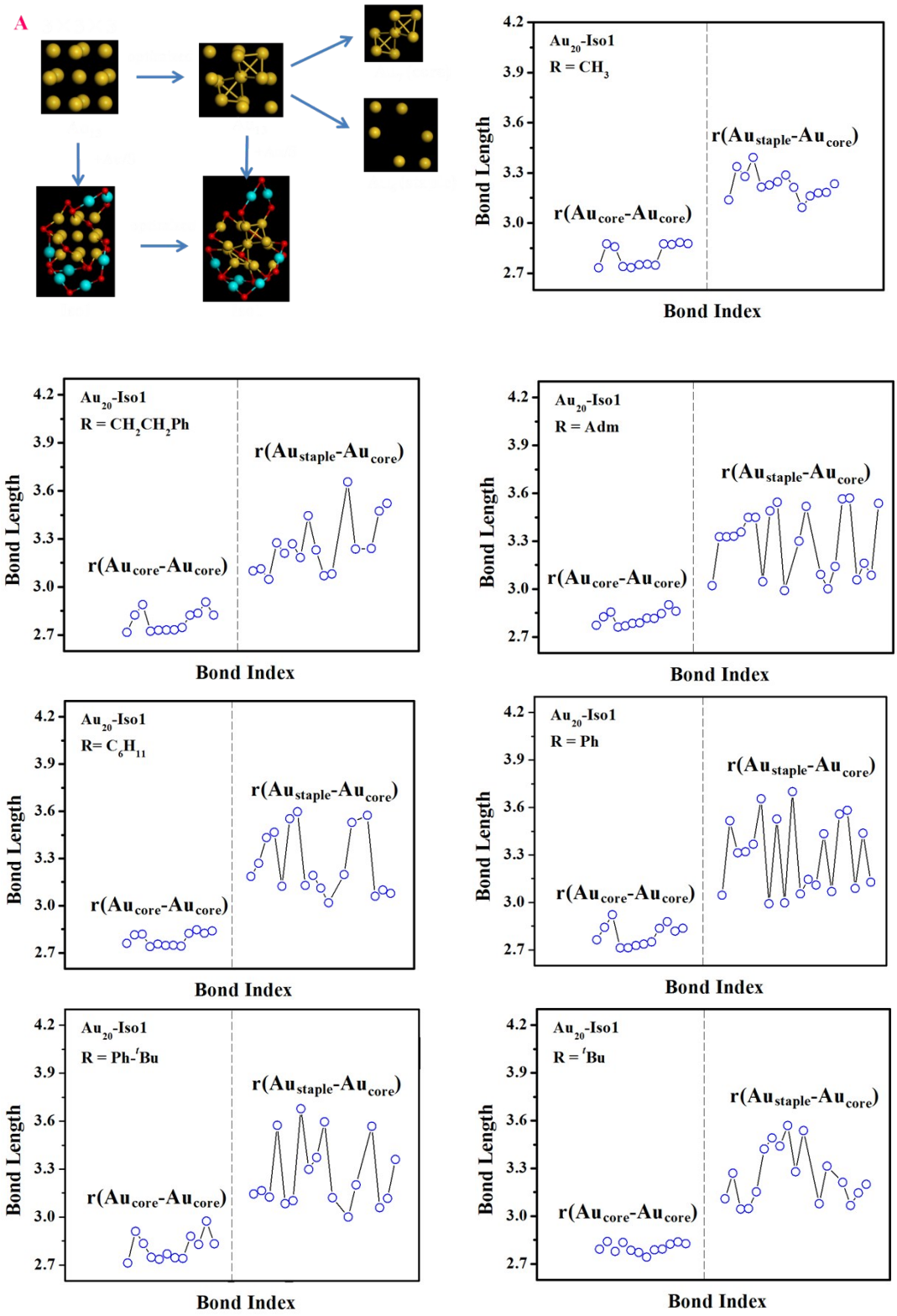


Figure S3. The Au-Au bond lengths (in unit of Å) in the 13-atom nanocrystal kernel of the **Au_{20}-Iso1** protected by different SR ligand after DFT-D optimizations.

