Supporting information

Identifying the Real Chemistry of the Synthesis and Reversible Transformation of AuCd Bimetallic Clusters

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Contents

1. Experimental Methods

1.1 Chemicals. The following chemicals and solvents were purchased from various sources and used them without further purification. The water used in all experiments is ultrapure (resistivity 18.2 MΩ cm), produced with a PURELAB pure water system. Tetrachloroauric (III) acid ($HAuCl_4 \cdot 4H_2O$, 99.999% metal basis), tetraoctylammonium bromide (TOAB, 98%), tetrahydrofuran (99.8%), 2 - phenylethanethiol (PET, 98%), 2-methylbenzenthiol (2MBT, 98%), 4-methylbenzenthiol (4MBT, 98%), 2,4-dimethylbenzenethiol (2,4DMBT, 98%), 2,6-dimethylbenzenethiol (2,6DMBT, 98%), 4-tert-butyl-benzenethiol (TBBT, 98%), 4-methoxybenzenethiol (4MOBT, 98%), 4-(trifluoromethyl) thiophenol (4TMBT, 98%), 2-isopropyl thiophenol (2IPBT, 98%), cadmium acetate (98%), methanol (99.8%), ethanol (99.8%), toluene (99.8%), n-hexane (99.8%) and dichloromethane (DCM, 99.9%) were received from Adamas. Petroleum ether (99.8%) was received from Greagent. Sodium borohydride ($NaBH_4$) was received from Sinopharm Chemical Reagent Co., Ltd.

1.2 Synthesis of $[Au_{25}(PET)_{18}]^-$. The syntheses of $[Au_{25}(PET)_{18}]^-$ followed the procedures reported previously.[1]

1.3 Synthesis of AuCd bimetallic clusters using $[Au_{25}(PET)_{18}]^-$ as precursor. 15.8 mg of $[Au_{25}(PET)_{18}]^-$ crystal was dissolved in 1 mL toluene and then mixed with an aqueous solution of cadmium acetate (5.33 mg). Then excess mercaptan (50 μL of 2MBT, 50 μL of 3MBT, 50 μL of 4MBT, 56 μL of 2,4DMBT, 56 μL of 2,6MBT, 67 μL of TBBT, 61 μL of 2-IPBT, 72 μL of 4TMBT, 56 μL of 4MOBT, respectively) was added to the above solution. After the reaction at 60℃ for 1 hour, the crude product was washed with methanol to remove excess ligands. Finally, the synthesized product was completely dried under vacuum and stored in a refrigerator for further use.

1.4 Crystallization of $[Au_{19}Cd_3(SR)_{18}]^-$. $[Au_{19}Cd_3(4MOBT)_{18}]^-$, $[Au_{19}Cd_3(TBBT)_{18}]^-$ and $[Au_{19}Cd_3(2,4DMBT)_{18}]^-$ were crystallized by diffusion methanol into toluene solution of the prepared clusters, and red single crystals were obtained after two weeks.

$Au_{19}Cd_3(4DMBT)_{18}$ was crystallized by diffusing n-hexane into a DCM solution of the prepared cluster, and red acicular single crystal was obtained in 3~5 days.

1.5 Synthesis of $[Au_{25}(PET)_{18}]^0$. 10 mg of $[Au_{25}(PET)_{18}]^-$ was dissolved in DCM and then underwent thin-layer chromatography (TLC) separation. Under aerobic conditions, the $[Au_{25}(PET)_{18}]^-$ on the silica gel plate will be oxidized to $[Au_{25}(PET)_{18}]^0$. The yield rate of $[Au_{25}(PET)_{18}]^0$ was about 80%, and the product was stored at 4 °C for later use.

1.6 Synthesis of AuCd bimetallic clusters using $[Au_{25}(PET)_{18}]^0$ as precursor. 14.8 mg of $[Au_{25}(PET)_{18}]^0$ crystal was dissolved in 1 mL toluene and then mixed with an aqueous solution of cadmium acetate (5.33 mg). Then excess mercaptan (50 μL of 2MBT, 50 μL of 4MBT, 56 μL of 2,4DMBT, 56 μL of 2,6MBT, 67 μL of TBBT, 56 μL of 4MOBT, respectively) was added to the above solution. After the reaction at 60℃ for 1 hour, the crude product was washed with methanol to remove excess ligands. Finally, the synthesized product was completely dried under vacuum and stored in a refrigerator for further use.

1.7 Synthesis and crystallization of $Au_4Cd_4(2,4DMBT)_{12}$. 15.8 mg of $[Au_{19}Cd_3(SR)_{18}]^-$ was dissolved in 1 mL of toluene. 13.3 mg of cadmium acetate was dissolved in 200 μL of deionised water. 56 μL of 2,4DMBT and cadmium acetate aqueous solution were added to the sample vial at the same time and the reaction was performed at 60°C for 1 h. After the reaction, the crude products were washed with methanol and centrifuged to obtain a large amount of red precipitate. The precipitate was dissolved in toluene and the methanol was diffused into it, after one week the colourless and transparent single crystals were obtained.

2. Characterizations

Single crystal X-ray diffraction data was collected on a Bruker APEX II CCD diffractometer. Data were collected using graphite-monochromated and 0.5 mm-MonoCap-collimated Mo-Kα radiation (λ = 0.71073 Å) with the ω scan method. Data

were processed with the INTEGRATE program of the APEX2 software for reduction and cell refinement. Multi-scan absorption corrections were applied by using the SCALE program for area detector. The UV/vis/NIR absorption was measured on a P9 Dual Beam UV-Visible Spectrophotometer (Mapada, Shanghai) at room temperature. ESI-MS data of clusters were recorded on an Agilent Technologies ESI-TOF-MS spectrometer.

3. Computational methods

Quantum-chemical calculations were carried out with Amsterdam Density Functional (ADF 2019.304) program.[2-4] The scalar relativistic (SR) effects were introduced by the zero-order-regular approximation (ZORA).[5] Time-dependent DFT (TDDFT) calculations were performed using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional[6] to simulate the CD and UV-Vis spectra, with TZ2P basis sets utilized for all elements. The experimental crystal structures of Au_4Cd_4-R and Au_4Cd_4-S were used in the simulation without further optimization at the DFT level. The lowest 800 excited states were considered for these two enantiomers. The calculated UV-Vis spectrum was blue-shifted by the value (51 nm) of the difference of maximum absorption of the experimental and calculated spectra.[7]

4. References

(1) Wu, Z.; Suhan, J.; Jin, R. One-pot synthesis of atomically monodisperse, thiol-functionalized Au_{25} nanoclusters. *J. Mater. Chem.* **2009**, *19*, 622-626.

(2) Bomble, Y. J. Amsterdam Density Functional 2005. *J. Am. Chem. Soc*. **2006**, *128*, 3103-3103.

(3) te Velde, G.; Bickelhaupt, F. M.; Baerends, E. J.; Guerra, C. F.; Van Gisbergen, S. J. A.; Snijders, J. G.; Ziegler, T. Chemistry with ADF. *Journal of Computational Chemistry* **2001**, *22*, 931-967.

(4) Guerra, C. F.; Snijders, J. G.; te Velde, G.; Baerends, E. J. Towards an order-N DFT method. *Theoretical Chemistry Accounts*, **1998**, *99*, 391-403.

(5) Lenthe, E. v.; Baerends, E. J.; Snijders, J. G. Relativistic regular two-component Hamiltonians. *J. Chem. Phys.* **1993**, *99*, 4597-4610.

(6) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made simple. *Phys. Rev. Lett.* **1996**, *77*, 3865-3868.

(7) Rode, J. E.; Frelek, J. Circular dichroism spectroscopy and DFT calculations in determining absolute configuration and E/Z isomers of conjugated oximes. *Chirality* **2017**, *29*, 653-662.

