

SUPPORTING INFORMATION FOR:

**Combined Experimental and Computational
Study of the Photoabsorption of the
Monodoped and Nondoped Nanoclusters
 $\text{Au}_{24}\text{Pt}(\text{SR})_{18}$, $\text{Ag}_{24}\text{Pt}(\text{SR})_{18}$, and $\text{Ag}_{25}(\text{SR})_{18}$**

Pierpaolo D'Antoni¹, Luca Sementa², Sara Bonacchi³, Mattia Reato,³ Flavio Maran^{3,4*}, Alessandro Fortunelli^{2*}, and Mauro Stener^{1*}

¹*Dipartimento di Scienze Chimiche e Farmaceutiche, Università di Trieste, Via Giorgieri 1, I-34127 Trieste, Italy*

²*CNR-ICCOM & IPCF, Consiglio Nazionale delle Ricerche, via Giuseppe Moruzzi 1, I-56124 Pisa, Italy*

³*University of Padova, Department of Chemistry, Via Marzolo 1, I-35131 Padova, Italy*

⁴*Department of Chemistry, University of Connecticut, 55 North Eagleville Road, Storrs, Connecticut 06269, United States*

AgNO₃ (Sigma-Aldrich, ≥99.0%), HAuCl₄·3H₂O (Sigma-Aldrich, 99.9%), H₂PtCl₆·xH₂O (Alfa Aesar, 99.9%), tetra-*n*-octylammonium bromide (TOABr, Sigma-Aldrich, 98%), NaBH₄ (Sigma-Aldrich, 99%), 2,4-dimethylbenzenethiol (Sigma-Aldrich, 95%), *n*-butanethiol (Aldrich, 99.8%), dichloromethane (DCM, Sigma-Aldrich, ≥99.9%), tetrahydrofuran (THF, Sigma-Aldrich, 99.9%), toluene (Sigma-Aldrich, 99.7%), ethyl acetate (Sigma-Aldrich, 99.9%), methanol (Sigma-Aldrich, 99.8%), acetonitrile (Carlo Erba RS), hexane (Aldrich, ≥99%), pentane (Sigma-Aldrich, 99.8%), butyronitrile (Sigma-Aldrich, ≥99.0%), propionitrile (Sigma-Aldrich, 99%) were used as received.

[*n*-Oct₄N⁺][Ag₂₅(DMBT)₁₈⁻] and Au₂₄Pt(SC₄H₉)₁₈ were synthesized according to procedure described previously [1,2].

[*n*-Oct₄N⁺]₂[Ag₂₄Pt(SPhMe₂)₁₈²⁻] was synthesized according to a known procedure [3], with minor modifications. AgNO₃ (60 mg, 0.35 mmol) was dissolved in methanol (10 mL) and ethyl acetate (30 mL), and H₂PtCl₆·xH₂O (8 mg, 0.0155 mmol) dissolved in methanol (10 mL) was added. The solution was vigorously stirred for 15 min and then cooled to 0 °C in an ice bath. 2,4-dimethylbenzenethiol (0.2 mL, 1.5 mmol) and tetra-*n*-octylammonium bromide (241.96 mg, 0.44 mmol) were added under continuous stirring. After 15 min, a NaBH₄ aqueous solution (1 mmol) was added quickly under vigorous stirring. The reaction was allowed to proceed for 12 h at 0 °C, under a nitrogen atmosphere. Afterwards, the aqueous phase was removed, and the organic mixture was washed several times with methanol and then dried. [*n*-Oct₄N⁺]₂[Ag₂₄Pt(DMBT)₁₈²⁻] was stored at 4 °C in the dark.

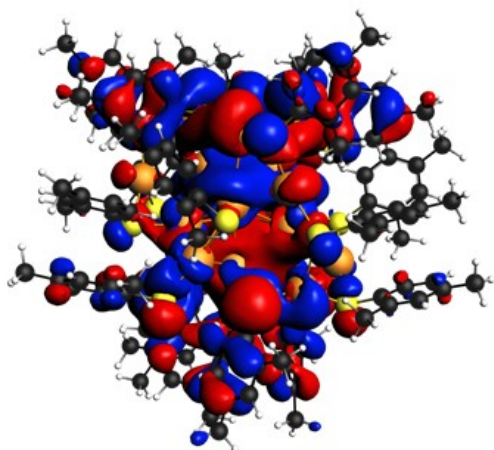
All clusters exhibit the same spectral features already described [1-4]. Figure S7-9 show a comparison of the UV-vis absorption spectra obtained at 77 and 297 K for the three clusters.

[1] M. Medves, L. Sementa, D. Toffoli, G. Fronzoni, K. R. Krishnadas, T. Bürgi, S. Bonacchi, T. Dainese, F. Maran, A. Fortunelli, M. Stener, *J. Chem. Phys.*, 2021, **155**, 084103.

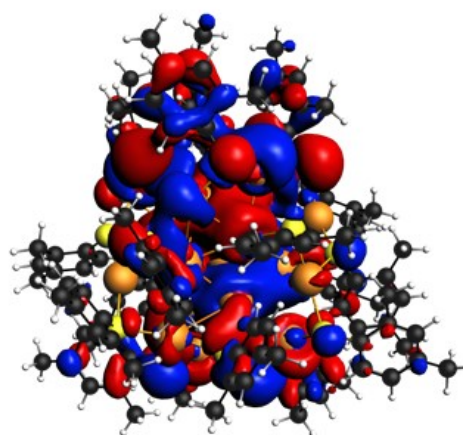
[2] W. Fei, S. Antonello, T. Dainese, A. Dolmella, M. Lahtinen, K. Rissanen, A. Venzo, and F. Maran, *J. Am. Chem. Soc.* 2019, **141**, 16033.

[3] X. Liu, J. Yuan, C. Yao, J. Chen, L. Li, X. Bao, J. Yang, and Z. Wu. *J. Phys. Chem. C* 2017, **121**, 13848.

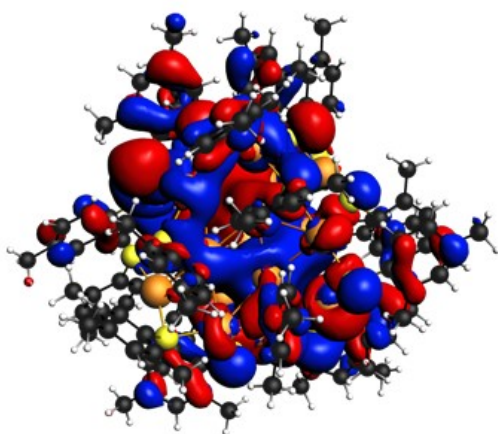
[4] M. S. Bootharaju, C. P. Joshi, M. R. Parida, O. F. Mohammed, and O. M. Bakr. *Angew. Chem. Int. Ed.* 2016, **55**, 922.