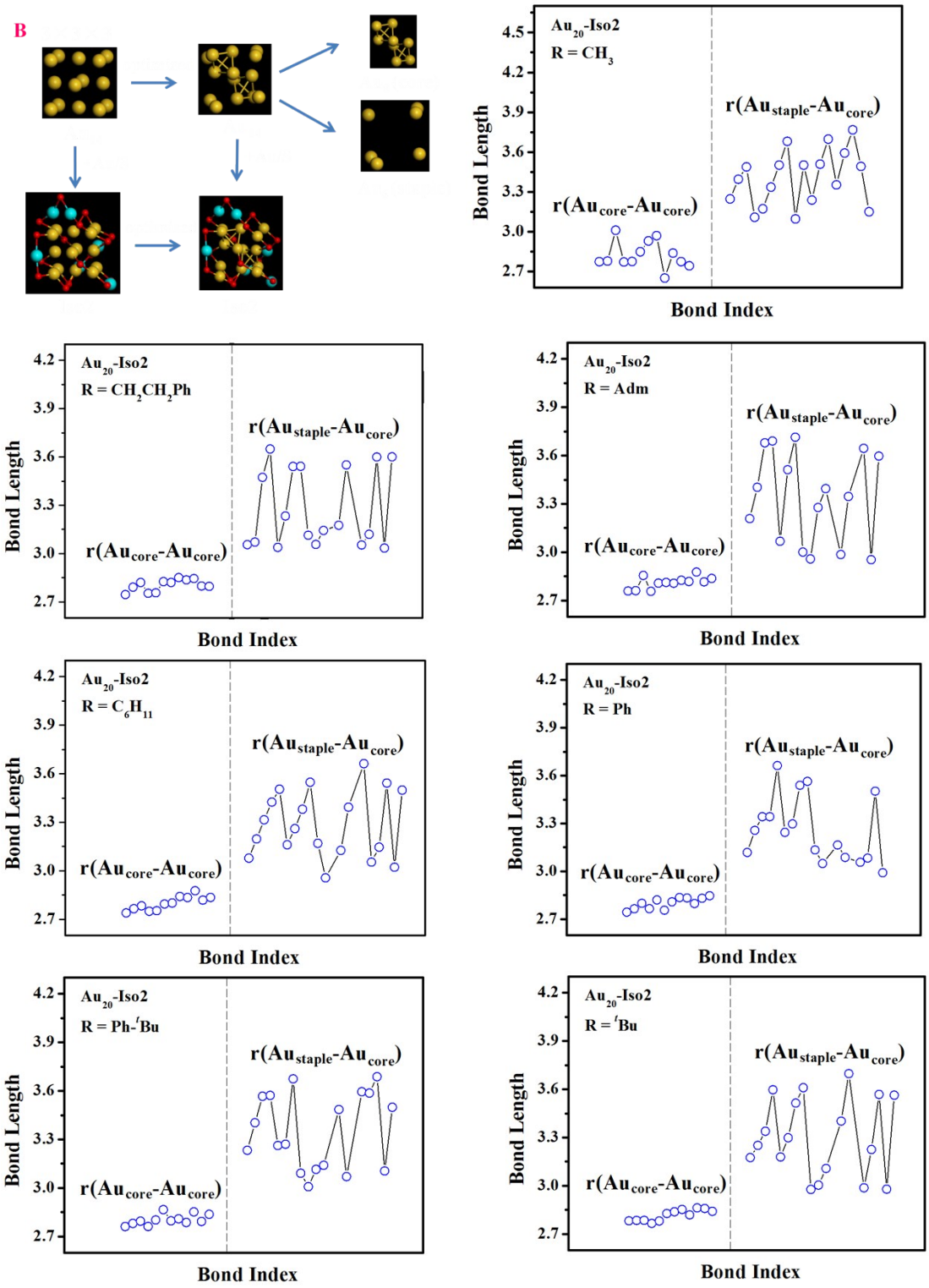


Figure S4. The Au-Au bond lengths (in unit of Å) in the 14-atom nanocrystal kernel of the **Au_{20}-Iso2** protected by different SR ligand after DFT-D optimizations.

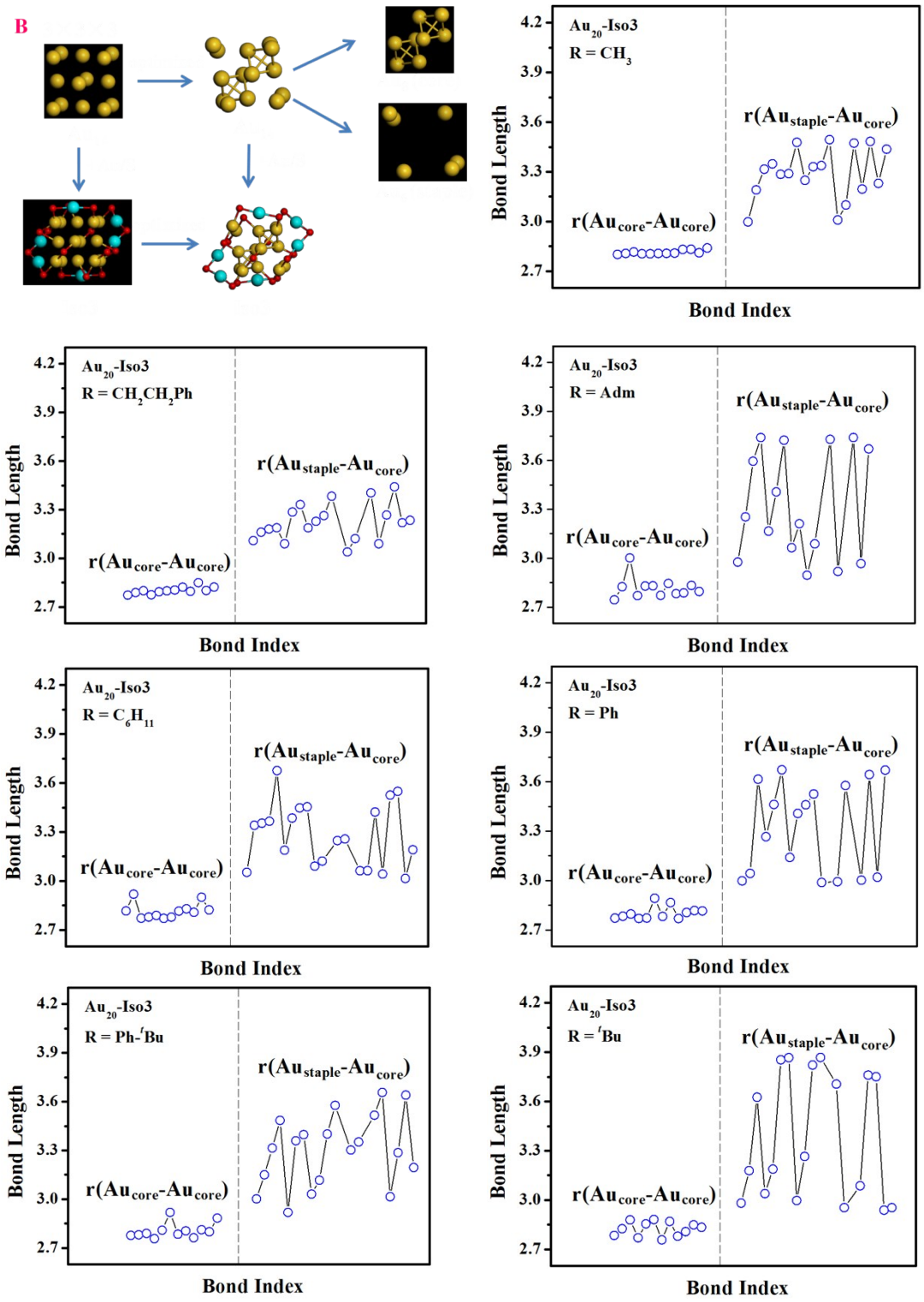
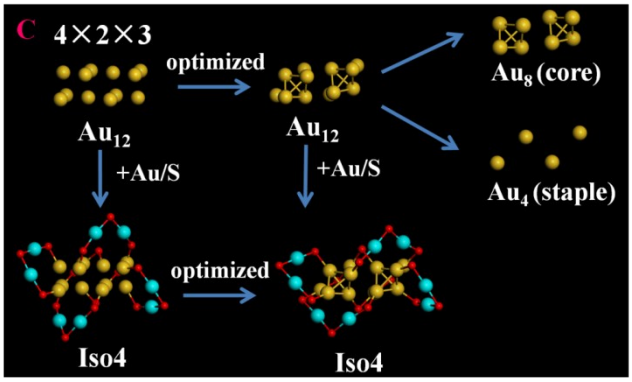
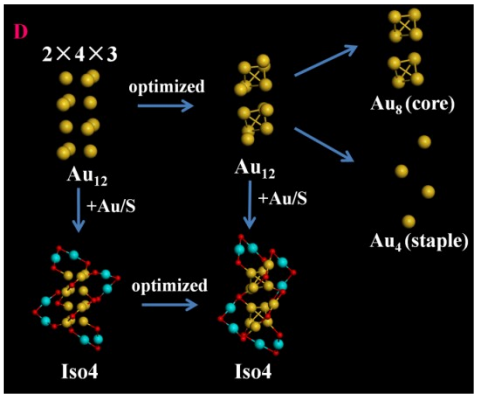
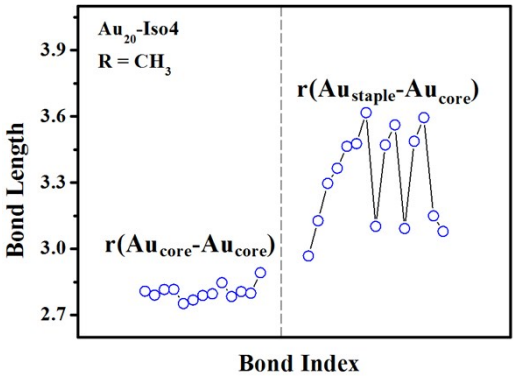
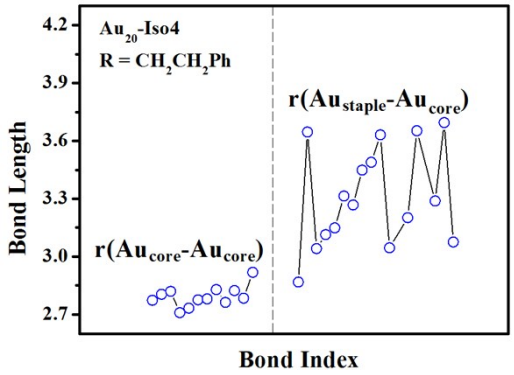