5. Supporting Figures/Tables:

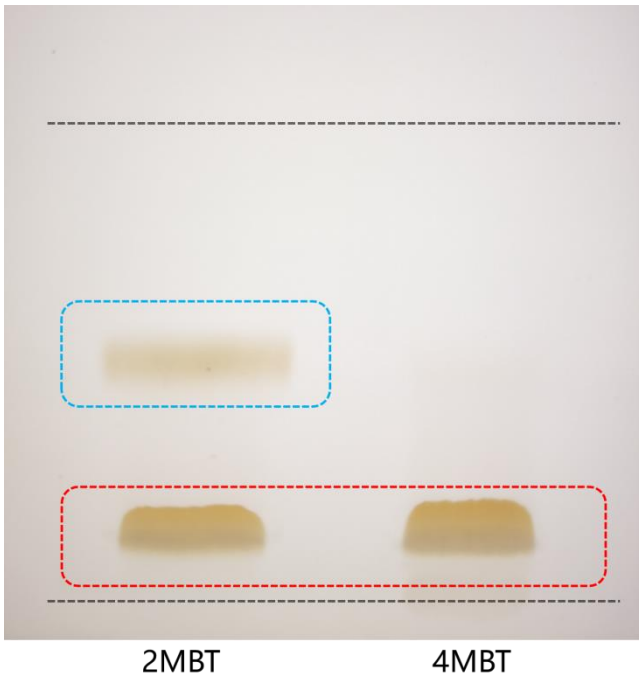

Figure S1. Photographs of isolated products of $[Au_{25}(PET)_{18}]^-$ doped by Cd assisted with 2MBT and 4MBT, respectively. The red and blue box indicate the $[Au_{19}Cd_3(SR)_{18}]^-$ and $Au_{24}Cd(SR)_{18}$, respectively.

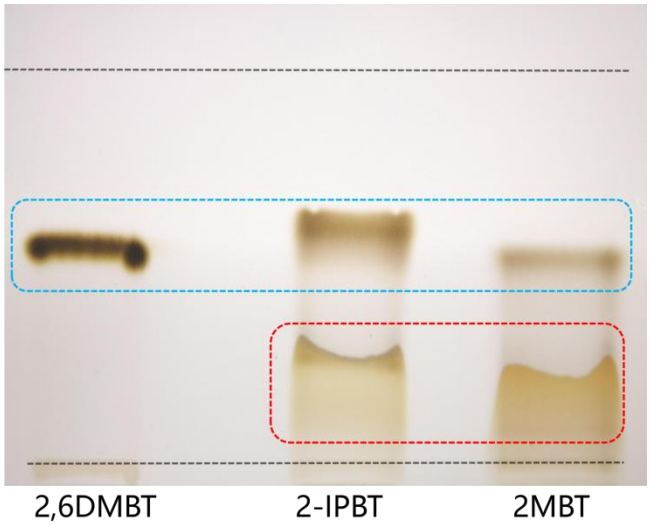

Figure S2. Photographs of isolated products of $[Au_{25}(PET)_{18}]^-$ doped by Cd assisted with 2,6DMBT, 2-IPBT and 2MBT, respectively. The red and blue box indicate the $[Au_{19}Cd_3(SR)_{18}]^-$ and $Au_{24}Cd(SR)_{18}$, respectively.

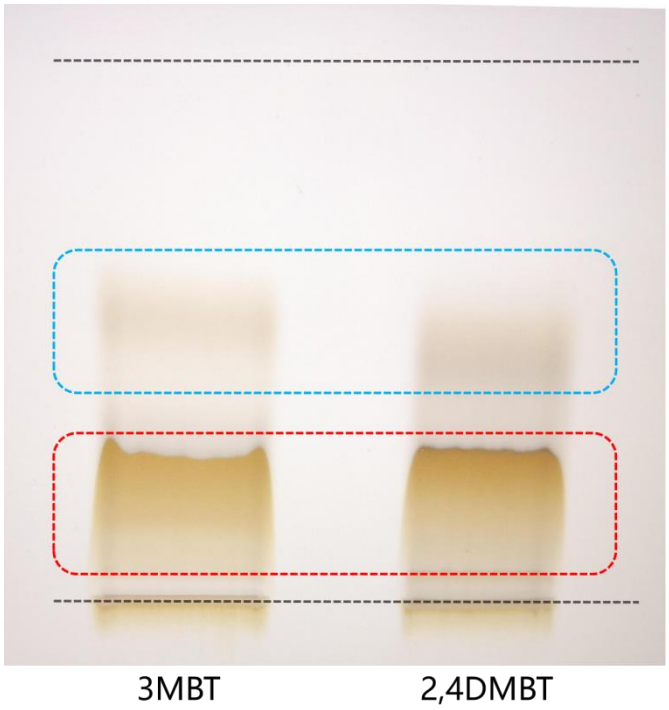

Figure S3. Photographs of isolated products of $[Au_{25}(PET)_{18}]^-$ doped by Cd assisted with 3MBT and 2,4DMBT, respectively. The red and blue box indicate the $[Au_{19}Cd_3(SR)_{18}]^-$ and $Au_{24}Cd(SR)_{18}$, respectively.

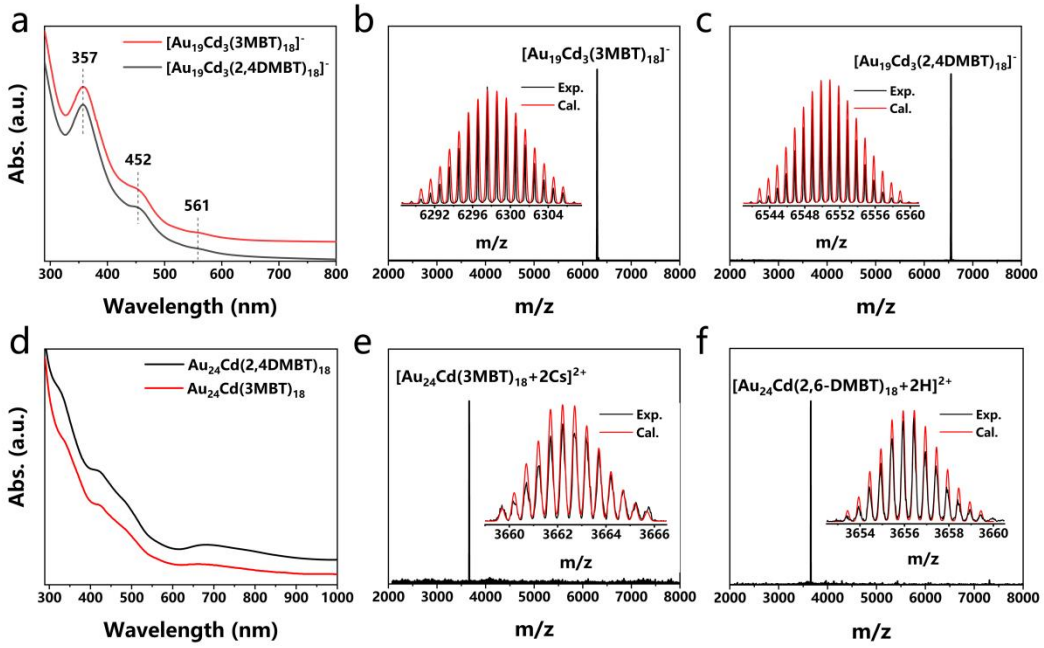

Figure S4. UV-Vis-NIR spectra and ESI-MS of $[Au_{19}Cd_3(SR)_{18}]^-$ and $Au_{24}Cd(SR)_{18}$ (SR=3MBT and 2,4DMBT). (a) UV-Vis-NIR spectra of $[Au_{19}Cd_3(SR)_{18}]^-$ and (d) $Au_{24}Cd(SR)_{18}$. ESI-MS of (b) $[Au_{19}Cd_3(3MBT)_{18}]^-$, (c) $[Au_{19}Cd_3(2,4DMBT)_{18}]^-$, (e) $Au_{24}Cd(3MBT)_{18}$ and (f) $Au_{24}Cd(2,4DMBT)_{18}$. Inset: the measured (black) and simulated (red) isotopic distribution patterns of the corresponding molecular ion peak.

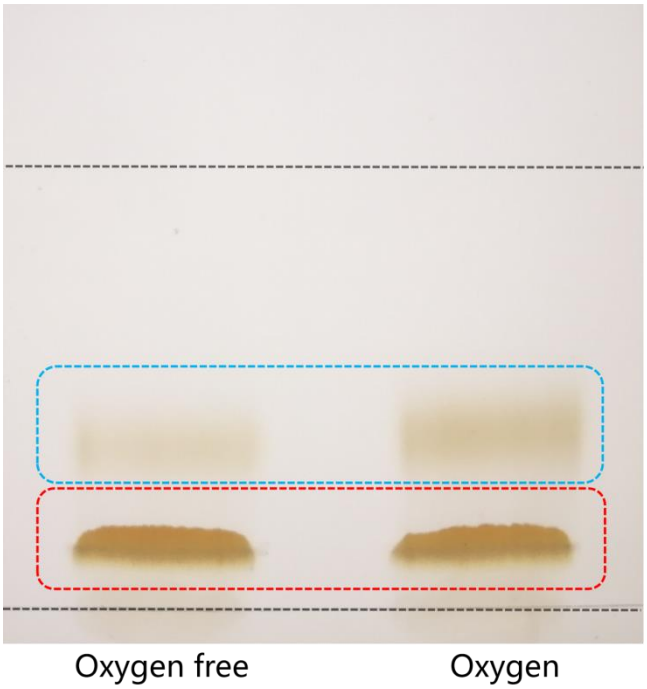

Figure S5. Photographs of the isolated products of $[Au_{25}(PET)_{18}]^-$ doped with Cd under oxygen or oxygen free conditions (using 2MBT as ligand). The red and blue box indicate the $[Au_{19}Cd_3(2MBT)_{18}]^-$ and $Au_{24}Cd(2MBT)_{18}$, respectively.