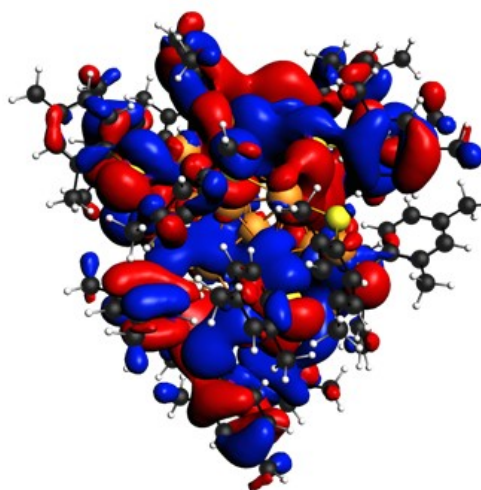
HOMO



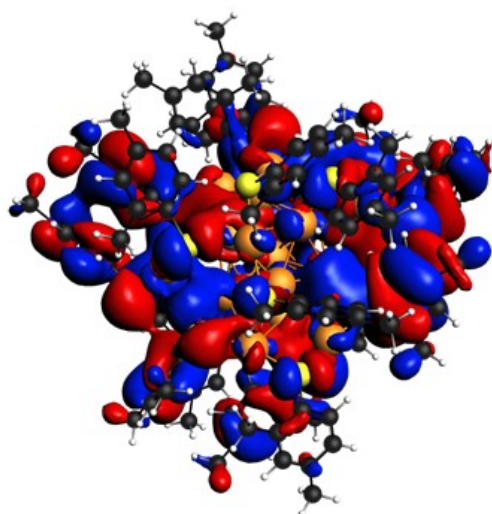
HOMO-1



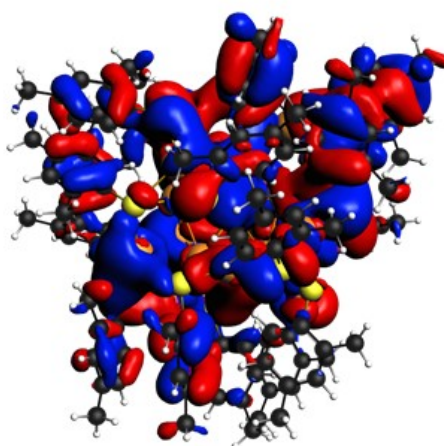
HOMO-2



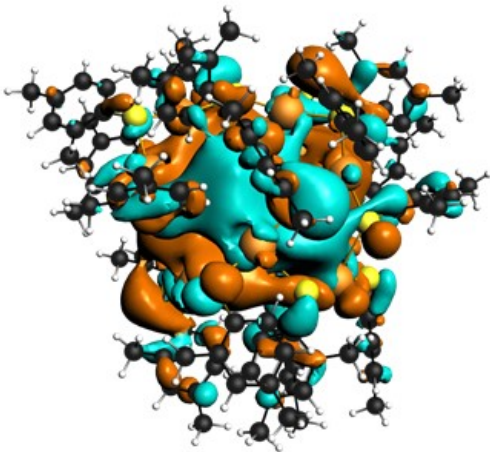
HOMO-20



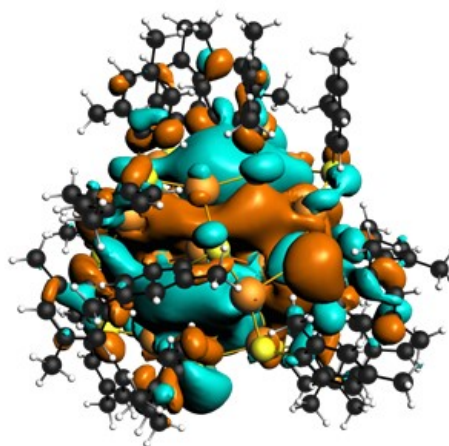
HOMO-21



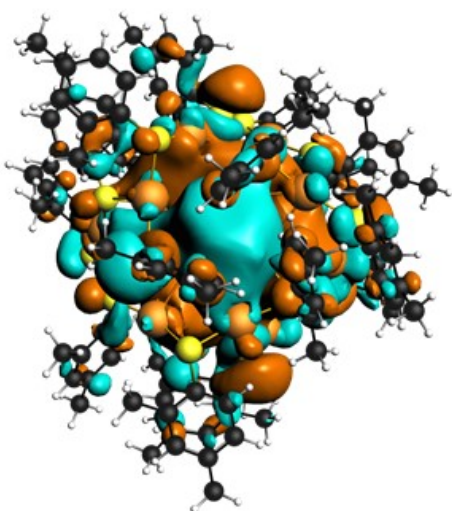
HOMO-23



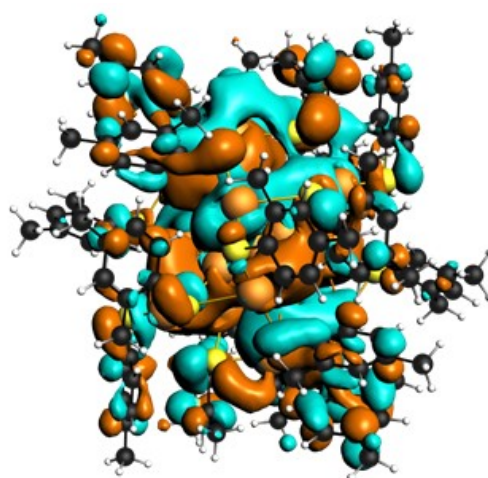
LUMO+2



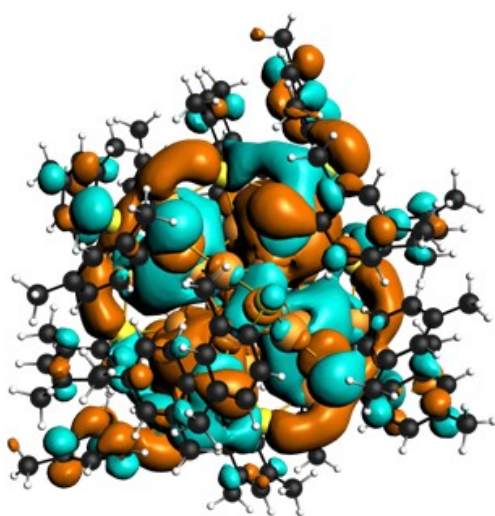
LUMO+3



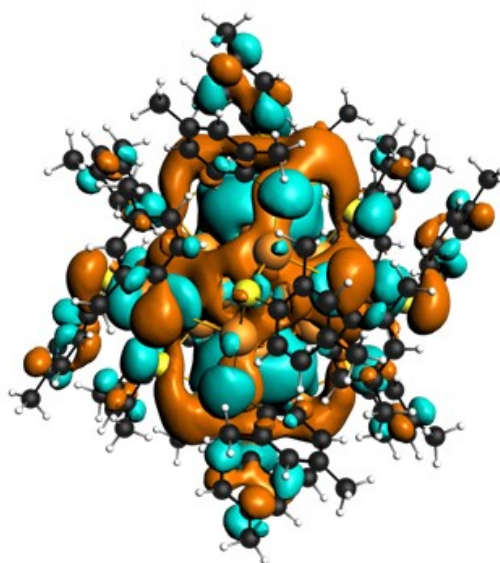
LUMO+4



LUMO+8



LUMO



LUMO+1

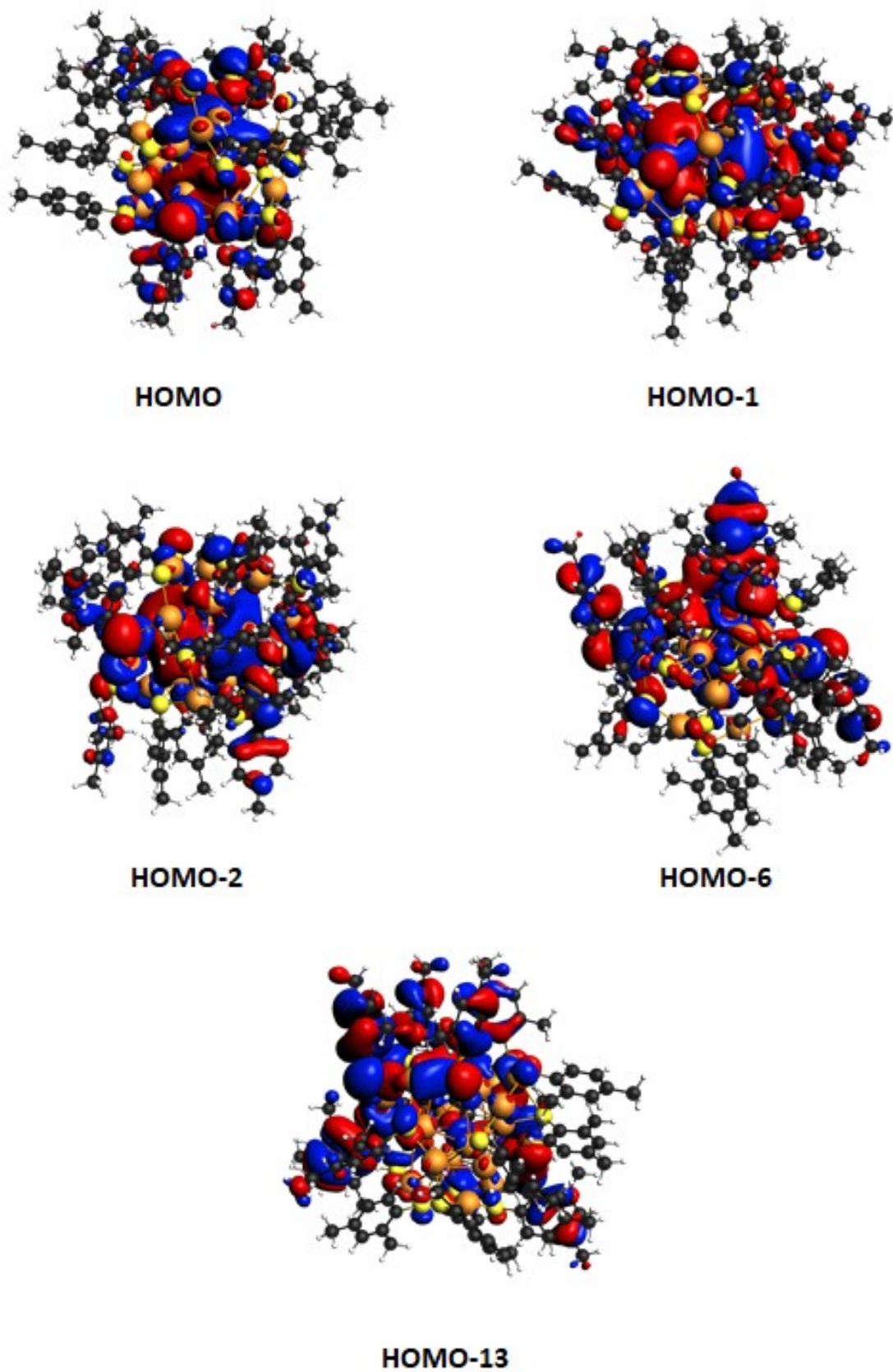


Figure S3 Occupied molecular orbital most involved in the main spectral features for $\text{Ag}_{24}\text{Pt}(\text{SR})_{18}^{2-}$.

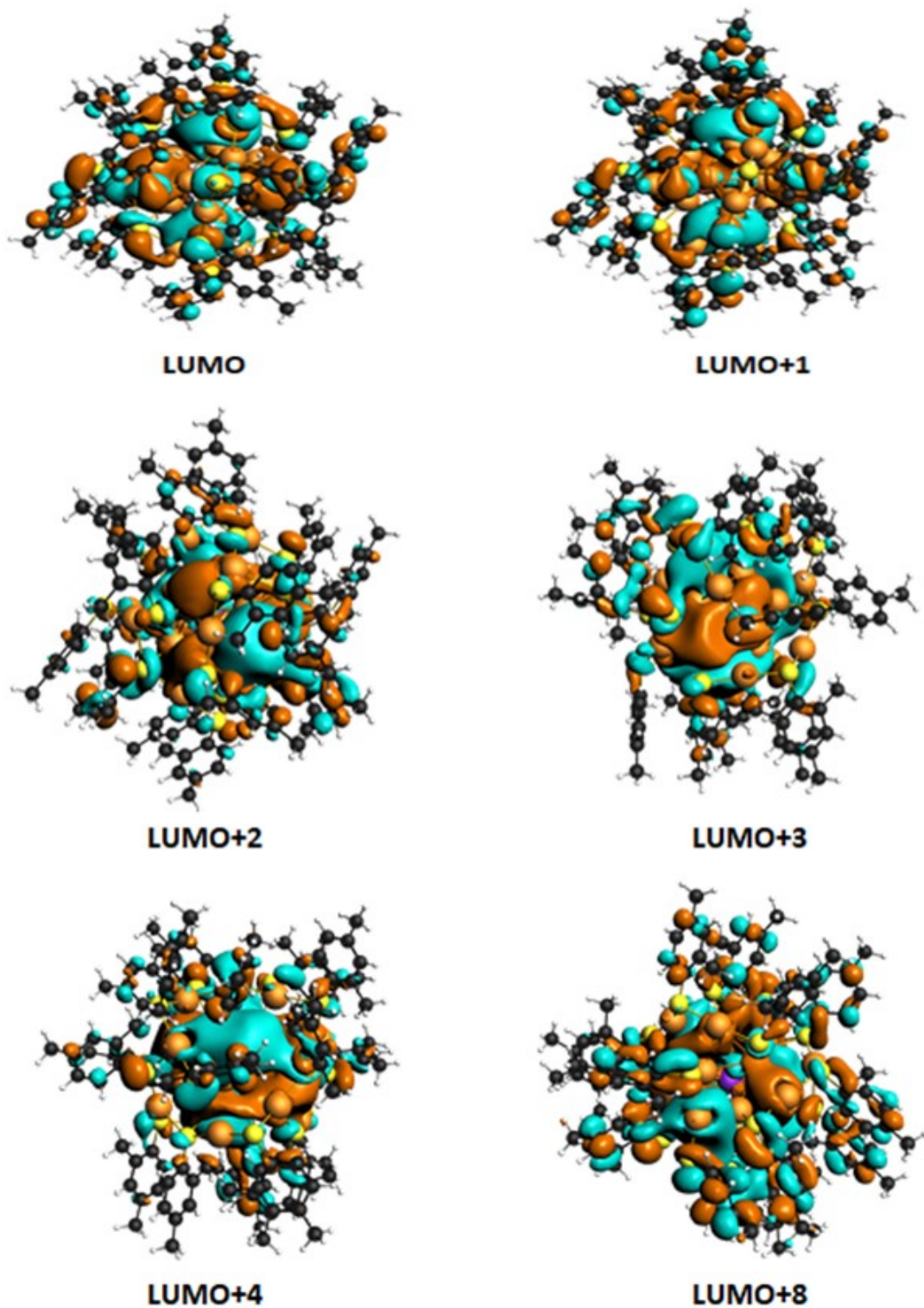
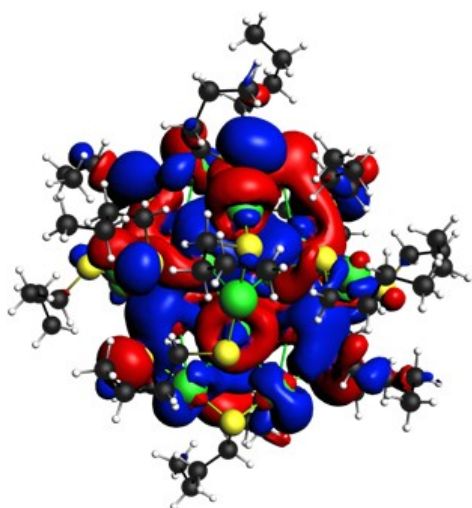
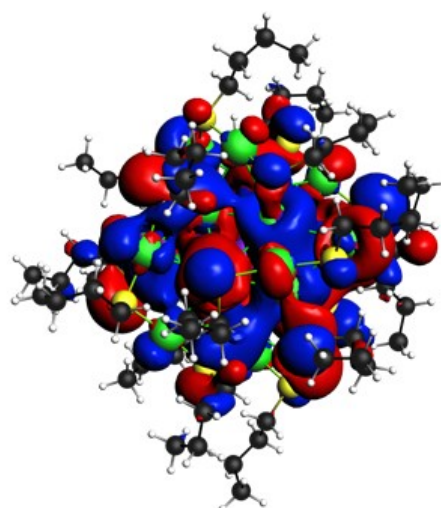


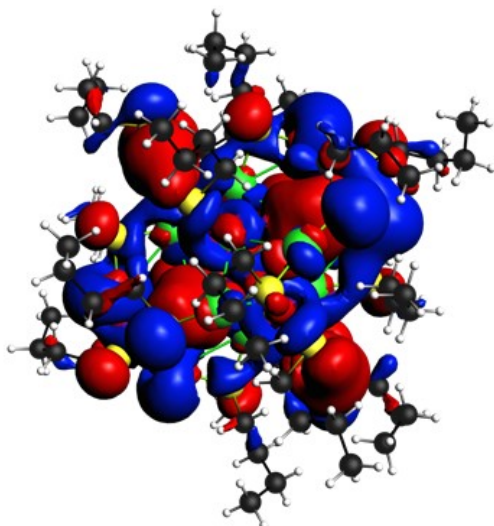
Figure S4 Virtual molecular orbital most involved in the main spectral features for $\text{Ag}_{24}\text{Pt}(\text{SR})_{18}^{2-}$.