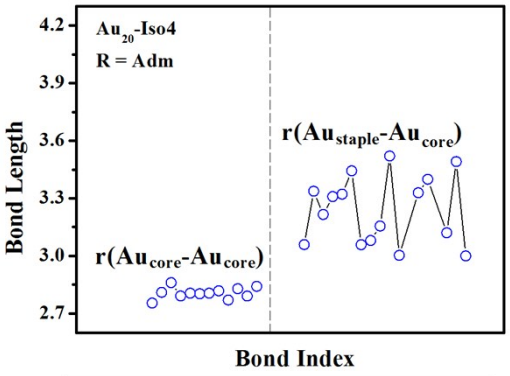
Figure S5. The Au-Au bond lengths (in unit of Å) in the 14-atom nanocrystal kernel of the **Au_{20}-Iso3** protected by different SR ligand after DFT-D optimizations.

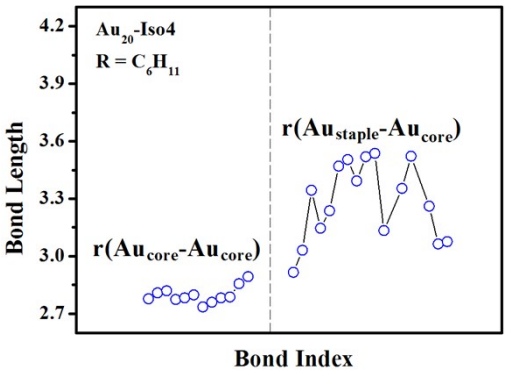

C
4×2×3
optimized
Au12
+Au/S
Au12
+Au/S
Au8 (core)
Au4 (staple)
optimized
Iso4
Iso4

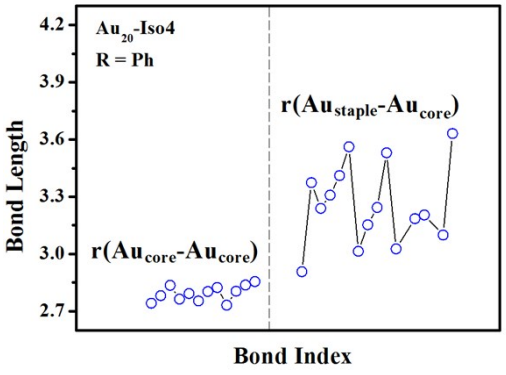

D
2×4×3
optimized
Au12
+Au/S
Au12
+Au/S
Au8 (core)
Au4 (staple)
optimized
Iso4
Iso4


Au20-Iso4
R = CH3
r(Austaple-Aucore)
r(Aucore-Aucore)
Bond Length
Bond Index


Au20-Iso4
R = CH2CH2Ph
r(Austaple-Aucore)
r(Aucore-Aucore)
Bond Length
Bond Index


Au20-Iso4
R = Adm
r(Austaple-Aucore)
r(Aucore-Aucore)
Bond Length
Bond Index


Au20-Iso4
R = C6H11
r(Austaple-Aucore)
r(Aucore-Aucore)
Bond Length
Bond Index


Au20-Iso4
R = Ph
r(Austaple-Aucore)
r(Aucore-Aucore)
Bond Length
Bond Index

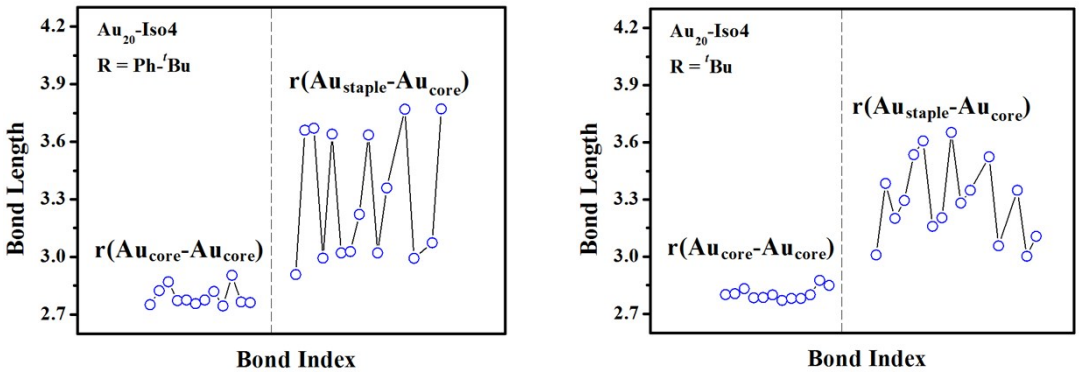


Figure S6. The Au-Au bond lengths (in unit of Å) in the 12-atom nanocrystal kernel of the **Au_{20}-Iso4** protected by different SR ligand after DFT-D optimizations.