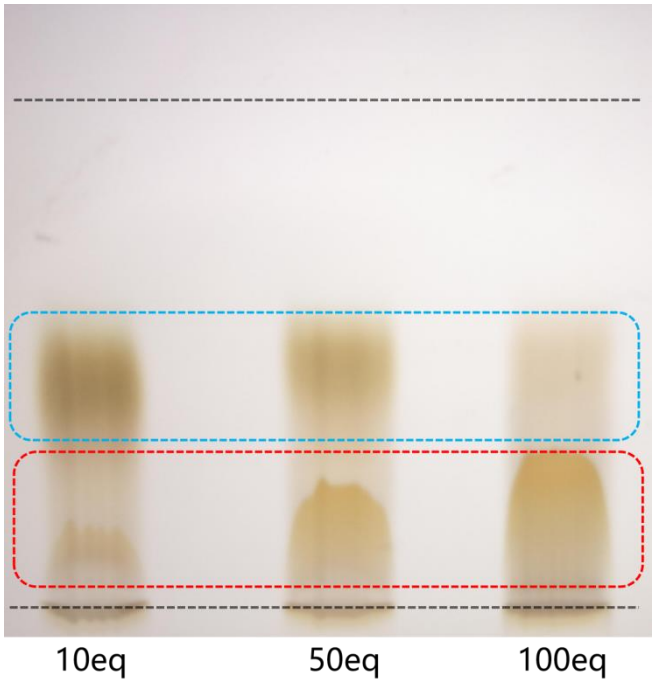

Figure S6. Photographs of the isolated products of $[Au_{25}(PET)_{18}]^-$ doped with Cd using different equivalent 2MBT ligand. The red and blue box indicate the $[Au_{19}Cd_3(2MBT)_{18}]^-$ and $Au_{24}Cd(2MBT)_{18}$, respectively.

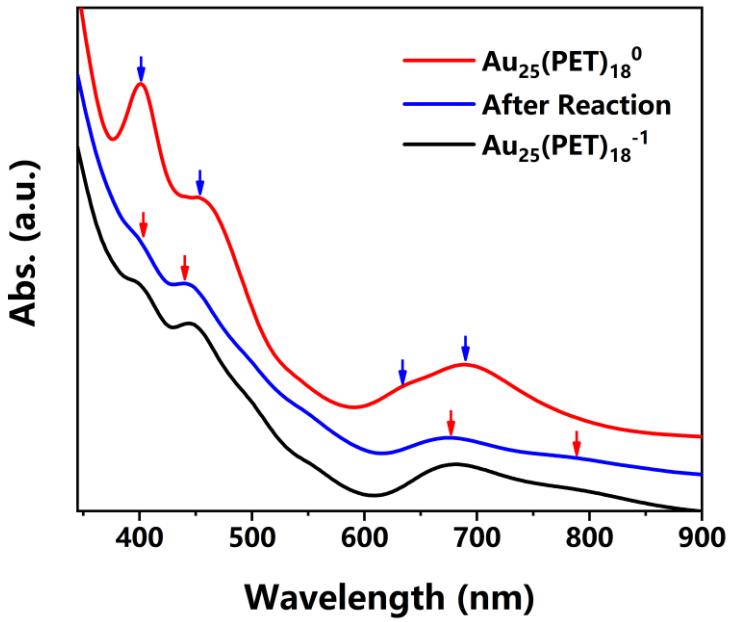

Figure S7. UV-vis-NIR spectra of $[Au_{25}(PET)_{18}]^-$ (black line), $[Au_{25}(PET)_{18}]^0$ (red line), and the product obtained by the addition of excess of phenylethanethiol (PET) to $[Au_{25}(PET)_{18}]^0$ (blue line), respectively.

Details of the transformation of $[Au_{25}(PET)_{18}]^0$ to $[Au_{25}(PET)_{18}]^-$. 10 mg of $[Au_{25}(PET)_{18}]^0$ was dissolved in acetonitrile (the solvent was purged with nitrogen and protected by nitrogen) and an excess amount (200 eq) of phenylethanethiol (as reducing agent) and TOAB (TOA^+ serving as the counter-ion for $[Au_{25}(PET)_{18}]^-$) were added into the vessel at the same time. The solution turns red within a few seconds under stirring at room temperature, and the UV-vis-NIR spectrum of the resulting product showed that the characteristic peak of $[Au_{25}(PET)_{18}]^0$ at ~ 400 nm was decreased, and the peak at 460 nm was enhanced and blue-shifted to 445 nm. The peak at 690 nm was blue-shifted to 680 nm, and the shoulder at 632 nm disappeared, while a new shoulder appeared around 800 nm, all of which is coincided with the UV-vis-NIR spectra of $[Au_{25}(PET)_{18}]^-$, indicating that Au_{25}^0 is reduced to Au_{25}^{-1} by excess thiol ligands.

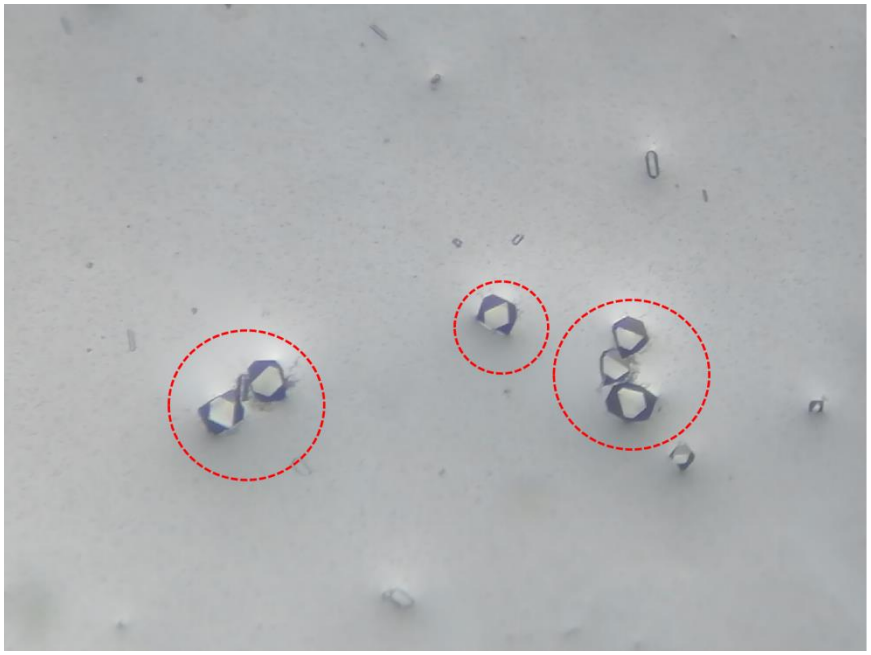

Figure S8. Photograph of the $Au_4Cd_4(2,4DMBT)_{12}$ single crystals.