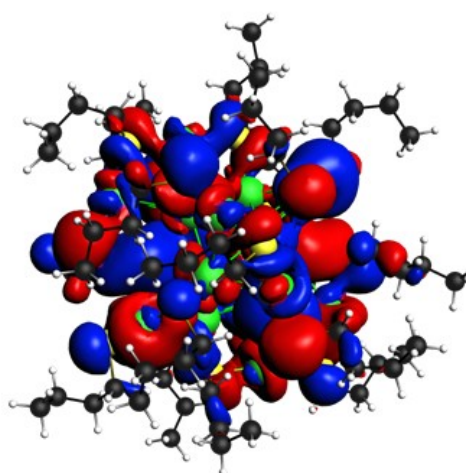
HOMO



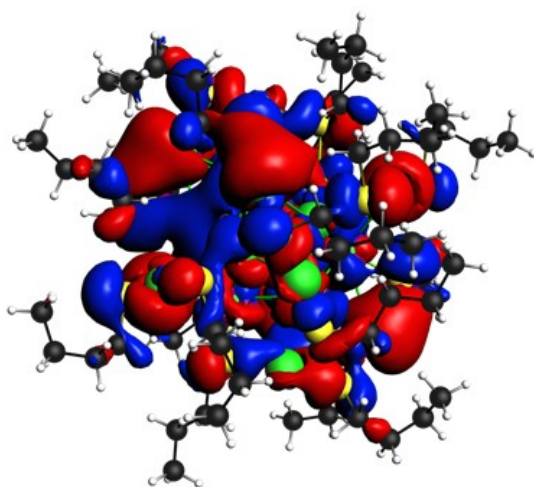
HOMO-1



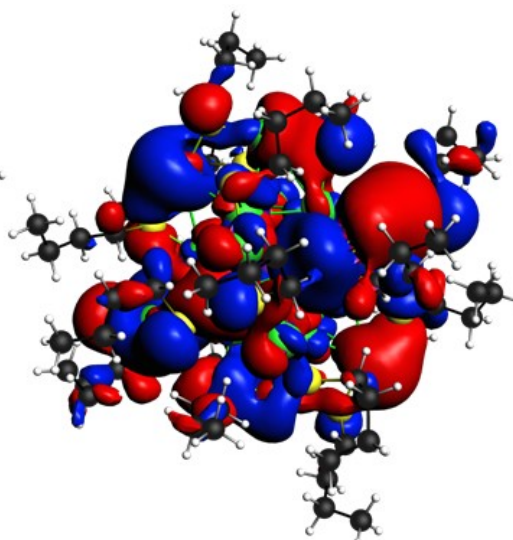
HOMO-3



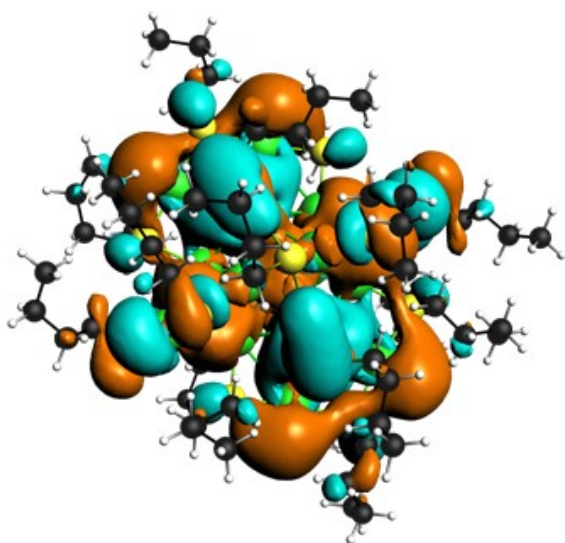
HOMO-6



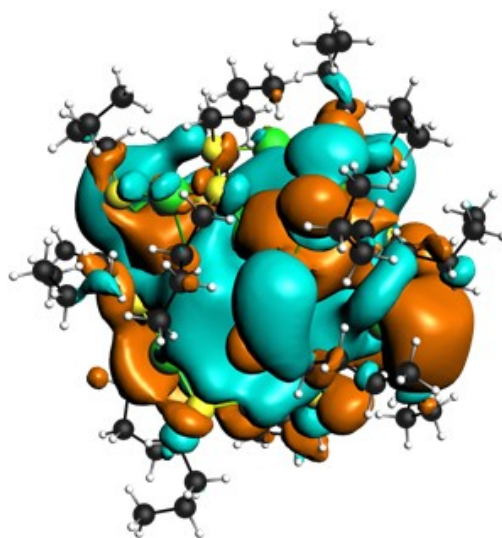
HOMO-8



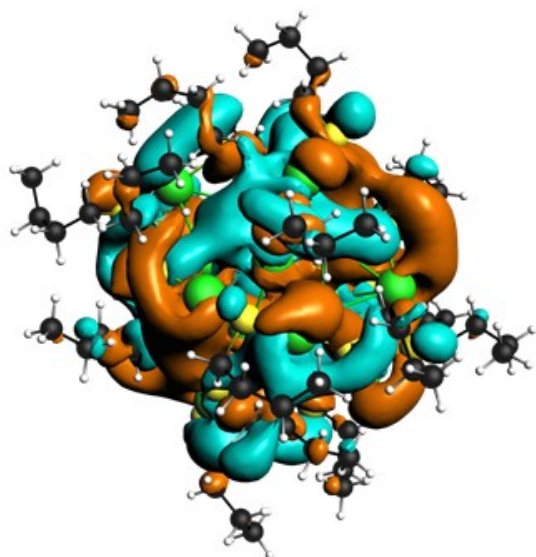
HOMO-14



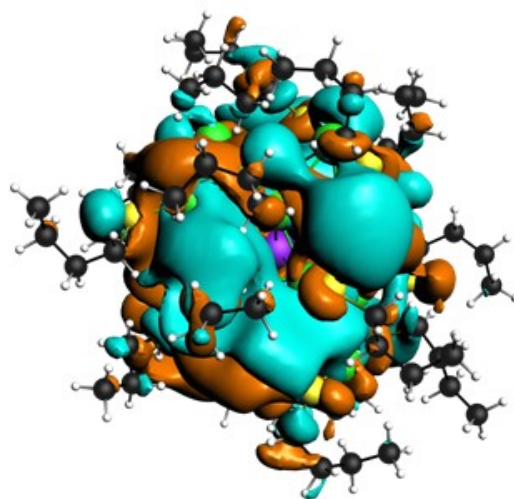
LUMO+2



LUMO+7



LUMO+8



LUMO+9

Figure S6 Virtual molecular orbital most involved in the main spectral features for $\text{Au}_{24}\text{Pt}(\text{SC}_4)_{18}$.

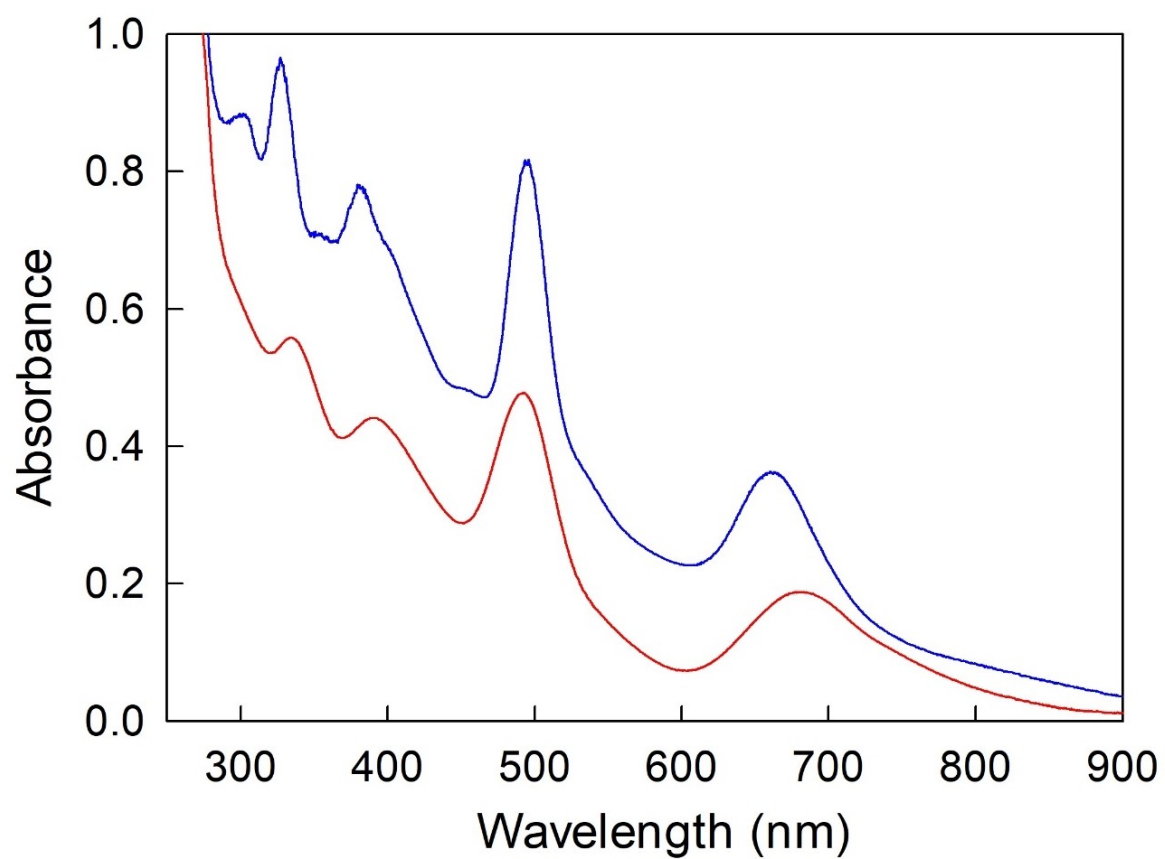


Figure S7. Comparison between room-temperature (297 K, red trace) and low-temperature (77 K, blue trace) UV-vis absorption spectra of $[\text{n-Oct}_4\text{N}^+][\text{Ag}_{25}(\text{SPhMe}_2)_{18}^-]$ in butyronitrile/propionitrile/dichloromethane (5/4/2 v/v/v) in a 1 mm cuvette.