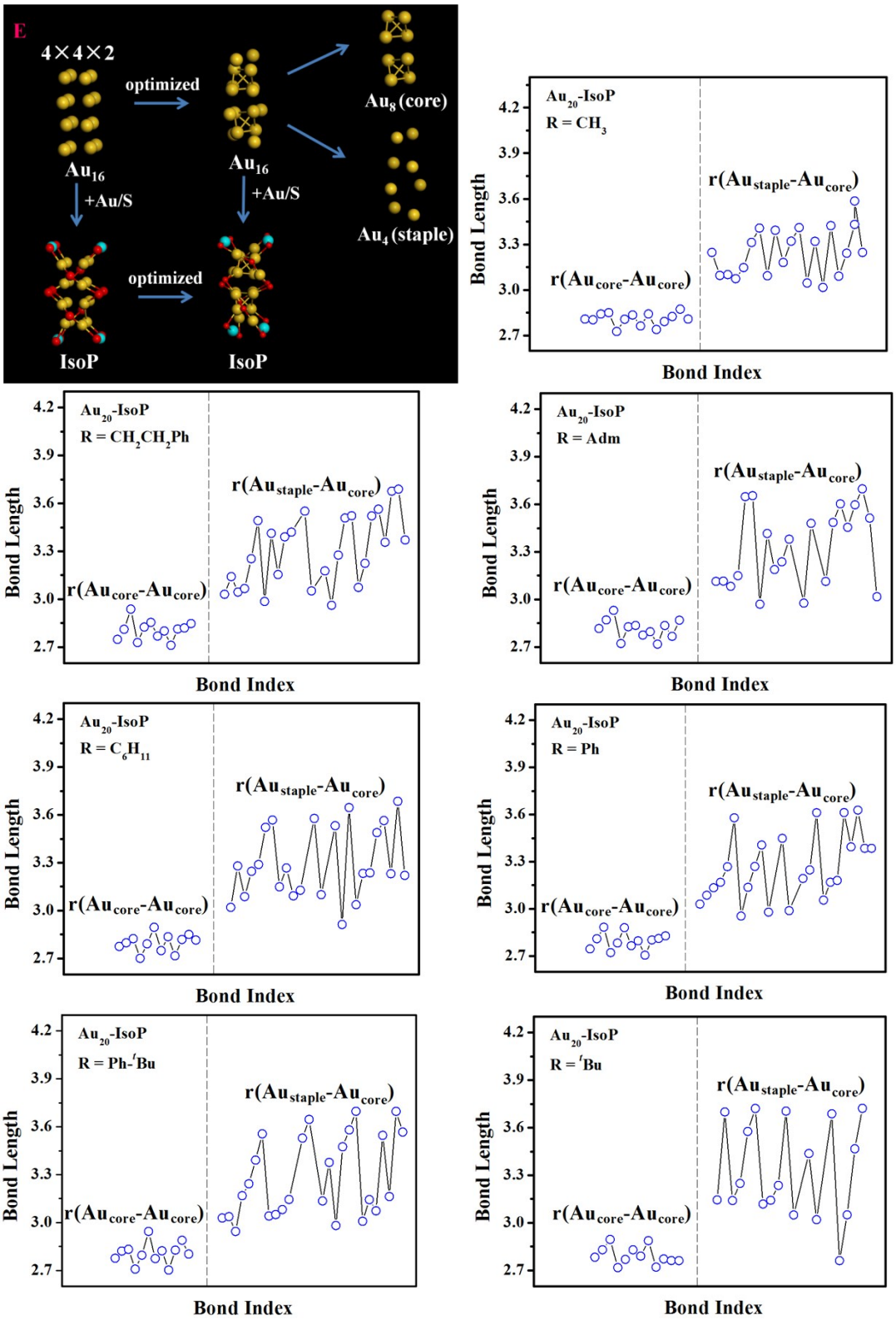
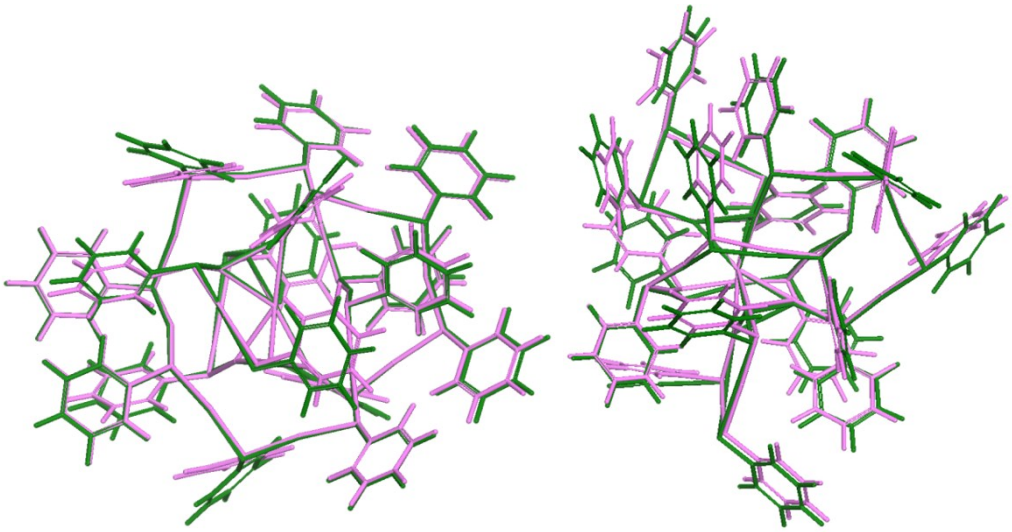
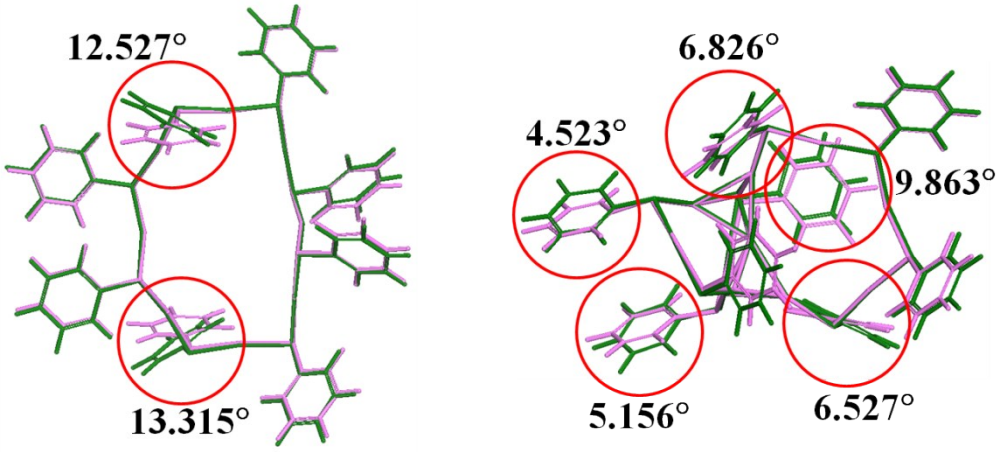


Figure S7. The Au-Au bond lengths (in unit of Å) in the 16-atom nanocrystal kernel of the **Au_{20}-IsoP** protected by different SR ligand after DFT-D optimizations.



Au_{20}-Exp. **Au_{20}-Iso1**

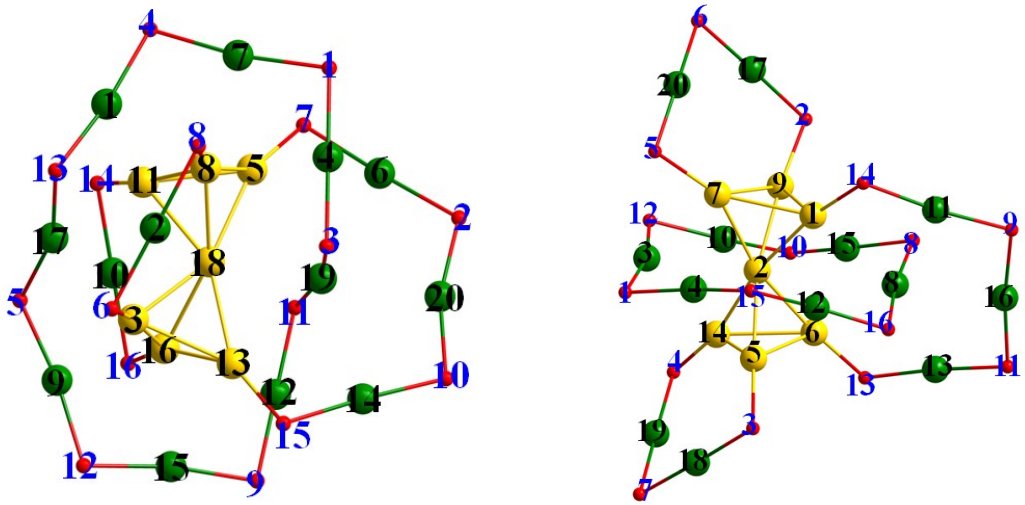
(a)



$Au_8(SPh)_8$ ring **$Au_{12}(SPh)_8$**

(b) The orientation of the phenyl rings in the Au_{20}-Exp.