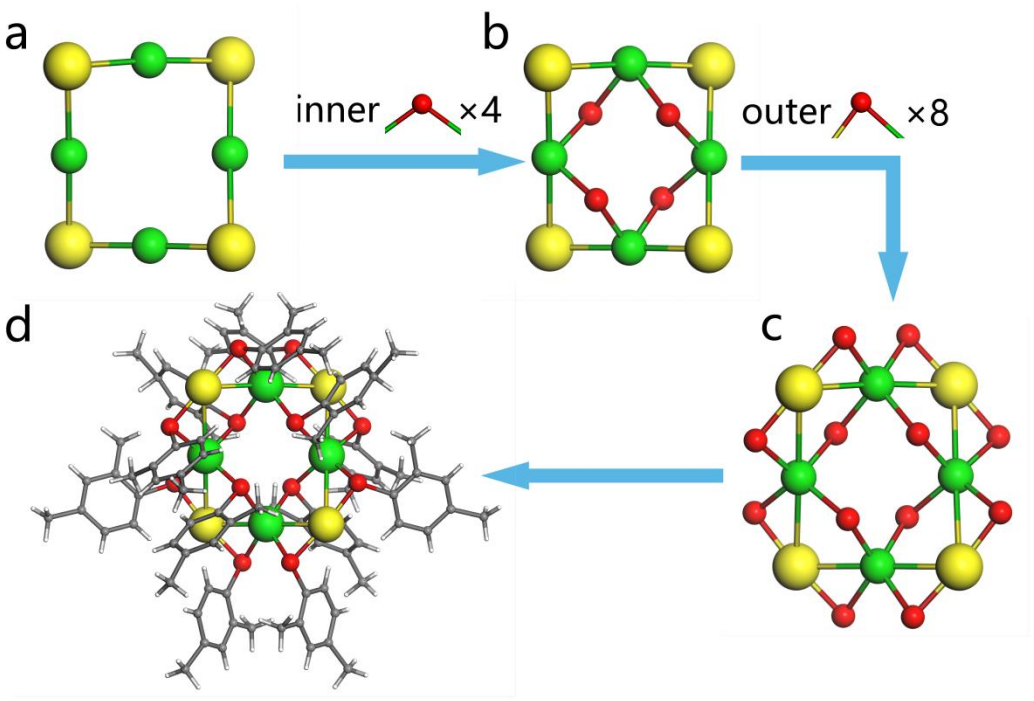

Figure S9. $Au_4Cd_4(2,4DMBT)_{12}$ cluster and its structural dissection. (a) Au_4Cd_4 framework. (b) Four simple bridging thiolates connected inside the Au_4Cd_4 framework. (c) Another eight simple bridging thiolates capped on the the Au_4Cd_4 framework. (d) Total structure of $Au_4Cd_4(2,4DMBT)_{12}$. Color codes: yellow sphere, Au; green sphere, Cd; red sphere, S; brown sphere, C.

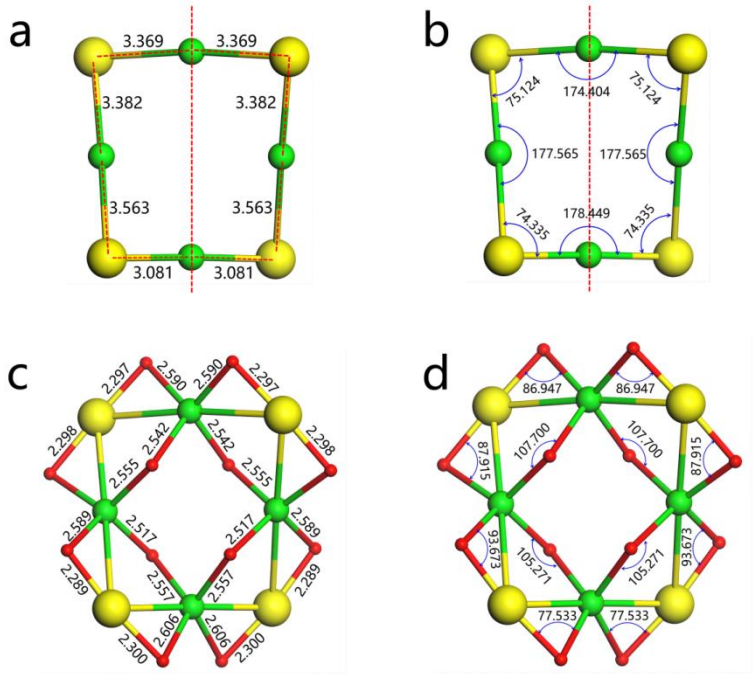

Figure S10. Interatomic distances/bond lengths and bond angles for $Au_4Cd_4(SR)_{12}$ cluster. Au-Cd interatomic distances (a) and Au-Cd-Au and Cd-Au-Cd bond angle in Au_4Cd_4 framework (b). Au-S and Cd-S bond lengths (c) and external Au-S-Cd and internal Cd-S-Cd bond angle in $Au_4Cd_4S_{12}$ framework (d).

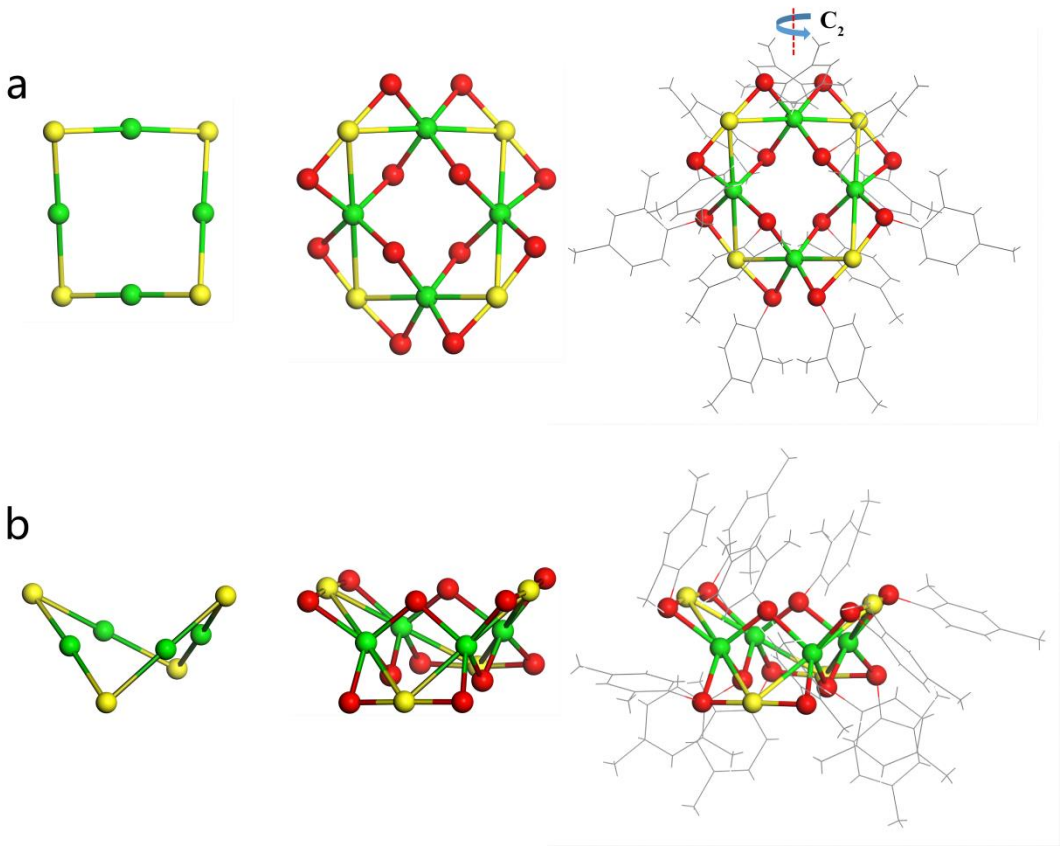

Figure S11. Different view directions of the overall structure of $Au_4Cd_4(2,4DMBT)_{12}$ and $Au_4Cd_4S_{12}$ framework. Color codes: yellow sphere, Au; green sphere, Cd; red sphere, S; brown sphere, C.