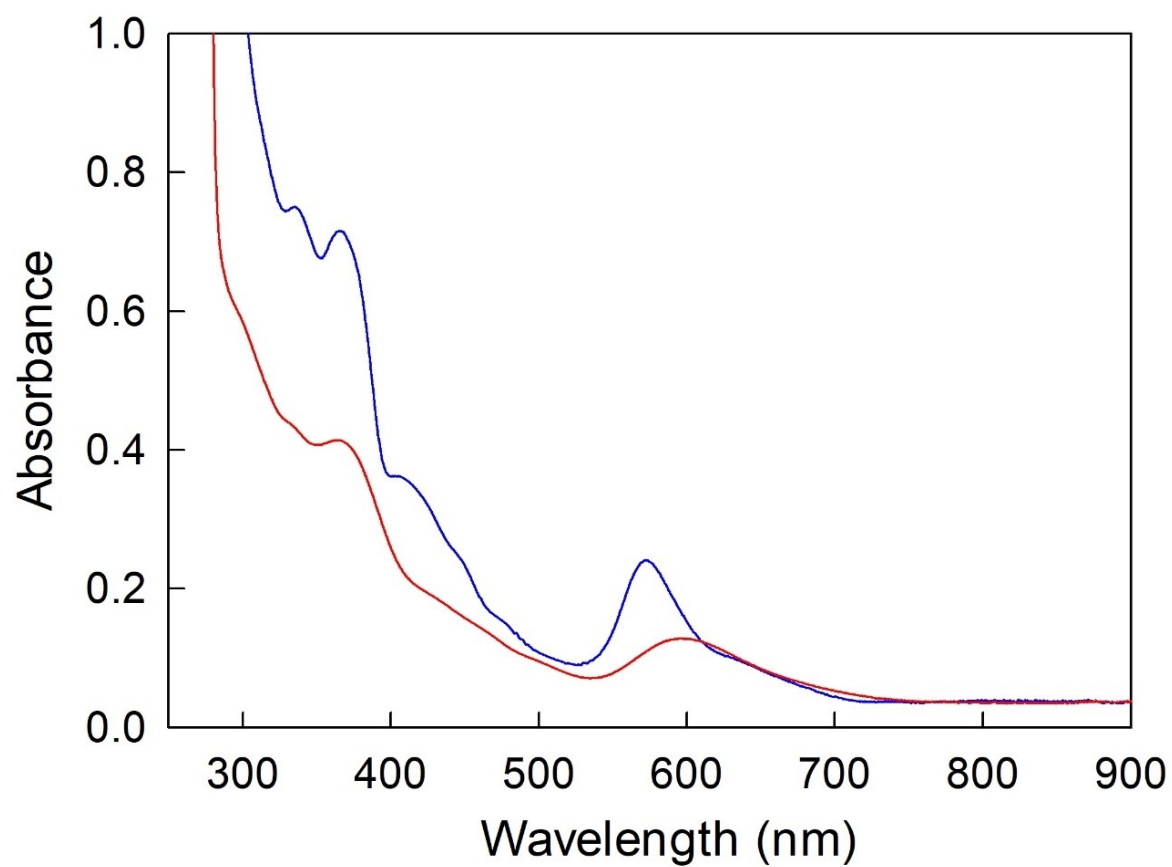


Figure S8. Comparison between room-temperature (297 K, red trace) and low-temperature (77 K, blue trace) UV-vis absorption spectra of Au₂₄Pt(SC₄H₉)₁₈ in tetrahydrofuran/toluene (1/1 v/v) in a 1 mm cuvette.

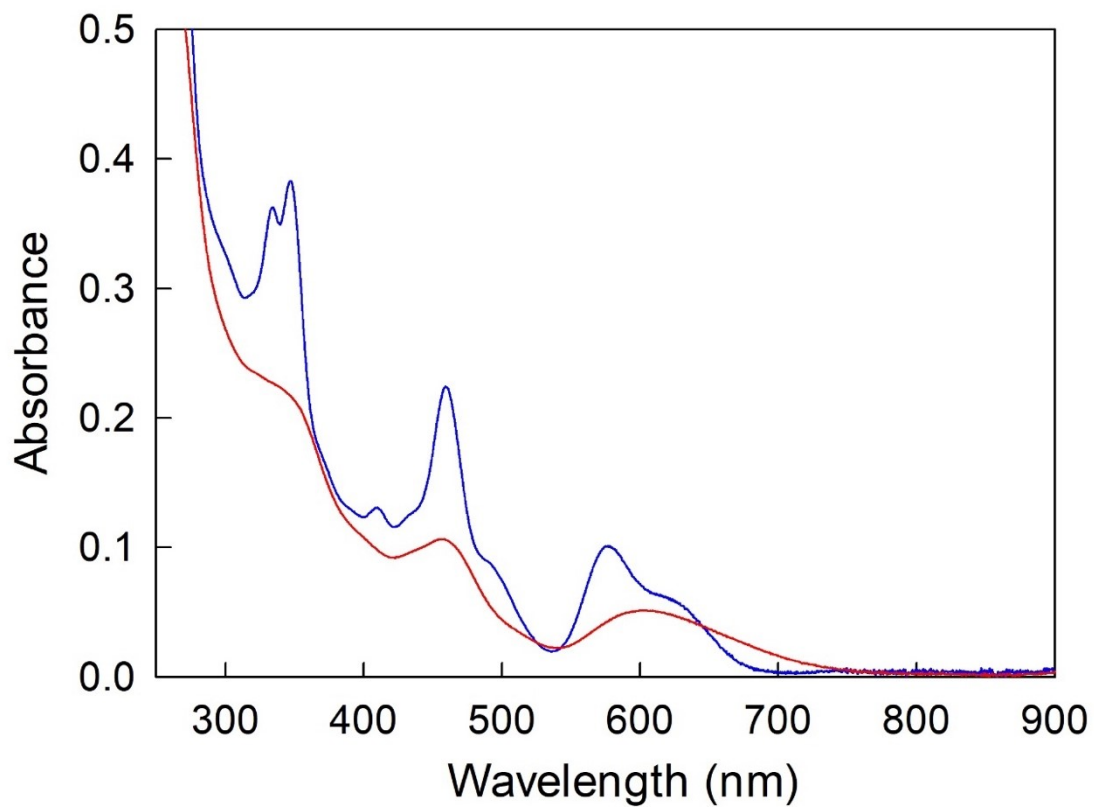


Figure S9. Comparison between room-temperature (297 K, red trace) and low-temperature (77 K, blue trace) UV-vis absorption spectra of $[n\text{-Oct}_4\text{N}^+]_2[\text{Ag}_{24}\text{Pt}(\text{SPhMe}_2)_{18}]^{2-}$ in butyronitrile/propionitrile/dichloromethane (5/4/2 v/v/v) in a 1 mm cuvette.

Table S1. Coordinates of the cluster Ag₂₅(DMBT)₁₈⁻.

Ag	9.7051410000	12.7878370000	6.9064770000
Ag	12.2961100000	13.6712290000	7.1545980000
Ag	11.4539950000	11.2901250000	8.4577670000
Ag	10.0242180000	15.5238710000	6.9829450000
Ag	10.4907870000	13.8292480000	9.3320730000
Ag	7.9998620000	14.3631030000	5.3685550000
Ag	7.1000580000	11.9149480000	6.7203860000
Ag	9.3730650000	10.0347610000	6.7637010000
Ag	8.5750650000	11.5808160000	9.1069460000
Ag	10.7424020000	14.0296420000	4.6755280000
Ag	9.0000760000	11.6877250000	4.4832880000
Ag	7.7379760000	14.1566970000	8.3184670000
Ag	11.6088580000	11.2937130000	5.5410100000
Ag	8.4981640000	14.0592400000	11.3804070000
Ag	13.0246050000	16.0834090000	5.7046410000
Ag	6.9900740000	8.8494200000	8.0596510000
Ag	8.4360930000	13.6877150000	2.3878960000
Ag	14.2988280000	11.4352280000	6.7177130000
Ag	11.7975600000	16.6151180000	9.0200500000
Ag	6.4533690000	9.7540130000	4.9653590000
Ag	11.5634350000	12.1444750000	2.6427010000
Ag	5.1653920000	14.2836730000	6.1776220000
Ag	7.2223280000	16.8275130000	7.3513830000
Ag	12.2391160000	8.6738210000	7.2997810000
Ag	10.3528250000	10.9404660000	11.2929760000
S	5.0005560000	16.6667260000	6.4845650000
S	14.7255400000	13.8025240000	6.6166460000
S	6.5531010000	14.8324470000	3.3942830000
S	7.9648620000	9.4517620000	10.1817800000
S	12.1167420000	9.6793240000	10.2245590000
S	12.6077460000	15.1259980000	3.5052420000
S	9.3894370000	17.7855180000	7.7898730000
S	6.9241420000	15.5232050000	10.2149340000
S	13.5927210000	17.4062290000	7.6430860000
S	13.3309940000	10.9869540000	3.7809020000
S	10.7421300000	15.6939710000	10.9935200000
S	10.0119820000	7.7423150000	7.4398830000
S	7.2678410000	10.8434540000	2.9651520000
S	4.7583320000	11.9201090000	5.8768290000
S	9.0379160000	12.2178470000	12.8397210000
S	5.8942320000	7.7765740000	6.2206690000
S	10.0661260000	12.7493730000	0.8914170000
S	14.6059040000	9.1126160000	7.1960400000
C	4.0021864859	17.0223951072	7.9233413494
C	2.7085531285	16.4742558461	8.0883851219
C	1.9750172369	16.8362669548	9.2277752218
C	2.4627405875	17.7149878420	10.2025643551
C	3.7333030672	18.2718187442	10.0012544025
C	4.4857963571	17.9324934714	8.8805031349

C	2.1260115442	15.4885638052	7.1144156912
C	1.6720378648	18.0062024698	11.4531602891
C	15.5665101299	14.1962766082	8.1461480167
C	16.9766800176	14.0956197325	8.2154939882
C	17.6116449632	14.5168564437	9.3953822022
C	16.9098670577	15.0270041215	10.4975832113
C	15.5129325216	15.0916688904	10.4126626698
C	14.8577960367	14.6737090412	9.2581799332
C	17.7830277321	13.5322096727	7.0758584783
C	17.6304282865	15.4884454902	11.7423528665
C	6.7041818299	16.5378942180	2.9003791719
C	6.1225615064	16.9457090748	1.6744615647
C	6.1979275815	18.3036775857	1.3293594484
C	6.7965580540	19.2652799297	2.1568062926
C	7.3571405067	18.8354600516	3.3666443733
C	7.3207470789	17.4903659277	3.7242268316
C	5.4186071663	15.9693856685	0.7673781399
C	6.8194810706	20.7247313839	1.7711725520
C	6.5550980793	9.7996699049	11.2257164903
C	5.8700511501	8.7278343679	11.8458828889
C	4.7995102809	9.0363530690	12.7000085780
C	4.3928212819	10.3518738130	12.9672376147
C	5.0818252332	11.3930509175	12.3322852049
C	6.1395182101	11.1158816116	11.4718441908
C	6.2580631355	7.2940704890	11.5968122261
C	3.2504078200	10.6428342238	13.9091929835
C	13.6821474834	10.1927985787	10.9089828022
C	14.2139189149	9.4800390626	12.0113199585
C	15.4630543992	9.8771180575	12.5128409076
C	16.2152004858	10.9157182351	11.9453722516
C	15.6803474879	11.5815665865	10.8357453122
C	14.4275171809	11.2342818259	10.3385489365
C	13.4942585391	8.3020491933	12.6141348108
C	17.5667448304	11.2958113522	12.4998492890
C	11.9565221686	16.5006759820	2.5652217918
C	12.8546584570	17.4427366175	2.0052366067
C	12.3248379691	18.4674449504	1.2069763775
C	10.9563587557	18.5803874458	0.9236209957
C	10.0880451526	17.6474428314	1.5027953289
C	10.5820598527	16.6321630615	2.3173101031
C	14.3386149550	17.3547377848	2.2389944229
C	10.4382266654	19.6568964008	0.0022967333
C	9.6372780017	18.9682955617	6.4806822969
C	9.1310647531	20.2812401921	6.6308148224
C	9.4167173422	21.2164531218	5.6236971446
C	10.1815533061	20.9024156396	4.4926016958
C	10.6563013948	19.5909181165	4.3641807512
C	10.3817564341	18.6397037736	5.3382072744
C	8.3095548887	20.6814933915	7.8279461051
C	10.5133909988	21.9383257512	3.4485869871
C	5.3277174931	14.9194385533	10.7268324428