Figure S8. (a) A comparison of the optimized structure of SPh protected **Au_{20}-Exp.** and **Au_{20}-Iso1** by the DFT (green color) and the DFT-D (pink color) methods. (b) Comparison of the phenyl orientations in the **Au_{20}-Exp.** optimized by the DFT and the DFT-D methods.



Au_{20}-Exp **Au_{20}-Iso1**

Figure S9. The serial number of the gold and sulfur atoms in the Au-S frameworks of the **Au_{20}-Exp.** and **Au_{20}-Iso1**. Color: S = red, Au = yellow, green.

Table S5 Comparison the bond lengths of Au-Au (in unit of Å) of the **Au_{20}-Exp.** after DFT and DFT-D optimizations. (SR = SPh). The serial number of the Au and S atoms is displayed in Figure S9.

Au_{20}-Exp.				
Au-Au		***r*(DFT-D)**	***r*(DFT)**	***Δr***
Au_3	**Au_8**	2.775	2.805	0.030
	Au_{10}	2.878	2.873	-0.005
	Au_{20}	2.754	2.768	0.014
Au_6	**Au_8**	2.750	2.772	0.022
	Au_9	2.875	2.806	-0.069
	Au_{17}	2.742	2.871	0.129
Au_8	**Au_9**	2.753	2.811	0.059
	Au_{10}	2.779	2.807	0.028
	Au_{17}	2.762	2.810	0.048
	Au_{20}	2.805	2.804	0.000
Au_9	**Au_{17}**	2.794	2.827	0.033
Au_{10}	**Au_{20}**	2.803	2.834	0.031
Average difference				0.027

Table S6. Comparison the Au-S bond lengths (in unit of Å) of **Au_{20}-Exp.** (SR = SPh) optimized by the DFT and DFT-D methods.The serial number of the Au and S atoms is displayed in the Figure S9.

Au_{20}-Exp.				
Au-S		***r*(DFT-D)**	***r*(DFT)**	***Δr***
Au_1	**S_2**	2.392	2.375	-0.017
	S_{10}	2.391	2.375	-0.016
Au_2	**S_2**	2.364	2.363	-0.001
	S_3	2.360	2.359	-0.001
Au_3	**S_4**	2.439	2.458	0.020
Au_4	**S_5**	2.347	2.358	0.011
	S_8	2.357	2.362	0.005
Au_5	**S_{10}**	2.364	2.364	0.000
	S_{11}	2.360	2.359	0.000
Au_6	**S_{12}**	2.442	2.461	0.019
Au_7	**S_{13}**	2.346	2.366	0.020
	S_{16}	2.357	2.365	0.008
Au_9	**S_1**	2.428	2.438	0.010
Au_{10}	**S_9**	2.427	2.439	0.012
Au_{11}	**S_5**	2.397	2.410	0.012
	S_{13}	2.395	2.409	0.014
Au_{12}	**S_6**	2.341	2.348	0.007
	S_7	2.340	2.343	0.003
Au_{13}	**S_{14}**	2.342	2.349	0.006
	S_{15}	2.340	2.345	0.005
Au_{14}	**S_7**	2.351	2.359	0.007
	S_{15}	2.351	2.358	0.007
Au_{15}	**S_1**	2.362	2.354	-0.008
	S_4	2.361	2.361	0.001
Au_{16}	**S_3**	2.357	2.355	-0.002
	S_8	2.362	2.363	0.000
Au_{17}	**S_6**	2.417	2.415	-0.001
Au_{18}	**S_9**	2.360	2.354	-0.006
	S_{12}	2.362	2.358	-0.004
Au_{19}	**S_{11}**	2.357	2.355	-0.001
	S_{16}	2.362	2.361	-0.001
Au_{20}	**S_{14}**	2.416	2.416	0.000
Average difference				0.003

Table S7. Comparison the bond lengths (in unit of Å) of Au-Au of the **Au_{20}-Iso1** (SR = SPh) after DFT and DFT-D optimizations. The serial number of the Au and S atoms is displayed in the Figure S9.

Au_{20}-Iso1				
Au-Au		***r*(DFT-D)**	***r*(DFT)**	***Δr***
Au_1	**Au_2**	2.712	2.745	0.032
	Au_7	2.934	2.871	-0.063
	Au_9	2.839	2.860	0.021
Au_2	**Au_5**	2.739	2.757	0.018
	Au_6	2.707	2.755	0.048
	Au_7	2.754	2.775	0.020
	Au_9	2.748	2.764	0.015
	Au_{14}	2.755	2.768	0.014
Au_5	**Au_6**	2.878	2.892	0.014
	Au_{14}	2.799	2.851	0.052
Au_6	**Au_{14}**	2.901	2.883	-0.019
Au_7	**Au_9**	2.803	2.860	0.057
Average difference				0.017

Table S8. Comparison the Au-S bond lengths (in unit of Å) of **Au_{20}-Iso1**(SR = SPh) after the geometric optimization by DFT and DFT-D methods. The serial number of the Au and S atoms is displayed in the Figure S9.

Au_{20}-Iso1				
Au-S		***r*(DFT-D)**	***r*(DFT)**	***Δr***
Au_1	**S_{14}**	2.394	2.405	0.011
Au_3	**S_1**	2.342	2.345	0.004
	S_{12}	2.348	2.341	-0.007
Au_4	**S_1**	2.341	2.354	0.014
	S_{15}	2.338	2.341	0.003
Au_5	**S_3**	2.421	2.425	0.004
Au_6	**S_{13}**	2.404	2.415	0.011
Au_7	**S_5**	2.421	2.431	0.010
Au_8	**S_8**	2.367	2.376	0.008
	S_{16}	2.360	2.370	0.010
Au_9	**S_2**	2.421	2.427	0.006
Au_{10}	**S_{10}**	2.342	2.342	0.000
	S_{12}	2.339	2.342	0.003
Au_{11}	**S_9**	2.351	2.359	0.008
	S_{14}	2.336	2.347	0.011
Au_{12}	**S_{15}**	2.359	2.354	-0.005
	S_{16}	2.347	2.352	0.004
Au_{13}	**S_{11}**	2.353	2.361	0.008