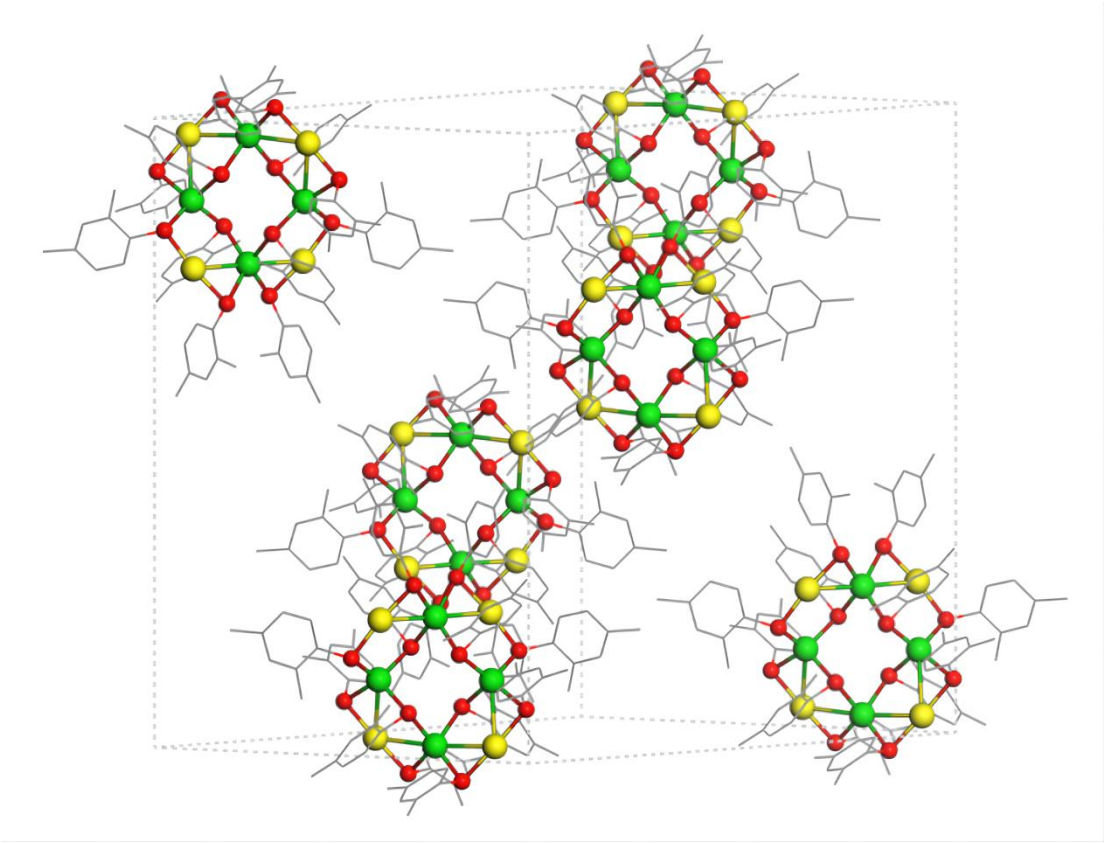

Figure S12. Three pairs of $Au_4Cd_4(2,4DMBT)_{12}$ enantiomers in a unit cell. Color codes: yellow sphere, Au; green sphere, Cd; red sphere, S. All H atoms are omitted for clarity.

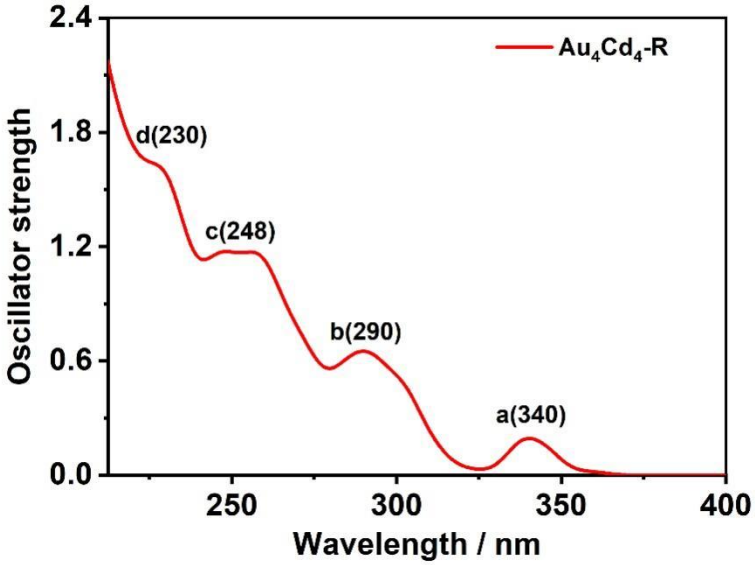

Figure S13. The calculated absorption spectrum of Au_4Cd_4-R at the TDDFT/PBE level. The spectrum is fitted with a Gaussian function with a width at half-maximum of 12 nm.

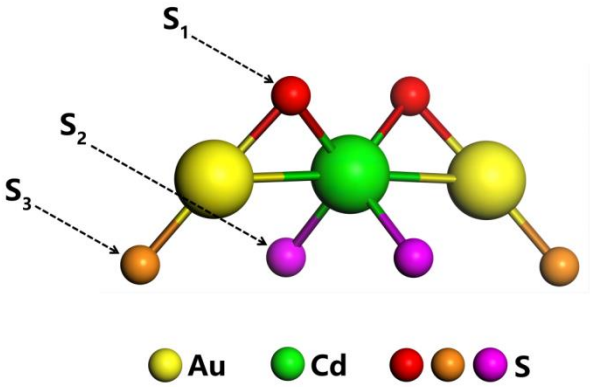

Figure S14. The Au_2CdS_6 motif in $Au_4Cd_4(SR)_{12}$ and $[Au_{19}Cd_3(SR)_{18}]^-$ clusters.

Table S1. Comparison of various bond lengths/interatomic distances between $Au_4Cd_4(2,4DMBT)_{12}$ and $[Au_{19}Cd_3(2,4DMBT)_{18}]^-$.

Type	Average bond lengths/interatomic distances		Differences
	$Au_4Cd_4(2,4DMBT)_{12}$	$[Au_{19}Cd_3(2,4DMBT)_{18}]^-$	
Cd-S_1 / Å	2.5580	2.5848	1.05%
Cd-Au / Å	3.3488	3.3455	0.10%
Cd-S_2 / Å	2.5428	2.5755	1.29%
Au-S_3 / Å	2.2960	2.2870	0.39%

Bond lengths/interatomic distances difference (%) was calculated using $Au_4Cd_4(2,4DMBT)_{12}$ as the reference.

Table S2. Crystal data and structure refinement of $[Au_{19}Cd_3(4TMBT)_{18}]^-$.

Empirical formula	$C_{126}H_{72}Au_{19}Cd_3F_{54}S_{18}$	
Formula weight	7268.6	
Temperature	296 K	
Wavelength	0.71073Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a=15.1732(12) Å	α=90.340(2)°
	b=22.1077(15) Å	β=92.313(3)°
	c=77.549(6) Å	γ=93.817(3)°
Volume	25934(3)Å^3	
Z	4	
Density (calculated)	1.862 Mg/m^3	
Absorption coefficient	11.150mm^{-1}	
F(000)	12988.0	
Crystal size	0.200 × 0.200 × 0.100 mm^3	
Theta range for data collection	1.915 to 24.108	
Index ranges	$-17 \le h \le 17$, $-25 \le k \le 25$, $-89 \le l \le 89$	
Reflections collected	149843	
Independent reflections	78572 [R(int) = 0.0540]	
Completeness to theta = 24.108°	95.2 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	78572 / 42048 / 3961	
Goodness-of-fit on F^2	1.127	
Final R indices [I>2sigma(I)]	R_1 = 0.0868, wR_2 = 0.2569	
R indices (all data)	R_1 = 0.1261, wR_2 = 0.2689	
Extinction coefficient	n/a	
Largest diff. peak and hole	3.388 and -2.376 e.Å^{-3}	

Table S3. Crystal data and structure refinement of $[Au_{19}Cd_3(TBBT)_{18}]^-$.

Empirical formula	$C_{180}H_{234}Au_{19}Cd_3S_{18}$	
Formula weight	7054.30	
Temperature	296 K	
Wavelength	0.71073Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a=47.857(19) Å	α=90°
	b=15.217(7) Å	β=90.932(11)°
	c=71.73(3) Å	γ=90°
Volume	52228(40)Å^3	
Z	8	
Density (calculated)	1.794 Mg/m^3	
Absorption coefficient	11.041 mm^{-1}	
F(000)	25976	
Crystal size	0.200 × 0.100 × 0.100 mm^3	
Theta range for data collection	1.868 to 24.439	
Index ranges	$-55 \le h \le 55$, $-13 \le k \le 17$, $-83 \le l \le 73$	
Reflections collected	129651	
Independent reflections	42091 [R(int) = 0.1704]	
Completeness to theta = 24.108°	97.5 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	42091 / 8273 / 1969	
Goodness-of-fit on F^2	0.930	
Final R indices [I>2sigma(I)]	R_1 = 0.0787, wR_2 = 0.1915	
R indices (all data)	R_1 = 0.2230, wR_2 = 0.2568	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.169 and -1.388 e.Å^{-3}	

Table S4. Crystal data and structure refinement of $[Au_{19}Cd_3(MOBT)_{18}]^-$.

Empirical formula	$C_{126}H_{126}Au_{19}Cd_3O_{18}S_{18}$
Formula weight	6584.90
Temperature	296 K
Wavelength	0.71073Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a=18.7128(19) Å α=90° b=32.533(3) Å β=101.032(3)° c=31.483(3) Å γ=90°
Volume	18812(3) $Å^3$
Z	4
Density (calculated)	2.325 Mg/m^3
Absorption coefficient	15.325 mm^{-1}
F(000)	11836
Crystal size	0.100 × 0.100 × 0.100 mm^3
Theta range for data collection	1.874 to 25.078
Index ranges	$-15 \le h \le 22, -38 \le k \le 38, -37 \le l \le 37$
Reflections collected	124278
Independent reflections	33194 [R(int) = 0.1026]
Completeness to theta = 24.108°	99.3 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	33194 / 5076 / 1442
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	$R_1 = 0.0783$, $wR_2 = 0.1990$
R indices (all data)	$R_1 = 0.1292$, $wR_2 = 0.2239$
Extinction coefficient	0.000186(10)
Largest diff. peak and hole	2.032 and -2.150 $e.Å^{-3}$

Table S5. Crystal data and structure refinement of $[Au_{19}Cd_3(2,4DMBT)_{18}]^-$.