C	4.8129314396	15.3020717426	11.9910125297
C	3.5230058055	14.8737022900	12.3345950536
C	2.7217219405	14.1060629429	11.4765992520
C	3.2611352337	13.7290137439	10.2414667728
C	4.5453751758	14.1231502446	9.8782503366
C	5.6116043355	16.1419147113	12.9511681805
C	1.3106312887	13.7289604468	11.8540265851
C	13.3421120001	19.1255311941	7.2416805436
C	12.8895793032	20.0709634007	8.1953873925
C	12.7955958779	21.4130450933	7.8018380570
C	13.1453361038	21.8630067281	6.5225451481
C	13.6253748233	20.9162370657	5.6081329353
C	13.7167941884	19.5736409326	5.9627945464
C	12.5129665823	19.6978124127	9.6037647884
C	12.9684009988	23.3117715810	6.1407777698
C	13.1420923219	9.3534298838	3.0835649475
C	13.8019322261	9.0397173609	1.8708445361
C	13.6883114618	7.7311781903	1.3791251689
C	12.9619130783	6.7303277263	2.0397035473
C	12.2980062373	7.0756447388	3.2229905731
C	12.3834057801	8.3679596188	3.7302568336
C	14.5913082151	10.0716809629	1.1126816978
C	12.8967052171	5.3222053898	1.5011337297
C	12.1136501610	15.1993102189	12.0281891406
C	12.6983024379	16.1388844307	12.9074742873
C	13.7170333330	15.6936956493	13.7646723544
C	14.1547161200	14.3633588004	13.7975375651
C	13.5581969154	13.4519550689	12.9148271317
C	12.5641322147	13.8698384365	12.0391059894
C	12.2298934003	17.5675816382	12.9641705109
C	15.2177444191	13.9030889961	14.7613362913
C	9.7769182756	6.7077611997	6.0031328201
C	10.1647703567	5.3467491781	6.0604770452
C	9.8974727717	4.5374244733	4.9448047631
C	9.2520276834	5.0134267673	3.7943269548
C	8.8751610340	6.3620823811	3.7641205663
C	9.1439259732	7.1924668449	4.8479894691
C	10.8286604263	4.7650700906	7.2809305527
C	8.9620828599	4.1068130512	2.6220099754
C	7.9548664818	9.5576248265	1.9425597718
C	7.0892295348	8.7797639608	1.1365893869
C	7.6636069359	7.8268067060	0.2821999174
C	9.0483039341	7.6245563306	0.1910465425
C	9.8827901214	8.4021432116	1.0058502438
C	9.3399349426	9.3453443048	1.8710592929
C	5.5948567224	8.9509020184	1.1937805283
C	9.6303698531	6.6045636074	-0.7563461953
C	3.6796916552	11.4099554932	7.2023320670
C	2.2800575248	11.4587453897	7.0039423204
C	1.4529419544	11.0042650825	8.0435226875
C	1.9574443498	10.4829072095	9.2422122632

C	3.3480667786	10.4361634916	9.4059881076
C	4.1922602394	10.9094140104	8.4082012990
C	1.6788618955	11.9473453530	5.7120117424
C	1.0461483463	9.9718079608	10.3304019938
C	10.0784205923	12.8296321528	14.1473969915
C	10.8448683240	11.9433981220	14.9404411750
C	11.5798803301	12.4765897347	16.0100765828
C	11.5849351036	13.8393605793	16.3270340441
C	10.8063783473	14.6963000871	15.5358033593
C	10.0665722831	14.1988705799	14.4685930106
C	10.9137186818	10.4697588711	14.6523084395
C	12.4242534927	14.3806291034	17.4568548838
C	4.1854705411	7.6777714607	6.7434564363
C	3.1021972134	7.9417899731	5.8714855192
C	1.7997239900	7.7367869217	6.3493481202
C	1.5227689369	7.2697861677	7.6415580372
C	2.6106855946	6.9939250060	8.4794518609
C	3.9163868985	7.1962681557	8.0364011419
C	3.3080476505	8.4208770973	4.4608990792
C	0.0986201289	7.0996954191	8.1101275176
C	10.9429362509	14.0347844505	0.0176161162
C	10.2545676059	14.9869126493	-0.7703017699
C	11.0087808986	15.9349122271	-1.4750751352
C	12.4073116480	15.9856021665	-1.4283176365
C	13.0693824580	15.0203826688	-0.6583734526
C	12.3487264991	14.0602156843	0.0468892039
C	8.7543903450	15.0382079186	-0.8302396874
C	13.1641896727	17.0767701213	-2.1419098922
C	15.3188327018	8.4485837768	5.7049847117
C	15.1248586028	7.0989501610	5.3226016732
C	15.7831160224	6.6368358101	4.1751558335
C	16.6227851364	7.4445341173	3.3972168059
C	16.8186241535	8.7688172366	3.8087845596
C	16.1767335845	9.2604086692	4.9425021384
C	14.2226954728	6.1684150620	6.0834968292
C	17.2584376102	6.9105403307	2.1385706471
H	0.9859997197	16.3993806310	9.3608554271
H	4.1416002396	18.9685273855	10.7310243114
H	5.4735902575	18.3723759401	8.7425280004
H	2.2309021451	15.8260067483	6.0743227345
H	1.0644564217	15.3077508935	7.3218560455
H	2.6473806740	14.5175549261	7.1902561376
H	1.9095296030	18.9968236969	11.8624132968
H	1.9054454911	17.2625441804	12.2322649486
H	0.5902606499	17.9616705841	11.2698520876
H	18.6965025673	14.4342271678	9.4521348572
H	14.9278827972	15.4488642363	11.2575116773
H	13.7682787873	14.7108814309	9.2221577935
H	17.4915743764	12.4898744749	6.8683973701
H	18.8556470075	13.5519235391	7.3031229006
H	17.6104541947	14.0936944795	6.1463664760

H	18.6029800848	14.9916215232	11.8556528145
H	17.0324706371	15.2866507681	12.6417001225
H	17.8182521071	16.5728335266	11.7125797324
H	5.7618600381	18.6191971269	0.3821966598
H	7.8459474305	19.5478174604	4.0275239495
H	7.7882585246	17.1696312920	4.6553607921
H	5.0965765325	16.4576524396	-0.1603189105
H	4.5330048713	15.5435706189	1.2623538735
H	6.0630954504	15.1162561958	0.5087445627
H	6.8158968984	20.8575843477	0.6811952444
H	7.7076194174	21.2284580207	2.1769331834
H	5.9373276146	21.2519109626	2.1666585322
H	4.2640528047	8.2127862148	13.1713362620
H	4.7805021273	12.4271471766	12.4871342875
H	6.6420617306	11.9413534735	10.9658243696
H	6.1958924575	7.0435022606	10.5257459872
H	5.6090828034	6.6063070533	12.1518949695
H	7.3012888570	7.1068443708	11.8908971282
H	2.5588422106	9.7935134937	13.9824112269
H	2.6815700566	11.5234637501	13.5795861235
H	3.6181750766	10.8557846487	14.9248079955
H	15.8639504912	9.3436598262	13.3740937149
H	16.2296940582	12.3959116966	10.3704366254
H	14.0125993544	11.7928652577	9.4986355407
H	13.4145320769	7.4812334908	11.8854194303
H	12.4639010052	8.5531628010	12.9034441030
H	14.0233194820	7.9285806758	13.4991533475
H	17.7942100790	12.3516057238	12.2987916958
H	18.3676581770	10.6963066926	12.0400264748
H	17.6204079911	11.1317350581	13.5842993725
H	13.0143136634	19.1989947178	0.7856697921
H	9.0157840446	17.7198167468	1.3328498100
H	9.8872763434	15.9236563485	2.7717051989
H	14.5817613887	17.3905848381	3.3132956735
H	14.8673496140	18.1726353411	1.7349479773
H	14.7376850368	16.3984168133	1.8692840800
H	9.4071218833	19.9375007235	0.2572780947
H	10.4330376493	19.3073133438	-1.0426710196
H	11.0621113596	20.5600153577	0.0387912611
H	9.0270394683	22.2279770387	5.7349708826
H	11.2413368180	19.3050111898	3.4938634621
H	10.7564286960	17.6225635142	5.2167292894
H	8.8586098986	20.5068314440	8.7646848103
H	7.3862674403	20.0837309109	7.8924412931
H	8.0309732997	21.7409671903	7.7778245970
H	9.8732998677	22.8256667612	3.5342770178
H	10.4037288634	21.5288865513	2.4343188061
H	11.5583688792	22.2710160640	3.5496289553
H	3.1296214181	15.1594064965	13.3101022664
H	2.6783923076	13.1181583733	9.5560095005
H	4.9504070468	13.8147930998	8.9132803134

H	6.5367928027	15.6262036705	13.2566136642
H	5.0302520598	16.3696869973	13.8526297272
H	5.9231707815	17.0874566918	12.4840633354
H	1.2040855652	13.5768263779	12.9366539052
H	0.9925338590	12.8110244371	11.3423151045
H	0.6045109840	14.5251481627	11.5687381635
H	12.4365764173	22.1374783478	8.5320382940
H	13.9189595736	21.2283502458	4.6074992570
H	14.0754346683	18.8451072898	5.2366870003
H	11.5763436004	19.1123093442	9.6263444283
H	12.3541787642	20.5934616004	10.2165209841
H	13.2926091709	19.0862708735	10.0800088297
H	13.1962372729	23.9834278717	6.9792663812
H	11.9273920317	23.5089759603	5.8387363118
H	13.6136473649	23.5895136409	5.2970398481
H	14.1867209879	7.4900305060	0.4405917339
H	11.6954773959	6.3365325374	3.7465447421
H	11.8449703284	8.6215282748	4.6447801674
H	15.3818420355	10.5044800055	1.7422848983
H	13.9472706893	10.9075728731	0.7957218778
H	15.0542557462	9.6356799032	0.2193337245
H	11.9490800787	4.8366088055	1.7716715266
H	13.7088980887	4.7042919408	1.9158474879
H	12.9985723738	5.2989694762	0.4081273236
H	14.1737143857	16.4163805568	14.4402472715
H	13.8803635396	12.4126993386	12.9003594023
H	12.1173979832	13.1469349088	11.3545913007
H	12.3008808595	18.0549030182	11.9804787284
H	12.8211735315	18.1481558688	13.6825347861
H	11.1711775657	17.6232652294	13.2591136238
H	14.7712888125	13.3019505903	15.5689419564
H	15.7436884251	14.7473081910	15.2246727402
H	15.9595140714	13.2658507678	14.2587805385
H	10.2034001204	3.4922657670	4.9836864454
H	8.3908874729	6.7770722386	2.8823540316
H	8.8668213053	8.2464599939	4.7923607968
H	11.7414010924	5.3194303552	7.5468614202
H	11.0947772678	3.7133491133	7.1207694371
H	10.1657375670	4.8274739740	8.1566583445
H	9.0280623489	4.6556694624	1.6723410762
H	7.9451218478	3.6897473818	2.6858851618
H	9.6600296393	3.2603857654	2.5814424677
H	7.0000311768	7.2214804964	-0.3343299558
H	10.9610464646	8.2602230627	0.9832630305
H	10.0030339887	9.9217496962	2.5171179817
H	5.0933005310	8.2771027803	0.4888840085
H	5.3005488384	9.9845710083	0.9617668003
H	5.2123372725	8.7416650938	2.2048251360
H	10.4642297724	6.0607524200	-0.2900550118
H	10.0284237278	7.0874653576	-1.6621370752
H	8.8789819471	5.8717305207	-1.0768381248