	S_{13}	2.334	2.348	0.013
Au_{14}	S_4	2.421	2.432	0.011
Au_{15}	S_8	2.329	2.340	0.011
	S_{10}	2.360	2.360	0.000
Au_{16}	S_9	2.346	2.351	0.005
	S_{11}	2.356	2.358	0.002
Au_{17}	S_2	2.318	2.330	0.012
	S_6	2.362	2.363	0.001
Au_{18}	S_3	2.323	2.330	0.007
	S_7	2.363	2.364	0.001
Au_{19}	S_4	2.333	2.338	0.004
	S_7	2.360	2.361	0.002
Au_{20}	S_5	2.337	2.342	0.005
	S_6	2.366	2.368	0.002
Average difference				0.006

XYZ coordinates of four$Au_{20}(SCH_3)_{16}$ isomers

Au_{20}-Iso1

S	36.233280380	5.043973913	-1.853683462
Au	33.299944202	3.107029534	-6.623204634
Au	32.950552595	3.438401699	-3.933832115
Au	34.066389178	5.908765561	-2.090749908
Au	36.326332596	3.479280211	-3.596986899
Au	34.083821083	1.421449428	-2.466062756
Au	31.292962963	1.408329528	-3.157717553
Au	34.283502962	5.442215005	-5.264512343
Au	31.362403019	0.429030517	-6.163274348
Au	31.455674457	5.037988914	-5.603945133
Au	30.486670907	5.627400709	-2.633069673
Au	32.424437978	0.625612127	-9.255249483
Au	34.945816163	0.694340450	-5.475787796
Au	29.450422224	-1.575299517	-4.380194264
Au	32.308022446	3.331939415	-1.264572598
Au	29.168684176	2.994311827	-4.750503513
Au	30.191059695	-2.014744566	-7.943540491
Au	31.259829720	8.057838141	-7.375337170
Au	35.181261016	0.352265139	0.639071981
Au	33.168849632	2.511655150	1.937179047
Au	34.384811382	8.526352936	-6.724720320
S	29.832597982	6.277243230	-6.891229620
S	35.422272899	-0.370920017	-1.565489725
S	31.520877236	3.840017392	0.954098789
S	35.876635910	7.247319335	-5.454897210
S	32.755359514	9.817632162	-7.836050208
S	34.871066099	1.153972354	2.829945648
S	29.309995703	1.535538356	-6.580888768
S	30.978288182	-1.086239778	-9.951087696
S	28.510234802	4.415961926	-2.997797637
S	29.311093304	-3.165381171	-6.099366191
S	32.114660601	7.209331684	-2.047736260
S	29.537224211	-0.118220196	-2.553769940
S	33.918023778	2.373910945	-8.817598619
S	36.939731281	1.908115941	-5.226392201
S	33.304753497	-0.910040799	-5.946910182
C	33.326648291	3.744748606	-9.889625834
H	33.505227953	3.467056482	-10.940283888
H	32.259683250	3.949392161	-9.732495173
H	33.911240798	4.641980556	-9.636066892
C	33.143888542	9.638944360	-9.624843175

H	34.026796947	10.257791249	-9.843622408
H	33.342965526	8.593575482	-9.894686259
H	32.281932782	10.013676595	-10.197799046
C	28.284456443	3.366958180	-1.513111706
H	27.420605176	2.710302704	-1.694230079
H	29.178382241	2.764214105	-1.312413597
H	28.080556547	4.034259343	-0.662118187
C	32.241752666	8.372686276	-3.456953162
H	31.312680487	8.962137905	-3.490682275
H	33.095893162	9.040629119	-3.268905345
H	32.384866819	7.842476085	-4.406343137
C	37.172534547	-0.027626165	-1.995760280
H	37.811255049	-0.676343886	-1.377658731
H	37.309276791	-0.274141253	-3.059645372
H	37.429829896	1.027294572	-1.830346875
C	33.994481269	-0.192563090	3.724727808
H	33.641300085	0.215889241	4.683808164
H	33.144440176	-0.576174029	3.145458172
H	34.715731305	-1.002705922	3.913011862
C	32.008345107	5.568337273	1.331513344
H	31.864362873	5.739349514	2.408982459
H	33.052108596	5.764091010	1.051582380
H	31.346527359	6.232902123	0.757314213
C	29.550460115	2.594535338	-8.055488768
H	28.629328078	3.177026669	-8.207548619
H	30.402579519	3.272919977	-7.922367748
H	29.724872793	1.931547584	-8.917169719
C	33.139177075	-1.898998033	-4.414273200
H	32.943639449	-1.257699401	-3.546113359
H	32.306667340	-2.605386707	-4.560515566
H	34.080344201	-2.450167977	-4.266773467
C	37.134047681	6.660814117	-6.657551387
H	37.759375354	7.518521506	-6.950349224
H	37.753748376	5.909718158	-6.144335203
H	36.671186540	6.213696841	-7.546810789
C	28.578174825	6.960755630	-5.741277923
H	27.974462624	7.701279038	-6.288937952
H	27.938005905	6.126705421	-5.415752230
H	29.044929439	7.425634046	-4.863031725
C	32.121157354	-2.368097219	-10.605878076
H	31.521859509	-3.252431328	-10.869655653
H	32.600520163	-1.962948889	-11.509858173
H	32.884700712	-2.640130840	-9.866092896
C	36.232920156	4.068544464	-0.301790847

H	35.425160861	3.326635331	-0.290713111
H	37.208068036	3.564854305	-0.217924280
H	36.107992781	4.771389596	0.536532502
C	30.307296010	-1.104461093	-1.207965341
H	29.596868564	-1.886242753	-0.898873648
H	31.252542752	-1.560651472	-1.530775476
H	30.499434132	-0.420875703	-0.366552815
C	27.511343666	-3.258427866	-6.460268935
H	27.373705887	-3.895421059	-7.346703793
H	27.018850556	-3.721322548	-5.592172188
H	27.086986022	-2.262308474	-6.644739457
C	37.184429453	2.822054497	-6.794799037
H	36.339491547	3.492097275	-6.998729184
H	38.119555959	3.395004705	-6.704217403
H	37.277398699	2.083631037	-7.604974006

Au_{20}-Iso2

S	2.898768518	6.543832254	25.273075359
Au	4.162208192	7.975662130	21.030516596
Au	4.399008182	5.577763069	23.626292159
Au	1.502133063	7.630525669	23.743239645
Au	4.273172941	5.828208639	19.251481536
Au	4.347321596	3.686382055	21.486089726
Au	6.384176054	3.619636732	23.441883356
Au	2.292849702	5.908010544	21.289382461
Au	6.592666577	8.177280801	23.540253085
Au	2.143699426	7.738018953	19.149765865
Au	6.274895436	5.767872437	21.596204972
Au	4.382142012	2.799594773	25.665385043
Au	7.092804533	3.461840881	18.511540226
Au	1.777141364	3.094075966	23.280584730
Au	6.849022739	5.429560691	25.827452029
Au	3.727489357	10.276378001	18.573228301
Au	1.101927679	10.009540151	20.977397263
Au	8.512333080	2.164731068	21.578190776
Au	6.562696702	7.886347271	18.786675830
Au	2.346657441	2.612135922	18.547838028
Au	0.863154746	5.644547811	17.068801207
S	9.015185364	2.353820435	19.297375520
S	2.121441972	11.639061116	19.619792939
S	0.430361498	4.703288372	22.243629428
S	8.240004110	6.911560692	24.650865794