Empirical formula	$C_{144}H_{162}Au_{19}Cd_3S_{18}$	
Formula weight	6549.59	
Temperature	193(2) K	
Wavelength	1.34139 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a=19.7023(11) Å	α=74.779(3)°
	b=32.6182(18) Å	β=79.545(3)°
	c=32.7460(16) Å	γ=85.474(3)°
Volume	19958.1(19) $Å^3$	
Z	1	
Density (calculated)	2.257 Mg/m^3	
Absorption coefficient	20.609 mm^{-1}	
F(000)	12368	
Crystal size	0.2 × 0.2 × 0.1 mm^3	
Theta range for data collection	1.222 to 48.432	
Index ranges	$-21 \le h \le 21, -36 \le k \le 36, -33 \le l \le 36$	
Reflections collected	182811	
Independent reflections	57621 [R(int) = 0.1951]	
Completeness to theta = 24.108°	99.4 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	57621 / 31488 / 3594	
Goodness-of-fit on F^2	0.983	
Final R indices [I>2sigma(I)]	R_1 = 0.0854, wR_2 = 0.1896	
R indices (all data)	R_1 = 0.2523, wR_2 = 0.2490	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.564 and -1.343 $e.Å^{-3}$	

Table S6. Crystal data and structure refinement of $Au_4Cd_4(2,4DMBT)_{12}$.

Empirical formula	$C_{96}H_{110}Au_4Cd_4S_{12}$	
Formula weight	3224.29	
Temperature	190(2) K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a=23.804(4) Å	α=90°
	b=29.872(5) Å	β=124.916(7)°
	c=18.804(3) Å	γ=90°
Volume	10964(3)Å^3	
Z	4	
Density (calculated)	1.953 Mg/m^3	
Absorption coefficient	15.079 mm^{-1}	
F(000)	6040	
Crystal size	0.12 × 0.1 × 0.1 mm^3	
Theta range for data collection	2.476 to 54.471	
Index ranges	$-28 \le h \le 28$, $-35 \le k \le 36$, $-22 \le l \le 22$	
Reflections collected	55155	
Independent reflections	10152 [R(int) = 0.0711]	
Completeness to theta = 24.108°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10152 / 249 / 452	
Goodness-of-fit on F^2	1.816	
Final R indices [I>2sigma(I)]	R_1 = 0.1236, wR_2 = 0.3204	
R indices (all data)	R_1 = 0.1506, wR_2 = 0.3408	
Extinction coefficient	n/a	
Largest diff. peak and hole	5.998 and -3.065 e.Å^{-3}	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Au_4Cd_4(2,4DMBT)_{12}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Au(1)	3735(1)	7276(1)	2522(1)	49(1)
Au(2)	5351(1)	5274(1)	4496(1)	67(1)
Cd(1)	5000	7262(1)	2500	49(1)
Cd(2)	4597(1)	6259(1)	3551(1)	54(1)
Cd(3)	5000	5219(1)	2500	60(1)
S(3)	5561(1)	6722(1)	3785(1)	49(1)
S(2)	4006(1)	7829(1)	1933(1)	51(1)
S(1)	3462(1)	6665(1)	2983(2)	58(1)
S(4)	4098(1)	5785(1)	2187(2)	55(1)
S(5)	5047(1)	5858(1)	4986(2)	65(1)
S(6)	5564(1)	4714(1)	3860(2)	72(1)
C(19)	5849(5)	6140(3)	5782(6)	57(2)
C(27)	5831(4)	7102(3)	4657(5)	48(2)
C(26)	6515(4)	7240(3)	5159(6)	50(2)
C(39)	3425(4)	5520(3)	2171(6)	55(2)
C(13)	4338(4)	8276(3)	2690(6)	52(2)
C(28)	5393(4)	7255(3)	4844(6)	63(2)
C(25)	7025(4)	7048(3)	5019(6)	66(3)
C(5)	3448(4)	6809(3)	3881(6)	60(2)
C(34)	2757(5)	5664(3)	1590(7)	70(3)
C(38)	3560(5)	5170(3)	2737(7)	74(3)
C(18)	5831(5)	6436(3)	6317(7)	67(3)
C(20)	6430(5)	6074(3)	5825(7)	67(3)
C(30)	6289(5)	7720(3)	5995(7)	79(3)
C(14)	4177(5)	8717(3)	2377(7)	72(3)
C(33)	2566(5)	6023(3)	932(7)	88(3)
C(21)	7033(5)	6274(3)	6472(8)	81(3)
C(29)	5627(5)	7557(3)	5526(7)	77(3)
C(31)	6707(5)	7556(3)	5789(7)	69(3)
C(41)	6454(5)	4739(3)	4291(7)	73(3)
C(12)	4724(5)	8224(3)	3554(7)	76(3)
C(22)	7055(6)	6565(4)	7042(8)	84(3)

C(46)	6680(6)	4481(3)	3911(7)	77(3)
C(43)	7589(6)	5009(4)	5353(8)	105(4)
C(15)	4415(5)	9076(3)	2949(8)	77(3)
C(4)	3231(5)	6481(4)	4193(8)	82(3)
C(23)	6449(6)	6638(3)	6943(7)	82(3)
C(42)	6906(6)	5013(3)	5013(7)	85(3)
C(37)	3046(6)	4972(4)	2740(8)	89(3)
C(10)	4799(6)	9014(4)	3837(9)	89(4)
C(11)	4966(6)	8579(4)	4157(8)	101(4)
C(45)	7385(7)	4496(4)	4288(9)	103(4)
C(6)	3601(5)	7237(3)	4226(6)	66(3)
C(35)	2237(5)	5457(4)	1592(8)	92(4)
C(3)	3201(6)	6602(5)	4865(9)	114(5)
C(48)	8593(6)	4784(5)	5323(10)	157(7)
C(16)	3758(6)	8808(3)	1403(8)	98(4)
C(17)	5198(6)	6532(3)	6274(8)	95(4)
C(47)	6233(6)	4186(4)	3171(8)	111(4)
C(8)	3051(6)	6017(4)	3840(9)	115(5)
C(9)	5043(6)	9417(4)	4474(9)	135(6)
C(32)	6532(6)	8045(4)	6707(8)	127(5)
C(36)	2386(6)	5114(4)	2165(9)	99(4)
C(7)	3547(6)	7347(4)	4903(8)	100(4)
C(40)	1805(6)	4892(5)	2161(10)	163(7)
C(24)	7711(6)	6806(4)	7747(8)	125(5)
C(44)	7832(7)	4760(5)	4976(11)	112(4)
C(2)	3330(8)	7018(6)	5212(10)	119(6)
C(1B)	3146(19)	7059(14)	5870(20)	116(8)
C(1A)	3434(19)	7242(12)	6038(17)	117(8)

Table S8. Bond lengths [Å] and angles [°] for $Au_4Cd_4(2,4DMBT)_{12}$.

Au(1)-Cd(1)	3.0812(5)
Au(1)-S(2)	2.300(2)
Au(1)-S(1)	2.289(2)
Au(2)-Cd(2)	3.3820(8)
Au(2)-Cd(3)	3.3686(10)
Au(2)-S(5)	2.297(2)
Au(2)-S(6)	2.297(3)
Cd(1)-S(3)#1	2.557(2)
Cd(1)-S(3)	2.557(2)
Cd(1)-S(2)#1	2.606(2)
Cd(1)-S(2)	2.606(2)
Cd(2)-S(3)	2.5167(19)
Cd(2)-S(1)	2.589(2)
Cd(2)-S(4)	2.555(2)
Cd(2)-S(5)	2.567(3)
Cd(3)-S(4)	2.542(2)
Cd(3)-S(4)#1	2.542(2)
Cd(3)-S(6)	2.590(3)
Cd(3)-S(6)#1	2.590(3)
S(3)-C(27)	1.791(8)
S(2)-C(13)	1.779(9)
S(1)-C(5)	1.780(9)
S(4)-C(39)	1.796(8)
S(5)-C(19)	1.822(9)
S(6)-C(41)	1.799(10)
C(19)-C(18)	1.369(12)
C(19)-C(20)	1.373(11)
C(27)-C(26)	1.402(10)
C(27)-C(28)	1.377(11)
C(26)-C(25)	1.516(10)
C(26)-C(31)	1.377(12)
C(39)-C(34)	1.385(12)
C(39)-C(38)	1.397(12)
C(13)-C(14)	1.408(12)
C(13)-C(12)	1.339(12)
C(28)-H(28)	0.9300