H	0.3737028013	11.0506709723	7.9001755334
H	3.7757995441	10.0483980322	10.3269263227
H	5.2710366168	10.9019615816	8.5700025333
H	1.9568414873	11.2862409136	4.8772816119
H	2.0430876380	12.9506290500	5.4459330922
H	0.5844859994	11.9799447708	5.7762536778
H	0.0124917661	10.3143109196	10.1932846755
H	1.3909820566	10.2974366218	11.3221256348
H	1.0341258345	8.8706955421	10.3404274086
H	12.1731147464	11.7933276457	16.6167230967
H	10.7868337176	15.7631372550	15.7497975220
H	9.4723713801	14.8791381659	13.8580933957
H	11.4232847637	10.2908711404	13.6898284364
H	9.9134711866	10.0232565586	14.5635484521
H	11.4714456436	9.9383464657	15.4326411903
H	13.2725160598	14.9653398089	17.0674663464
H	12.8341282448	13.5749966661	18.0791285399
H	11.8437318869	15.0496693825	18.1077285573
H	0.9688238791	7.9510743262	5.6782856739
H	2.4388830060	6.6211749063	9.4876889489
H	4.7515107853	6.9780745499	8.7000019714
H	3.9763698753	7.7469541721	3.9060059675
H	3.7756146141	9.4200298899	4.4416764138
H	2.3550535458	8.4838956415	3.9219130253
H	0.0460097143	6.5186856762	9.0398898516
H	-0.5165798404	6.5894803961	7.3559760988
H	-0.3702638871	8.0771856828	8.3029920827
H	10.4752145174	16.6719058637	-2.0742416182
H	14.1564334241	15.0210142652	-0.6047558504
H	12.8819955782	13.3191214280	0.6428181302
H	8.3143653534	14.0493134853	-1.0182880025
H	8.4119639252	15.7315157492	-1.6078339071
H	8.3464505147	15.3908703542	0.1332420119
H	14.1852551745	16.7639872789	-2.3961077853
H	13.2426870653	17.9686991077	-1.4995979624
H	12.6590569065	17.3831348612	-3.0675019909
H	15.6223313519	5.6025981172	3.8736120616
H	17.4752575627	9.4222513103	3.2372161596
H	16.3383466628	10.2937475971	5.2491365330
H	14.3041071321	5.1423809145	5.7053294527
H	13.1689026117	6.4785629389	5.9767817934
H	14.4483045407	6.1684049564	7.1589325746
H	18.1425649482	7.4943403739	1.8519337323
H	16.5462153068	6.9551260977	1.2989940851
H	17.5626735691	5.8611504689	2.2506864035

Table S2. Coordinates of the cluster $\text{Ag}_{24}\text{Pt}(\text{DMBT})_{18}^{2-}$.

Pt	13.52185104	16.13425176	20.91360012
Ag	14.46235904	13.85480976	19.71394812
Ag	15.98960804	16.41321076	19.72697212
Ag	13.60193004	16.14609176	18.14875812
Ag	12.60831304	18.40891676	22.12511812
Ag	15.59441504	14.84227676	22.13524712
Ag	11.38703304	17.37679076	19.67950712
Ag	11.03109104	15.89953576	22.09907012
Ag	13.45198204	16.16520076	23.68365212
Ag	14.07544704	18.50051876	19.64882812
Ag	15.35743604	17.72470976	22.23770312
Ag	11.67234304	14.57557376	19.63956712
Ag	12.99525104	13.74492876	22.18705412
Ag	10.56211104	17.28103576	24.72354312
Ag	17.83459404	14.17551776	20.26153412
Ag	15.72659104	14.21560676	17.09844712
Ag	16.68031204	16.01959376	24.52818312
Ag	10.96547204	15.92404576	16.72972512
Ag	14.30836304	13.67119076	25.31540912
Ag	12.17304604	19.16623876	17.43244012
Ag	17.43408704	19.15709876	20.62331012
Ag	12.35764700	11.68593300	19.60858700
Ag	9.80616504	19.01273876	21.76826112
Ag	14.39079204	20.84185876	21.29592512
Ag	10.27950200	12.90313200	22.64780100
S	17.98429504	13.78896476	17.86078312
S	18.37196704	17.13750576	19.64680312
S	9.26652600	14.92833300	23.56584500
S	10.61932504	13.68593876	17.59972512
S	17.45358804	18.11604176	23.50015912
S	13.66845304	20.71307676	18.54439712
S	13.88393804	15.19227376	15.85914512
S	12.30766504	15.98947576	25.86183712
S	14.44401700	11.74263900	18.38028300
S	17.92815504	14.27999776	22.72103612
S	11.07305604	18.04957376	15.60590112
S	9.75904404	19.19199476	19.34348912
S	12.11660604	20.84165176	22.20297212
S	16.09426404	14.76355376	26.53126912
S	8.82184804	18.78695476	23.96902112
S	10.28681400	11.34528400	20.78566300
S	16.77237604	21.35636476	21.30750212
S	12.51413304	12.41224276	24.26133712
C	18.26048941	12.06040839	17.60985042
C	18.78653322	17.50428943	17.96593803
C	15.40109980	15.90393978	13.64297100
C	14.64908370	17.73511034	15.01511672
C	17.93991792	17.17222285	16.89340056
C	17.98194465	22.56625009	19.07179447

C 16.88336630 22.49753671 19.95627404
C 15.85002225 23.44001416 19.76980468
C 15.87493796 24.37422758 18.73983993
C 16.96701339 24.39120038 17.86653505
C 18.02654857 23.49949275 18.03084202
C 17.44289655 13.62363492 26.69259616
C 9.47518748 18.81435311 15.58337080
C 13.06884952 17.12356748 26.99210418
C 15.19679069 18.65275589 14.12301212
C 20.04444499 18.06978045 17.65116473
C 14.28570490 17.76580975 26.70154423
C 16.89118006 11.84197280 23.59706726
C 7.56827708 14.64655605 23.15003707
C 14.71475159 16.34663460 14.79841473
C 8.24773197 13.62880997 19.06566921
C 15.95995862 16.80938232 12.73485786
C 12.50911646 17.35055842 28.27119268
C 8.03675054 17.29713904 18.26700693
C 18.31601641 17.36444513 15.56879028
C 14.76338069 21.94349948 16.31937707
C 12.44231590 21.36037266 23.86846169
C 9.33284609 20.16296839 15.96871410
C 19.29117072 11.97271031 23.41514391
C 15.77579082 22.22466730 15.39741637
C 8.03672720 13.23938507 16.69708293
C 14.93145963 20.96281949 17.32335226
C 16.46216071 10.83784309 20.07294983
C 13.13903917 18.17538425 29.20895070
C 17.28899153 12.27283153 27.07624027
C 15.84521189 18.18223610 12.97723348
C 8.31424647 18.14494887 15.14059819
C 17.17242044 20.53311313 16.44151321
C 17.24968163 9.87483183 20.69384264
C 6.89765352 13.60865264 23.83325548
C 19.21624072 11.32344297 18.34472720
C 16.24522363 20.34329615 24.64659310
C 14.35866475 18.77462571 28.88203614
C 8.86529832 13.53555194 17.80531501
C 15.41166436 10.50340992 19.20203350
C 18.11588823 19.41703851 25.85172451
C 20.43317731 18.28858918 16.32600332
C 19.56647602 17.92458469 15.29152739
C 18.02863430 12.59131304 23.25314237
C 6.96471932 20.09548088 15.56635447
C 18.76186392 14.09212658 26.51532727
C 6.88120751 13.42911960 19.23296047
C 5.45911357 15.14086156 21.99682210
C 6.81494792 15.40439071 22.23158866
C 19.40589687 10.66506961 23.89580973
C 15.18013627 9.12842434 18.97058822
C 8.17819679 18.55366671 18.88143767

C	7.06551867	18.77339064	15.13337081
C	5.55526198	13.32444510	23.60796373
C	14.93847371	18.57258330	27.62755021
C	4.83938227	14.09590048	22.68253350
C	17.23327557	19.34616581	24.74769439
C	12.59891215	22.73094884	24.17601590
C	16.14905098	20.26038646	17.34405568
C	18.39195459	11.43224730	27.25746249
C	17.71924071	10.00025024	16.39337082
C	17.54228669	11.36205106	16.61682234
C	16.98719581	8.52599875	20.44693978
C	5.74561103	18.81183777	18.74767757
C	12.50934276	20.44813931	24.93662579
C	16.15144853	21.38669750	25.56162998
C	9.04693538	20.40826828	24.64833505
C	9.31070881	20.64650525	26.01516196
C	9.44387763	21.94407400	26.51841428
C	9.31319867	23.03093027	25.65340839
C	9.03071075	22.83756472	24.29707955
C	8.89331427	21.53927173	23.81648315
C	8.09927397	20.80555409	15.97175873
C	17.05819056	21.44353316	26.62435238
C	16.98286110	21.52575387	15.47852421
C	19.87221700	13.27159866	26.69026236
C	12.68643114	20.86233503	26.25164526
C	6.08766657	13.15619881	18.11484746
C	16.98670528	10.54590557	24.09342473
C	18.24775540	9.96644731	24.24508628
C	18.03392062	20.45463620	26.78481218
C	19.67721501	11.93776947	27.05937125
C	12.78284537	23.16761444	25.49068176
C	12.80768486	22.22640482	26.52292891
C	6.79784107	16.78854140	17.90007968
C	7.00148697	19.30549316	19.10637770
C	19.41540333	9.95780079	18.12958258
C	6.65602890	13.06403045	16.84132026
C	5.65552905	17.55189117	18.14891602
C	15.95349085	8.14220127	19.58826362
C	18.65266591	9.30003668	17.16404269
C	10.52871830	9.73358800	21.49450139
C	11.27143872	8.76459897	20.78639669
C	11.47668933	7.47620835	21.26775743
C	10.92197954	7.11258466	22.49892127
C	10.17295481	8.03137052	23.23548995
C	9.97952607	9.32082314	22.72972764
C	13.81048042	8.50847835	23.95011716
C	13.45084048	8.02408342	25.20824617
C	12.78681488	8.84601493	26.12696805
C	12.50924534	10.16529381	25.78116716
C	12.88343222	10.70241498	24.53299811
C	13.52199540	9.83922759	23.62241087

H	14.15234379	18.10201893	15.91307177
H	16.95560460	16.75609696	17.10870565
H	15.00004380	23.42514064	20.45159255
H	15.05290297	25.07045902	18.60144896
H	18.86725458	23.50757384	17.34425789
H	15.13092539	19.71886837	14.32067324
H	14.73109650	17.62747633	25.71638013
H	15.90698265	12.29057301	23.46856247
H	8.85877592	13.87166903	19.93413099
H	16.48590829	16.44493716	11.85783721
H	8.93131001	16.69839992	18.08962176
H	17.64305741	17.09705661	14.76040834
H	10.21772217	20.71101993	16.29101691
H	15.62958651	22.99395596	14.64591733
H	16.65614610	11.89268971	20.27304055
H	12.68344299	18.33883733	30.18059677
H	18.11262634	19.99422795	16.49523275
H	18.05535569	10.16819157	21.36057444
H	7.46010344	13.01801171	24.55319800
H	15.53273230	20.29429847	23.82410755
H	21.40094837	18.72993057	16.10927646
H	18.90666613	15.13283069	26.22860584
H	6.43095786	13.49453732	20.21854854
H	4.91041950	15.73078315	21.26785576
H	20.38572711	10.21732163	24.02711917
H	6.18234994	18.22499711	14.82183251
H	5.06352259	12.51131467	24.13472757
H	15.87895659	19.05115400	27.37514439
H	16.29947306	19.49038181	18.10105403
H	18.24414727	10.39108279	27.52593928
H	17.12967851	9.48076149	15.64318480
H	16.80905945	11.90642669	16.02267662
H	4.85528768	19.40622253	18.92559101
H	12.40503816	19.38288311	24.72682035
H	15.38014607	22.14374421	25.45474823
H	9.67680788	22.09918012	27.56721707
H	8.93432178	23.69009623	23.63112329
H	8.66914596	21.38292352	22.76182155
H	8.01038778	21.83615860	16.30291929
H	20.87577378	13.65361317	26.52779013
H	12.71292970	20.13740905	27.05886478
H	16.09568289	9.99379875	24.37480033
H	18.72028670	20.48618259	27.62530431
H	12.88162976	24.22720013	25.70399935
H	6.71935620	15.81326262	17.42914230
H	20.13140501	9.40995651	18.73402934
H	6.04148986	12.84977743	15.97259406
H	15.75818659	7.09304940	19.39101407
H	11.70628712	9.03910023	19.82549173
H	12.06285042	6.76216218	20.69561092
H	9.74882886	7.75425758	24.19522388