S	3.414768605	1.729082564	20.429910326
S	8.004984949	6.553544922	20.080064463
S	-0.149353027	8.593836227	22.366837306
S	5.261738063	9.097079856	17.242202446
S	5.644215882	3.998451562	27.252588313
S	1.301386886	3.389757301	16.592000748
S	8.048618791	1.931014199	23.876089897
S	5.134174134	4.338585860	17.567781765
S	3.006945694	1.405756679	24.368559904
S	0.480132354	7.938194524	17.428192861
S	5.152302530	9.683885719	22.455024732
C	-0.354229334	3.841672770	20.826004795
C	1.833714210	0.741795988	25.621279932
C	6.926848372	2.786260049	27.765931103
C	8.854973332	8.053248669	25.955720165
C	6.294152848	10.632127420	21.374134356
C	9.114196055	7.706195894	20.975182637
C	6.393864029	10.393002075	16.601566020
C	3.036088379	12.668003260	20.835802455
C	-1.029777710	9.769668018	23.472977573
C	3.829378849	7.872021591	26.128133359
C	-1.096092131	8.002724077	18.372105390
C	-0.366109100	2.617511772	16.616119391
C	4.837026571	0.790896658	19.749508116
C	7.087116604	0.368684982	23.998693639
C	10.336417266	3.627962979	19.237460769
C	5.717395185	5.364679990	16.165301415
H	0.392474126	3.333339821	20.196311681
H	-0.874005517	4.605411967	20.226465774
H	-1.081451135	3.115954284	21.221092261
H	2.395443910	0.093833006	26.310513016
H	1.075414692	0.144881809	25.091037153
H	1.346656545	1.549774563	26.182419538
H	7.482293795	2.407193391	26.896498906
H	6.423154526	1.958034842	28.286159667
H	7.617112992	3.291877670	28.458596198
H	9.393134627	8.877029468	25.463164439
H	9.550826047	7.490790335	26.596605700
H	8.030281645	8.453159206	26.560360440
H	5.679923977	11.255279844	20.705584199
H	6.908302645	9.961053106	20.756986333
H	6.930620570	11.269783802	22.007519588
H	9.746777239	8.224445864	20.236891452
H	9.741222745	7.102492442	21.648715740

H	8.546997152	8.430568619	21.577564125
H	5.810519070	11.056403132	15.946383635
H	7.181027137	9.894547964	16.014813295
H	6.849370759	10.975145846	17.413451094
H	3.751913313	13.300261760	20.288406421
H	3.559640028	12.047343512	21.576001034
H	2.299257269	13.308107136	21.346752541
H	-1.562411009	9.176593763	24.232398769
H	-1.754268726	10.334364193	22.866484314
H	-0.331794187	10.461227551	23.963207628
H	4.316164938	8.552231268	25.415842450
H	4.595712939	7.385568406	26.752949579
H	3.122787306	8.426830240	26.765407553
H	-1.113783120	7.260821397	19.179908103
H	-1.925847302	7.823977464	17.669925108
H	-1.183304214	9.011146639	18.804903026
H	-0.238078838	1.535005484	16.469319982
H	-0.949801953	3.035001659	15.781611591
H	-0.884576357	2.803824452	17.565606233
H	5.458062965	1.414105031	19.089777465
H	4.442925280	-0.074622686	19.194311167
H	5.443243404	0.445601774	20.600974643
H	7.789725030	-0.475664225	23.919419841
H	6.325693843	0.302571695	23.212252830
H	6.591723633	0.356394424	24.981929797
H	10.605935598	3.780582055	18.180767576
H	11.206800192	3.242631524	19.789893984
H	9.991601890	4.575705664	19.673424394
H	4.838044597	5.866414729	15.735729897
H	6.167640716	4.693152995	15.417634400
H	6.447345460	6.117221285	16.494310831

Au_{20}-Iso3

S	4.801358023	9.657361350	22.228759884
Au	4.107032178	7.667990301	21.063980558
Au	4.525493220	5.407856122	23.454104862
Au	4.292915878	5.855220814	18.917029142
Au	4.738349052	3.594718103	21.321841408
Au	6.769505464	3.732816431	23.291336937
Au	2.395481787	5.446135143	20.947969357
Au	6.333015615	8.379233518	23.461724641
Au	2.097215291	7.594176069	19.113898680

Au	6.451963168	5.844223662	21.462619415
Au	5.136432047	2.609530142	25.593782964
Au	6.998836350	3.312668872	18.150459466
Au	2.453946358	2.863854042	23.285698263
Au	-0.162527666	8.644597833	21.023751485
Au	7.139478100	5.554549544	25.735433616
Au	3.950472948	8.738340453	16.951693510
Au	1.241698484	7.224714068	24.049159251
Au	8.500926270	1.934885459	21.236070728
Au	6.601042570	8.458623238	19.237055477
Au	2.485607211	3.163313167	18.713496784
Au	1.702934231	5.935812634	16.633017196
S	8.535954221	1.706295615	18.909317153
S	0.411268526	9.321930249	18.842242850
S	0.825123580	4.334964150	22.434739010
S	8.111942503	7.386310729	24.638772333
S	4.241997143	1.917735764	19.658638620
S	8.079757416	6.792898504	19.970723455
S	3.206162303	6.567962325	25.138595360
S	5.187180664	10.137934154	18.384187946
S	6.369274716	3.849872906	27.162938563
S	0.596911339	4.184525684	17.742198834
S	-0.816985524	7.923557688	23.151653514
S	8.579158083	2.153921215	23.579929127
S	5.518756407	4.796399478	17.112342501
S	3.888356835	1.214448090	24.179921381
S	2.762361730	7.552268571	15.297566141
C	3.374394399	0.546188929	20.514227454
C	-0.306369910	3.257873178	21.453352885
C	0.143318871	3.044742903	16.371860614
C	1.400725193	8.712140530	14.880599649
C	6.627082457	6.035285524	16.336739073
C	9.304245714	7.689832928	21.001240127
C	6.267469838	11.082114422	17.233473629
C	7.645835249	0.127882522	18.603665258
C	10.082328991	3.174890858	23.858045628
C	7.860186020	2.812672276	27.434889670
C	2.815985984	0.271629238	25.339096430
C	2.591576086	5.305027101	26.318641591
C	-1.197716205	9.477024510	24.057174483
C	8.384543296	8.586240596	26.005761354
C	3.438073748	10.132143269	23.360812372
C	1.387167397	10.860110521	19.098685724
H	4.110492137	0.029431551	21.149478944