C(28)-C(29)	1.399(12)
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(5)-C(4)	1.398(12)
C(5)-C(6)	1.389(12)
C(34)-C(33)	1.503(13)
C(34)-C(35)	1.406(13)
C(38)-H(38)	0.9300
C(38)-C(37)	1.381(11)
C(18)-C(23)	1.391(13)
C(18)-C(17)	1.509(12)
C(20)-H(20)	0.9300
C(20)-C(21)	1.376(13)
C(30)-C(29)	1.385(13)
C(30)-C(31)	1.371(12)
C(30)-C(32)	1.482(13)
C(14)-C(15)	1.392(13)
C(14)-C(16)	1.525(14)
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(21)-H(21)	0.9300
C(21)-C(22)	1.367(14)
C(29)-H(29)	0.9300
C(31)-H(31)	0.9300
C(41)-C(46)	1.372(13)
C(41)-C(42)	1.412(14)
C(12)-H(12)	0.9300
C(12)-C(11)	1.415(13)
C(22)-C(23)	1.379(14)
C(22)-C(24)	1.530(14)
C(46)-C(45)	1.409(15)
C(46)-C(47)	1.465(14)
C(43)-H(43)	0.9300
C(43)-C(42)	1.376(14)
C(43)-C(44)	1.379(17)
C(15)-H(15)	0.9300

C(15)-C(10)	1.380(15)
C(4)-C(3)	1.369(16)
C(4)-C(8)	1.496(15)
C(23)-H(23)	0.9300
C(42)-H(42)	0.9300
C(37)-H(37)	0.9300
C(37)-C(36)	1.370(15)
C(10)-C(11)	1.398(15)
C(10)-C(9)	1.561(14)
C(11)-H(11)	0.9300
C(45)-H(45)	0.9300
C(45)-C(44)	1.360(17)
C(6)-H(6)	0.9300
C(6)-C(7)	1.405(13)
C(35)-H(35)	0.9300
C(35)-C(36)	1.382(15)
C(3)-H(3)	0.9300
C(3)-C(2)	1.360(18)
C(48)-H(48A)	0.9600
C(48)-H(48B)	0.9600
C(48)-H(48C)	0.9600
C(48)-C(44)	1.549(17)
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(47)-H(47A)	0.9600
C(47)-H(47B)	0.9600
C(47)-H(47C)	0.9600
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(32)-H(32A)	0.9600

C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(36)-C(40)	1.548(13)
C(7)-H(7)	0.9300
C(7)-C(2)	1.398(16)
C(40)-H(40A)	0.9600
C(40)-H(40B)	0.9600
C(40)-H(40C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(2)-C(1B)	1.553(19)
C(2)-C(1A)	1.59(2)
C(1B)-H(1BA)	0.9600
C(1B)-H(1BB)	0.9600
C(1B)-H(1BC)	0.9600
C(1A)-H(1AA)	0.9600
C(1A)-H(1AB)	0.9600
C(1A)-H(1AC)	0.9600

S(2)-Au(1)-Cd(1)	55.67(5)
S(1)-Au(1)-Cd(1)	120.30(6)
S(1)-Au(1)-S(2)	172.59(8)
Cd(3)-Au(2)-Cd(2)	75.12(2)
S(5)-Au(2)-Cd(2)	49.32(6)
S(5)-Au(2)-Cd(3)	124.33(7)
S(6)-Au(2)-Cd(2)	125.26(7)
S(6)-Au(2)-Cd(3)	50.14(7)
S(6)-Au(2)-S(5)	173.97(10)
Au(1)#1-Cd(1)-Au(1)	178.45(3)
S(3)-Cd(1)-Au(1)#1	92.66(4)
S(3)-Cd(1)-Au(1)	88.32(4)
S(3)#1-Cd(1)-Au(1)#1	88.32(4)
S(3)#1-Cd(1)-Au(1)	92.66(4)
S(3)-Cd(1)-S(3)#1	101.41(10)
S(3)#1-Cd(1)-S(2)	100.04(7)
S(3)-Cd(1)-S(2)	130.73(6)
S(3)-Cd(1)-S(2)#1	100.04(7)

S(3)#1-Cd(1)-S(2)#1	130.73(6)
S(2)#1-Cd(1)-Au(1)#1	46.80(5)
S(2)-Cd(1)-Au(1)	46.80(5)
S(2)-Cd(1)-Au(1)#1	131.83(5)
S(2)#1-Cd(1)-Au(1)	131.83(5)
S(2)#1-Cd(1)-S(2)	98.50(10)
S(3)-Cd(2)-Au(2)	103.56(5)
S(3)-Cd(2)-S(1)	117.26(7)
S(3)-Cd(2)-S(4)	108.94(7)
S(3)-Cd(2)-S(5)	107.42(7)
S(1)-Cd(2)-Au(2)	137.87(5)
S(4)-Cd(2)-Au(2)	80.74(5)
S(4)-Cd(2)-S(1)	94.82(8)
S(4)-Cd(2)-S(5)	118.08(8)
S(5)-Cd(2)-Au(2)	42.76(6)
S(5)-Cd(2)-S(1)	110.41(8)
Au(2)#1-Cd(3)-Au(2)	174.41(3)
S(4)-Cd(3)-Au(2)	81.19(5)
S(4)#1-Cd(3)-Au(2)	95.06(6)
S(4)-Cd(3)-Au(2)#1	95.05(5)
S(4)#1-Cd(3)-Au(2)#1	81.19(5)
S(4)#1-Cd(3)-S(4)	96.22(10)
S(4)-Cd(3)-S(6)#1	106.26(8)
S(4)#1-Cd(3)-S(6)#1	120.15(8)
S(4)#1-Cd(3)-S(6)	106.26(8)
S(4)-Cd(3)-S(6)	120.15(8)
S(6)-Cd(3)-Au(2)	42.91(6)
S(6)#1-Cd(3)-Au(2)#1	42.91(6)
S(6)#1-Cd(3)-Au(2)	142.14(6)
S(6)-Cd(3)-Au(2)#1	142.14(6)
S(6)-Cd(3)-S(6)#1	108.30(11)
Cd(2)-S(3)-Cd(1)	105.27(8)
C(27)-S(3)-Cd(1)	100.5(3)
C(27)-S(3)-Cd(2)	108.3(3)
Au(1)-S(2)-Cd(1)	77.53(6)
C(13)-S(2)-Au(1)	105.9(3)
C(13)-S(2)-Cd(1)	106.8(3)
Au(1)-S(1)-Cd(2)	93.68(7)

C(5)-S(1)-Au(1)	110.1(3)
C(5)-S(1)-Cd(2)	109.0(3)
Cd(3)-S(4)-Cd(2)	107.70(9)
C(39)-S(4)-Cd(2)	98.5(3)
C(39)-S(4)-Cd(3)	110.6(3)
Au(2)-S(5)-Cd(2)	87.92(9)
C(19)-S(5)-Au(2)	104.7(3)
C(19)-S(5)-Cd(2)	104.3(3)
Au(2)-S(6)-Cd(3)	86.95(8)
C(41)-S(6)-Au(2)	107.8(4)
C(41)-S(6)-Cd(3)	102.7(3)
C(18)-C(19)-S(5)	115.9(7)
C(18)-C(19)-C(20)	121.7(9)
C(20)-C(19)-S(5)	122.4(7)
C(26)-C(27)-S(3)	117.5(6)
C(28)-C(27)-S(3)	122.2(6)
C(28)-C(27)-C(26)	120.3(8)
C(27)-C(26)-C(25)	121.6(8)
C(31)-C(26)-C(27)	117.0(8)
C(31)-C(26)-C(25)	121.3(8)
C(34)-C(39)-S(4)	119.7(7)
C(34)-C(39)-C(38)	119.2(8)
C(38)-C(39)-S(4)	121.2(7)
C(14)-C(13)-S(2)	119.1(7)
C(12)-C(13)-S(2)	124.2(7)
C(12)-C(13)-C(14)	116.7(9)
C(27)-C(28)-H(28)	120.0
C(27)-C(28)-C(29)	120.0(8)
C(29)-C(28)-H(28)	120.0
C(26)-C(25)-H(25A)	109.5
C(26)-C(25)-H(25B)	109.5
C(26)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(4)-C(5)-S(1)	117.2(8)
C(6)-C(5)-S(1)	121.9(7)
C(6)-C(5)-C(4)	120.8(9)