H	14.32412765	7.87273096	23.23513965
H	12.50614908	8.45571962	27.10122901
H	12.00451597	10.81607378	26.49179018
C	19.99092907	18.16015823	13.83004023
H	21.04235817	18.35475565	13.79094177
H	19.76742508	17.28988933	13.24902558
H	19.45791598	18.99950738	13.43470489
C	21.03547600	18.45106362	18.76654838
H	20.60354641	19.21175607	19.38273328
H	21.25071023	17.58884594	19.36249711
H	21.94074459	18.81750629	18.32938874
C	19.16038898	21.58126979	19.18441228
H	19.33515538	21.35049727	20.21450972
H	18.92643625	20.68289116	18.65235782
H	20.03836425	22.02605185	18.76461667
C	16.99396029	25.38448704	16.68999118
H	17.20276776	26.36737717	17.05772264
H	17.75463869	25.09438520	15.99565027
H	16.04319722	25.38183918	16.19913217
C	18.12115057	21.86444613	14.49812397
H	17.79058812	22.61830167	13.81450838
H	18.96729621	22.22502754	15.04485846
H	18.39645648	20.98533417	13.95381816
C	13.45075930	22.74190909	16.21370231
H	12.72601355	22.16715454	15.67583540
H	13.08147259	22.95269430	17.19558668
H	13.63277599	23.66061737	15.69626147
C	16.46329765	19.18010406	11.98032349
H	16.47004538	18.74831744	11.00133688
H	15.88321821	20.07915539	11.96961991
H	17.46607840	19.40616291	12.27735575
C	15.57908844	14.40022370	13.36233244
H	16.46470769	14.04889386	13.84930872
H	14.73086874	13.86498461	13.73508228
H	15.66535629	14.24200334	12.30761723
C	19.19752208	18.34231734	26.06769353
H	18.77564210	17.51273562	26.59562482
H	19.56591002	18.01138985	25.11918031
H	20.00253865	18.75610505	26.63833182
C	16.99039152	22.58627725	27.60298951
H	17.97277360	22.79223181	28.02820502
H	16.61825396	23.48915843	27.11883609
H	16.31353078	22.34050060	28.42485517
C	20.87478085	11.03907087	27.23127748
H	21.38597445	11.26450834	28.16979992
H	20.57857297	9.99013052	27.24558519
H	21.58593838	11.19037262	26.41774934
C	15.91986475	11.69470767	27.31881238
H	15.27191527	12.42122979	27.81163268
H	15.45361418	11.41667707	26.36689373
H	15.97840456	10.79831458	27.93749563

C	18.34132079	8.58921317	24.84925179
H	17.86079834	7.85004584	24.20469386
H	19.37899587	8.29430069	25.00191219
H	17.82515225	8.56743472	25.81112863
C	20.52880434	12.77551329	23.12136673
H	20.59040043	13.01167929	22.05692973
H	20.48744337	13.72421110	23.66040728
H	21.42920984	12.23615161	23.41262601
C	20.06465224	11.98996247	19.39308322
H	20.31705950	13.01170718	19.10631964
H	19.51548895	12.02409359	20.34020502
H	20.98641136	11.43115355	19.55878654
C	18.79886819	7.81533328	16.95340220
H	19.17298074	7.60676459	15.94902047
H	19.48624172	7.37909949	17.67779862
H	17.82830513	7.32573798	17.05646594
C	14.12205034	8.69451357	17.98977046
H	13.17937937	8.49813254	18.50615642
H	13.94403476	9.47151894	17.24613433
H	14.42306202	7.77796033	17.48212976
C	17.85136783	7.47062833	21.08332550
H	18.89218486	7.60080220	20.78097958
H	17.80638173	7.54559904	22.17033478
H	17.52656611	6.47150361	20.79326711
C	9.12259350	10.24604554	23.55301971
H	9.75365775	10.92652578	24.13432118
H	8.46643349	10.84292164	22.91870647
H	8.50655704	9.68437347	24.25634206
C	11.11383332	5.71489127	23.02507029
H	11.92560957	5.69433949	23.75468155
H	10.20880140	5.36213178	23.52073467
H	11.36591048	5.02587395	22.21914952
C	13.89763570	10.31037910	22.24756371
H	13.01178534	10.68246405	21.72664169
H	14.62071595	11.12698688	22.28020648
H	14.32023891	9.49713170	21.66053354
C	13.79837258	6.61707668	25.61845419
H	14.40012408	6.63113564	26.52973256
H	12.89210776	6.04559859	25.83121325
H	14.36036881	6.10499500	24.83767079
C	7.45593646	16.51355054	21.45137177
H	8.16123030	17.06363220	22.07435714
H	8.00819130	16.10776893	20.59854916
H	6.70796279	17.21015380	21.07359227
C	3.38057382	13.81773639	22.43064392
H	2.78070018	14.69600234	22.67713903
H	3.21449147	13.58598798	21.37658016
H	3.03019704	12.97831960	23.03031846
C	7.10330368	20.66688849	19.74047390
H	7.13733117	20.57179972	20.83041607
H	8.01800264	21.16827465	19.42090474

H	6.24518407	21.28626281	19.47762860
C	4.30352908	16.99501422	17.78654230
H	4.36299994	16.39083233	16.88094777
H	3.93681742	16.35720812	18.59474925
H	3.57980252	17.79507075	17.63057121
C	5.61971194	20.77402977	15.59974522
H	5.43637347	21.29696378	14.65828899
H	4.82096688	20.04652812	15.74606133
H	5.57834151	21.50677598	16.40634087
C	8.38632761	16.71897880	14.66842397
H	9.32370682	16.52663498	14.14594731
H	8.32893708	16.04685210	15.52953133
H	7.55410864	16.48702629	14.00328046
C	8.66972512	13.04093540	15.34542246
H	8.93818310	14.00063001	14.89683416
H	9.58955771	12.46146429	15.44804738
H	7.99158994	12.52269385	14.66791910
C	4.60441333	12.96079088	18.29064226
H	4.05748119	13.32854841	17.42209220
H	4.37534580	11.89964649	18.41171178
H	4.24815765	13.48651003	19.17711931
C	15.07773325	19.63105759	29.89062800
H	14.43094351	19.88036250	30.73137111
H	15.95463290	19.10345176	30.27269797
H	15.42331071	20.55704451	29.42880546
C	11.23382662	16.63797955	28.63176977
H	11.35768375	15.56300097	28.48335806
H	10.95119481	16.82715718	29.66660396
H	10.41853873	16.96038295	27.98010172
C	12.56281417	23.74247008	23.06236051
H	13.53995820	23.79038947	22.57154227
H	11.82739512	23.45342055	22.31040263
H	12.31918158	24.73580468	23.44018247
C	12.98547188	22.67195491	27.95065563
H	12.93687496	23.75724994	28.03444860
H	12.21317210	22.23493252	28.58542954
H	13.95400481	22.33985475	28.33052870
C	9.49316344	24.43259210	26.17698151
H	8.52240980	24.88478368	26.39213794
H	10.08046831	24.43326961	27.09543459
H	9.99850867	25.05620692	25.43847192
C	9.46596575	19.50390275	26.98147901
H	8.80010106	18.67943934	26.72493165
H	10.49593738	19.13489011	26.95246853
H	9.25328347	19.82637619	28.00160472

Table S3. Coordinates of the cluster Au₂₄Pt(SC₄H₉)₁₈.

Pt	11.6704390000	7.9577070000	7.7376600000
Au	13.8908360000	9.1653750000	8.8562160000
Au	13.9844400000	7.3771760000	6.3164070000
Au	12.4336250000	10.1849640000	6.3083600000
Au	9.7152220000	9.5165580000	6.4662080000
Au	11.8330610000	8.1907310000	10.5035640000
Au	12.0309730000	5.4261820000	6.6393770000
Au	14.8143010000	7.8188090000	11.5688850000
Au	13.6348470000	5.5253130000	3.8151310000
Au	13.5719460000	12.3459690000	8.2404530000
Au	16.5294790000	7.5385100000	8.4314190000
Au	14.0581510000	8.9877110000	3.6289630000
Au	10.4213250000	12.6281530000	6.6138420000
Au	9.4500420000	6.7500380000	6.6191040000
Au	9.3564390000	8.5382380000	9.1589140000
Au	10.9072530000	5.7304490000	9.1669610000
Au	13.6256560000	6.3988550000	9.0091130000
Au	11.5078170000	7.7246820000	4.9717560000
Au	11.3099050000	10.4892320000	8.8359440000
Au	8.5265770000	8.0966040000	3.9064350000
Au	9.7060320000	10.3901000000	11.6601900000
Au	9.7689320000	3.5694440000	7.2348670000
Au	6.8113990000	8.3769040000	7.0439020000
Au	9.2827280000	6.9277020000	11.8463580000
Au	12.9195530000	3.2872600000	8.8614780000
S	16.9311620000	7.8847150000	10.6640430000
S	12.7655730000	7.7611580000	12.6340520000
S	16.3300810000	7.4212510000	6.1545350000
S	8.6174470000	11.5003370000	5.7119410000
S	13.8267030000	11.0271180000	4.6317630000
S	14.3208630000	7.1271590000	2.3197510000
S	12.9937160000	3.7846100000	5.1857800000
S	15.3349660000	11.0152890000	8.9462830000
S	12.0672120000	13.9446480000	7.5457660000
S	6.4097160000	8.0306980000	4.8112770000
S	10.5753060000	8.1542550000	2.8412690000
S	7.0107980000	8.4941620000	9.3207860000
S	14.7234310000	4.4150760000	9.7633800000
S	9.5141750000	4.8882950000	10.8435570000
S	9.0200160000	8.7882550000	13.1555700000
S	10.3471620000	12.1308030000	10.2895410000
S	8.0059120000	4.9001250000	6.5290380000
S	11.2736660000	1.9707650000	7.9295540000
C	16.7958293514	5.7000368252	5.6784494103
C	16.3335262584	4.5762426618	6.5981001850
C	16.6135303670	3.1918712686	5.9946388056
C	16.1429629623	2.0522587487	6.9071944834
C	8.7848525342	11.7035824581	3.8806642439
C	7.8461149270	12.7883723577	3.3400447201