H	2.986256472	-0.143841998	19.749333411
H	2.555212134	0.921270368	21.144652910
H	-0.242555029	2.223308864	21.814964578
H	-0.057086001	3.302508247	20.385170675
H	-1.325855334	3.643811500	21.613474536
H	-0.660090563	3.520211911	15.788862245
H	-0.227158192	2.108528259	16.817391128
H	1.003541484	2.834923976	15.723056209
H	0.885589006	9.055973783	15.788857073
H	0.691614939	8.182146806	14.226328720
H	1.833460670	9.567040998	14.339582707
H	6.003479641	6.868468384	15.974945167
H	7.127062227	5.545468759	15.486418578
H	7.371959209	6.415019470	17.047341141
H	9.942035262	8.288319434	20.333268032
H	9.916348733	6.939939429	21.525699956
H	8.811154676	8.337806708	21.739105097
H	5.640959651	11.807953855	16.692029021
H	6.776982758	10.421821881	16.518850553
H	7.011717171	11.620275908	17.840600035
H	8.215130250	-0.686171884	19.077093247
H	7.608157076	-0.030355225	17.514690830
H	6.625226433	0.166077292	19.006789760
H	10.105834313	4.044291384	23.188093988
H	10.964368384	2.540430122	23.681848110
H	10.074941649	3.517023369	24.904005006
H	8.274938272	2.464385979	26.478901675
H	7.565210220	1.949225971	28.051004266
H	8.602316593	3.419346979	27.976455024
H	3.462813521	-0.359210443	25.966695125
H	2.150897543	-0.366883990	24.738406573
H	2.218581815	0.940442851	25.971428295
H	3.455854250	4.907258153	26.871570784
H	2.081992776	4.485674992	25.793029197
H	1.899089454	5.799299800	27.017878926
H	-1.424226664	9.208909265	25.100309751
H	-2.082584229	9.938291123	23.593582438
H	-0.352950307	10.177956224	24.030776463
H	8.745971754	9.526627087	25.561480720
H	9.150972023	8.173520718	26.678799595
H	7.458203875	8.771758982	26.564144894
H	3.104947224	9.292063151	23.985077723
H	2.595817199	10.469905975	22.737170850
H	3.790942343	10.962949274	23.993135804

H	1.945940743	11.061498258	18.172651754
H	2.099276079	10.749012917	19.926828275
H	0.687020064	11.685807209	19.302738903

Au_{20}-Iso4

Au	14.134276997	32.468623614	47.513176064
Au	11.581426971	33.946438402	47.185669084
Au	14.111319794	34.773849442	49.131165187
Au	11.616021583	32.162594378	49.342534258
Au	11.704080470	29.731392654	47.219535036
Au	13.626063202	36.610882944	46.089092029
Au	9.571656551	32.029875351	47.439322832
Au	15.892883201	34.611468158	47.019117926
Au	11.750211012	34.856084222	51.528211156
Au	6.533963260	35.151247217	48.725097946
Au	14.201829384	32.557315617	51.808488291
Au	19.093884788	31.586737267	48.211468635
Au	9.722711810	34.202626042	49.272562045
Au	16.158547635	32.950881572	49.371856231
Au	9.119120968	32.466059516	51.758848293
Au	6.403612494	32.714659501	46.539856005
Au	16.730103330	35.239449473	51.351490272
Au	18.612899811	33.236873226	45.487697688
Au	8.861028091	29.920255217	49.462062911
Au	16.397747592	37.298075433	48.371642452
S	12.659665786	36.473768101	50.071798880
S	12.730825440	30.879934010	51.058386631
S	8.263040868	35.949663224	50.076848369
S	18.097682828	31.850629808	50.307994328
S	7.390107734	31.371928286	50.588115548
S	17.990642341	36.659463138	49.967984040
S	8.015538985	31.182255714	45.812475414
S	17.184677652	35.027887149	45.032445548
S	10.713342112	33.491392314	53.159513546
S	4.842937590	34.283605896	47.338912007
S	15.723881813	33.904771613	53.004012088
S	20.003517920	31.422187997	46.047588084
S	10.229372848	28.324074868	48.410822147
S	13.346406732	30.833728619	45.948922499
S	14.902779384	38.395906307	46.919086579
S	12.225835528	34.996613286	45.132378303
C	8.656032577	31.864992082	44.230706683

C	3.786885990	33.308022538	48.485853803
C	8.883994337	37.448466691	49.212924561
C	13.732424295	37.537211319	51.111995975
C	9.688029653	34.714839777	54.075199997
C	6.637773184	30.292733538	51.876332270
C	9.144039462	27.624932783	47.106376730
C	14.719628108	29.614295643	45.869596257
C	13.812042710	29.648541171	50.238349424
C	14.663024375	35.007478698	54.013179416
C	19.171044169	35.558962084	49.093306551
C	15.979427165	38.855074373	45.504332743
C	10.719682596	35.942860303	44.665036114
C	17.533607827	30.177571477	50.805307352
C	21.693550746	32.137897291	46.177386565
C	16.068489096	34.411824119	43.708879899
H	8.813879902	32.948491064	44.298659243
H	7.930102536	31.638427305	43.434396761
H	9.613634035	31.367208135	44.017700059
H	4.396483810	32.688972426	49.156780552
H	3.126528134	32.670691117	47.879367382
H	3.180890241	34.014945403	49.072571466
H	8.183847022	38.276166805	49.408272432
H	8.971149918	37.278753524	48.132154054
H	9.875805374	37.681228519	49.629211169
H	14.214522567	38.269727599	50.444096373
H	14.512627919	36.950969621	51.618797780
H	13.102684630	38.063225728	51.847382669
H	9.021623203	34.158990609	54.751973541
H	9.095683527	35.332233675	53.386636900
H	10.364068931	35.350670879	54.666655983
H	7.405173884	29.776827900	52.468472788
H	5.994592542	29.555008598	51.371914404
H	6.023647005	30.926990118	52.533664759
H	8.358496612	27.032856882	47.600945806
H	9.757425947	26.967451755	46.472093525
H	8.689217358	28.420991665	46.500284752
H	14.396631798	28.771770055	45.238046911
H	14.993307698	29.248485185	46.867310329
H	15.587589461	30.110723094	45.409301322
H	14.464370442	30.126451405	49.494159616
H	13.165825947	28.906480922	49.742802868
H	14.415996661	29.155402161	51.016421228
H	14.195524072	34.387668044	54.794439201
H	13.874954697	35.475047762	53.404967510

H	15.303177868	35.773197752	54.479109269
H	19.745920906	36.181113366	48.390569223
H	18.656487051	34.757107983	48.549109630
H	19.848417473	35.127117265	49.845494339
H	15.338861047	39.281364411	44.717103579
H	16.523915490	37.981309796	45.120077075
H	16.691511719	39.618488077	45.851976390
H	9.945127637	35.216625259	44.378457221
H	10.963397270	36.581947629	43.802340253
H	10.355881631	36.558281295	45.498611786
H	17.034446300	29.656123843	49.979499718
H	16.833725321	30.303469214	51.645718996
H	18.413579383	29.602911169	51.134492977
H	22.053223283	32.347369984	45.158767856
H	22.343740181	31.385733785	46.650527364
H	21.696847500	33.060857605	46.771763674
H	15.219652223	35.109166119	43.640293170
H	15.693031110	33.406260212	43.938153468
H	16.629202192	34.402565207	42.760974365