C	8.0409436242	14.1959419885	3.9264392395
C	12.5515708299	11.7855446529	3.5257951131
C	13.1478710326	12.3113861685	2.2220855727
C	12.0653095448	12.8528443595	1.2671165132
C	11.1349491393	11.7647661287	0.7078576842
C	16.1566937207	7.0318170789	2.0761299633
C	16.6182042061	5.9138544972	1.1369240640
C	16.4388542332	4.4706100420	1.6634466412
C	15.2805525502	3.7150195191	1.0035176361
C	11.5629635582	3.0332928206	4.2721780083
C	11.9342225507	2.4370948420	2.9151547210
C	12.9697252044	1.3071651162	2.9782036163
C	13.1528922377	0.6098856858	1.6231483871
C	16.3256402730	10.8738909973	7.3847056020
C	16.6322367788	12.2155459227	6.7268879306
C	17.4357626312	12.0417070103	5.4282605336
C	17.5563443542	13.3595936685	4.6520748401
C	12.9402302961	14.7235146182	6.1107378217
C	14.1025950573	15.6110804329	6.5603932767
C	13.7279868766	16.7121118000	7.5660982140
C	12.6044509522	17.6414362603	7.0861857026
C	17.7115736618	6.2894584585	11.1829217275
C	19.1339782114	6.1570529009	10.6327429068
C	19.6936498804	4.7299017492	10.7758782619
C	19.7823240714	4.2244070273	12.2233691533
C	12.6909143372	9.1521483681	13.8484525693
C	12.8875774059	8.6796429371	15.2949353057
C	11.6636111508	8.0271734567	15.9654806905
C	11.2966693405	6.6184075744	15.4736707399
C	6.5412055645	10.2124193090	9.7921778202
C	6.9932573297	11.3150760900	8.8439694464
C	6.6286408486	12.7144791414	9.3548167790
C	7.0987530247	13.8214347094	8.4025930799
C	14.4454527462	4.3137718969	11.5890016640
C	14.5358193035	2.9030437927	12.1841418486
C	15.9540508633	2.3418079568	12.3890936601
C	16.7068522178	1.9679400635	11.1037366295
C	10.7116290491	4.0762866586	12.0109127340
C	9.9996159146	3.4703945377	13.2210238244
C	9.0402562328	2.3234285046	12.8760726166
C	8.3088089268	1.7726342060	14.1067886192
C	7.2169261956	8.9937725907	13.5210744705
C	6.9992053778	9.9091897837	14.7324077429
C	7.4564238499	11.3685382400	14.5649919286
C	6.7284352425	12.1289726535	13.4502020735
C	11.6777443337	13.0422960368	11.1815193814
C	12.7637255328	12.1805915818	11.8209345415
C	14.0372813775	12.9774314505	12.1342382952
C	15.1245287947	12.1113215928	12.7841942886
C	7.0155943690	4.9406734094	8.1118070011
C	5.5197029893	5.0605023798	7.8286461860

C	4.7101294767	5.3044043963	9.1167161910
C	4.8632940822	4.2013713088	10.1756076176
C	10.3814359977	1.1798040710	9.3449004850
C	9.1497724426	0.3691577456	8.9229862796
C	9.4188862429	-1.0178648990	8.3115762754
C	10.0544531655	-1.0189895117	6.9115886896
C	5.6688037240	9.6489342064	4.3108056680
C	4.2861238277	9.8624147213	4.9336501787
C	3.7874141716	11.3109691257	4.7620770473
C	4.4909126470	12.3096573443	5.6943322322
C	10.6564748189	6.6092761242	1.8109117329
C	11.1077761550	6.9386520086	0.3876678986
C	11.3983718629	5.6759515684	-0.4445061306
C	10.1826750233	4.7578160410	-0.6407611326
C	9.4208498294	14.8057932065	3.6494097457
H	16.3599601689	5.5643984512	4.6779492484
H	17.8900680468	5.7152056034	5.5775399997
H	15.2540487869	4.6879419807	6.7820884968
H	16.8155098123	4.6796741531	7.5821872459
H	16.1019883038	3.1202696107	5.0221841059
H	17.6887519593	3.0904851751	5.7841914076
H	16.6303026361	2.0976695216	7.8906563212
H	16.3576902512	1.0681280657	6.4696384189
H	15.0580565697	2.1145186964	7.0819085652
H	9.8307053912	11.9162111312	3.6484069886
H	8.5434901880	10.7221222186	3.4431445662
H	7.9896831211	12.8206660236	2.2471463818
H	6.8044140753	12.4732492059	3.5013038611
H	10.2178384323	14.2131717204	4.1235059540
H	11.7937386673	11.0173017111	3.3421058469
H	12.0807160523	12.5882501282	4.1122667524
H	13.7013323084	11.4954488744	1.7323808487
H	13.8838552660	13.0972470897	2.4479184623
H	11.4739974728	13.6220168806	1.7850574777
H	12.5623578266	13.3706029848	0.4337831448
H	10.5723589531	11.2456985107	1.4950032346
H	11.7052081395	10.9952056503	0.1690542799
H	10.4018800452	12.1891305651	0.0080022243
H	16.4121382295	8.0142303230	1.6576737246
H	16.6337467004	6.9630946140	3.0601682614
H	16.1137939115	6.0248819386	0.1667110659
H	17.6851549301	6.1070683168	0.9413596103
H	17.3698504610	3.9074287941	1.5103344059
H	16.2805419696	4.4906011517	2.7521079198
H	14.3240993756	4.2280299908	1.1756892067
H	15.1866371962	2.6992207617	1.4097139597
H	15.4252597778	3.6313026898	-0.0822311796
H	11.1762556937	2.2608368937	4.9519488972
H	10.7918119901	3.8056867497	4.1742587727
H	11.0043284868	2.0576794931	2.4602732657
H	12.2953235903	3.2383869165	2.2511817898

H	13.9273818681	1.7158154397	3.3321319215
H	12.6615534851	0.5758601784	3.7399096244
H	13.9300351345	-0.1657449827	1.6630691615
H	13.4398834265	1.3253412903	0.8402010384
H	12.2216573574	0.1286299688	1.2936891499
H	17.2371246683	10.3321349692	7.6734953118
H	15.7631509074	10.2338715079	6.6953254042
H	15.6750406265	12.7096185319	6.4952438172
H	17.1614603317	12.8788023187	7.4262996597
H	18.4317839665	11.6364565030	5.6562910913
H	16.9375394638	11.2869604915	4.8012250111
H	18.0448649024	14.1392116862	5.2527238740
H	16.5631588878	13.7382310428	4.3708692469
H	18.1389399685	13.2393163413	3.7282629721
H	13.2942226880	13.9251611036	5.4481768781
H	12.1698823531	15.2956683598	5.5786258503
H	14.5336230912	16.0654474934	5.6535296503
H	14.8878956957	14.9725125895	6.9930768289
H	13.4356607231	16.2437218145	8.5164241450
H	14.6311112145	17.2989803370	7.7870834051
H	12.4311610245	18.4589452064	7.7996786628
H	11.6533158209	17.1029278926	6.9756485403
H	12.8429107017	18.0953029355	6.1143449429
H	17.6879953490	6.2838127621	12.2794285571
H	17.0786365372	5.4707165001	10.8188056410
H	19.1204741090	6.4311756736	9.5656498828
H	19.7925564500	6.8819295281	11.1318450755
H	19.0693225358	4.0436055103	10.1848518203
H	20.6910635522	4.6993960332	10.3139933017
H	20.2399026547	3.2262885280	12.2704530993
H	18.7905543400	4.1473923837	12.6897336099
H	20.3870398555	4.8977611229	12.8463318636
H	13.4587749168	9.8744443358	13.5590967053
H	11.7104461654	9.6269715620	13.7132735017
H	13.1659647675	9.5717637792	15.8805166605
H	13.7559504902	8.0063966983	15.3452785147
H	11.8565636395	7.9866605163	17.0479339104
H	10.7957673009	8.6912730881	15.8395056173
H	10.4952736558	6.1867636928	16.0897467254
H	12.1583560916	5.9390125008	15.5208310902
H	10.9431588169	6.6253981198	14.4332815886
H	6.9894979416	10.3595751402	10.7854182923
H	5.4479726465	10.1958132251	9.9029544756
H	8.0827099944	11.2413575687	8.7066967789
H	6.5557850615	11.1434062299	7.8488615961
H	7.0838874249	12.8646360627	10.3452813269
H	5.5402606654	12.7808130775	9.5041823168
H	6.8228650547	14.8177672022	8.7728023875
H	8.1926028376	13.7953515846	8.2830161144
H	6.6624286669	13.7003232335	7.4017992240
H	13.4679447935	4.7621257667	11.7894530315

H	15.1942322415	4.9847488934	12.0351410271
H	13.9382445382	2.2148065775	11.5657087673
H	14.0339558376	2.9464954142	13.1651298243
H	16.5436069368	3.0715465150	12.9650645222
H	15.8799096270	1.4517388562	13.0316479403
H	17.6800048545	1.5129381807	11.3347556382
H	16.1320000784	1.2522935586	10.5001303374
H	16.8890209695	2.8431678163	10.4670838531
H	11.4368595528	4.8383857436	12.3171009335
H	11.2464857098	3.3186770070	11.4193048635
H	10.7715055734	3.1117524748	13.9213306909
H	9.4582599944	4.2697080478	13.7503365872
H	9.6033492051	1.5183917981	12.3806917348
H	8.3091095491	2.6761444517	12.1341656954
H	9.0141400119	1.3876454975	14.8562099143
H	7.7109011029	2.5543333497	14.5956003992
H	7.6270069253	0.9524822677	13.8430529384
H	6.8528462461	7.9804274603	13.7303211636
H	6.7031639859	9.3512160847	12.6231049730
H	7.5077754154	9.4652845797	15.6012152980
H	5.9211783717	9.8913849803	14.9629139494
H	8.5394743828	11.3918501269	14.3729257733
H	7.3082800233	11.8844341807	15.5250314159
H	5.6376091333	12.0850183245	13.5723032244
H	7.0219319877	13.1876227985	13.4318986494
H	6.9730488958	11.7185153407	12.4611199306
H	11.1641706939	13.6655269570	11.9258836251
H	12.1056526844	13.7090178385	10.4196748075
H	13.0141808680	11.3510175006	11.1412165504
H	12.3577747331	11.7119824657	12.7281193718
H	13.7979212725	13.8348718820	12.7804908514
H	14.4180110679	13.4008215239	11.1913781639
H	14.8065423473	11.7358339247	13.7670024080
H	15.3615783689	11.2382698608	12.1571326523
H	16.0566405550	12.6728410647	12.9343644945
H	7.3819675539	5.7807742491	8.7115912197
H	7.2509870580	4.0211213506	8.6565902676
H	5.1686875539	4.1518569642	7.3183303497
H	5.3517830552	5.8984135776	7.1334355615
H	3.6505577137	5.4114639569	8.8433399694
H	5.0140721337	6.2717504020	9.5421540873
H	4.1974760281	4.3756871479	11.0324120515
H	4.6197014877	3.2120374661	9.7640874164
H	5.8888292481	4.1523599778	10.5678484233
H	10.0899240715	1.9831817226	10.0294462023
H	11.1247985792	0.5493768271	9.8508044958
H	8.5369351425	0.2391382120	9.8305901190
H	8.5422600894	0.9786178384	8.2349893071
H	8.4595501122	-1.5550016145	8.2672438123
H	10.0468268470	-1.5965117903	9.0049760250
H	9.4650881858	-0.4129291287	6.2096629866

H	11.0697554825	-0.6043605258	6.9175508520
H	10.1107199571	-2.0397369305	6.5082441184
H	5.6224467002	9.6447089855	3.2142045159
H	6.3655404330	10.4337404460	4.6232157831
H	4.3373782774	9.6191837498	6.0068584830
H	3.5738460104	9.1524605916	4.4899805758
H	2.7044251004	11.3383186574	4.9511749777
H	3.9113973480	11.6214410241	3.7139587581
H	4.1425939945	13.3376942138	5.5247533542
H	4.3013248416	12.0641651889	6.7486652154
H	5.5816965200	12.3065352564	5.5605558622
H	9.6684987544	6.1396763635	1.8372408819
H	11.3697472460	5.9330947986	2.3031643212
H	10.3413791927	7.5539238402	-0.1055278462
H	12.0192360858	7.5523058468	0.4412334400
H	12.2146174809	5.1157521164	0.0371535196
H	11.7883335669	5.9863858971	-1.4246805182
H	9.8278673254	4.3408653747	0.3115001107
H	9.3414913213	5.3005778122	-1.0935269917
H	10.4226724614	3.9094052400	-1.2965536177
H	7.8719687104	14.1586825719	5.0127193855
H	7.2579239836	14.8524871555	3.5201671194
H	9.4945648655	15.8247160396	4.0538694324
H	9.6325056864	14.8563111650	2.5723484190