C(39)-C(34)-C(33)	122.3(8)
C(39)-C(34)-C(35)	119.0(9)
C(35)-C(34)-C(33)	118.7(9)
C(39)-C(38)-H(38)	119.3
C(37)-C(38)-C(39)	121.3(10)
C(37)-C(38)-H(38)	119.3
C(19)-C(18)-C(23)	115.6(9)
C(19)-C(18)-C(17)	123.7(9)
C(23)-C(18)-C(17)	120.6(10)
C(19)-C(20)-H(20)	120.0
C(19)-C(20)-C(21)	120.0(10)
C(21)-C(20)-H(20)	120.0
C(29)-C(30)-C(32)	120.8(10)
C(31)-C(30)-C(29)	117.0(9)
C(31)-C(30)-C(32)	122.1(9)
C(13)-C(14)-C(16)	120.2(9)
C(15)-C(14)-C(13)	120.7(10)
C(15)-C(14)-C(16)	119.1(10)
C(34)-C(33)-H(33A)	109.5
C(34)-C(33)-H(33B)	109.5
C(34)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(20)-C(21)-H(21)	119.5
C(22)-C(21)-C(20)	121.1(10)
C(22)-C(21)-H(21)	119.5
C(28)-C(29)-H(29)	119.6
C(30)-C(29)-C(28)	120.8(9)
C(30)-C(29)-H(29)	119.6
C(26)-C(31)-H(31)	117.7
C(30)-C(31)-C(26)	124.6(9)
C(30)-C(31)-H(31)	117.7
C(46)-C(41)-S(6)	118.4(9)
C(46)-C(41)-C(42)	121.3(10)
C(42)-C(41)-S(6)	120.3(9)
C(13)-C(12)-H(12)	117.8
C(13)-C(12)-C(11)	124.4(10)

C(11)-C(12)-H(12)	117.8
C(21)-C(22)-C(23)	116.6(10)
C(21)-C(22)-C(24)	122.3(11)
C(23)-C(22)-C(24)	121.1(12)
C(41)-C(46)-C(45)	116.8(11)
C(41)-C(46)-C(47)	123.2(11)
C(45)-C(46)-C(47)	120.0(11)
C(42)-C(43)-H(43)	119.3
C(42)-C(43)-C(44)	121.3(13)
C(44)-C(43)-H(43)	119.3
C(14)-C(15)-H(15)	119.2
C(10)-C(15)-C(14)	121.7(10)
C(10)-C(15)-H(15)	119.2
C(5)-C(4)-C(8)	123.2(10)
C(3)-C(4)-C(5)	116.4(12)
C(3)-C(4)-C(8)	120.4(11)
C(18)-C(23)-H(23)	117.6
C(22)-C(23)-C(18)	124.7(11)
C(22)-C(23)-H(23)	117.6
C(41)-C(42)-H(42)	120.6
C(43)-C(42)-C(41)	118.9(11)
C(43)-C(42)-H(42)	120.6
C(38)-C(37)-H(37)	120.2
C(36)-C(37)-C(38)	119.5(11)
C(36)-C(37)-H(37)	120.2
C(15)-C(10)-C(11)	118.2(10)
C(15)-C(10)-C(9)	121.5(11)
C(11)-C(10)-C(9)	120.3(12)
C(12)-C(11)-H(11)	120.9
C(10)-C(11)-C(12)	118.3(12)
C(10)-C(11)-H(11)	120.9
C(46)-C(45)-H(45)	118.3
C(44)-C(45)-C(46)	123.3(13)
C(44)-C(45)-H(45)	118.3
C(5)-C(6)-H(6)	119.7
C(5)-C(6)-C(7)	120.5(9)
C(7)-C(6)-H(6)	119.7
C(34)-C(35)-H(35)	119.6

C(36)-C(35)-C(34)	120.7(10)
C(36)-C(35)-H(35)	119.6
C(4)-C(3)-H(3)	117.5
C(2)-C(3)-C(4)	125.1(12)
C(2)-C(3)-H(3)	117.5
H(48A)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(44)-C(48)-H(48A)	109.5
C(44)-C(48)-H(48B)	109.5
C(44)-C(48)-H(48C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-H(17A)	109.5
C(18)-C(17)-H(17B)	109.5
C(18)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(4)-C(8)-H(8A)	109.5
C(4)-C(8)-H(8B)	109.5
C(4)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-H(9A)	109.5
C(10)-C(9)-H(9B)	109.5
C(10)-C(9)-H(9C)	109.5

H(9A)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(37)-C(36)-C(35)	120.3(10)
C(37)-C(36)-C(40)	119.9(12)
C(35)-C(36)-C(40)	119.9(12)
C(6)-C(7)-H(7)	120.8
C(2)-C(7)-C(6)	118.5(12)
C(2)-C(7)-H(7)	120.8
C(36)-C(40)-H(40A)	109.5
C(36)-C(40)-H(40B)	109.5
C(36)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(43)-C(44)-C(48)	120.9(14)
C(45)-C(44)-C(43)	118.3(13)
C(45)-C(44)-C(48)	120.8(15)
C(3)-C(2)-C(7)	118.6(12)
C(3)-C(2)-C(1B)	112(2)
C(3)-C(2)-C(1A)	136.7(19)
C(7)-C(2)-C(1B)	129(2)
C(7)-C(2)-C(1A)	103.6(19)
C(2)-C(1B)-H(1BA)	109.5
C(2)-C(1B)-H(1BB)	109.5
C(2)-C(1B)-H(1BC)	109.5

H(1BA)-C(1B)-H(1BB)	109.5
H(1BA)-C(1B)-H(1BC)	109.5
H(1BB)-C(1B)-H(1BC)	109.5
C(2)-C(1A)-H(1AA)	109.5
C(2)-C(1A)-H(1AB)	109.5
C(2)-C(1A)-H(1AC)	109.5
H(1AA)-C(1A)-H(1AB)	109.5
H(1AA)-C(1A)-H(1AC)	109.5
H(1AB)-C(1A)-H(1AC)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $Au_4Cd_4(2,4DMBT)_{12}$. The anisotropicdisplacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	43(1)	56(1)	46(1)	0(1)	24(1)	1(1)
Au(2)	85(1)	56(1)	58(1)	3(1)	40(1)	-8(1)
Cd(1)	46(1)	55(1)	44(1)	0	26(1)	0
Cd(2)	51(1)	53(1)	57(1)	-4(1)	31(1)	-8(1)
Cd(3)	67(1)	55(1)	60(1)	0	38(1)	0
S(3)	43(1)	50(1)	48(2)	0(1)	24(1)	-5(1)
S(2)	48(1)	57(1)	42(1)	4(1)	22(1)	4(1)
S(1)	52(1)	63(1)	58(2)	2(1)	32(1)	-3(1)
S(4)	56(1)	55(1)	55(2)	-4(1)	33(1)	-7(1)
S(5)	73(2)	64(1)	64(2)	1(1)	43(2)	-13(1)
S(6)	97(2)	56(1)	60(2)	-1(1)	45(2)	-11(1)
C(19)	77(6)	48(5)	33(6)	5(4)	26(5)	-8(4)
C(27)	43(5)	55(5)	37(5)	3(4)	19(4)	-1(4)
C(26)	43(5)	51(5)	42(6)	0(4)	17(4)	-6(4)
C(39)	54(5)	60(5)	47(6)	-3(4)	28(5)	-16(4)
C(13)	55(5)	55(5)	33(6)	4(4)	19(5)	7(4)
C(28)	40(5)	74(6)	49(6)	-11(5)	13(5)	-4(4)
C(25)	39(5)	83(6)	67(7)	-4(5)	26(5)	-4(4)
C(5)	49(5)	77(6)	60(7)	17(5)	36(5)	15(4)
C(34)	57(6)	81(7)	52(7)	-3(5)	21(6)	-6(5)
C(38)	68(6)	86(7)	58(7)	-7(5)	32(6)	-18(5)
C(18)	60(6)	86(7)	52(7)	9(5)	30(6)	-8(5)
C(20)	63(6)	64(6)	80(8)	3(5)	46(6)	-8(5)
C(30)	53(6)	87(7)	64(8)	-27(6)	15(6)	6(5)
C(14)	53(6)	71(7)	75(9)	6(6)	29(6)	9(5)
C(33)	82(7)	94(8)	70(9)	-1(6)	34(7)	3(6)
C(21)	60(7)	89(8)	86(10)	14(7)	39(7)	-8(6)
C(29)	83(8)	91(7)	62(8)	1(6)	45(7)	12(6)
C(31)	63(6)	64(6)	65(8)	-13(5)	30(6)	-12(5)
C(41)	84(7)	58(6)	63(8)	18(5)	36(7)	3(5)
C(12)	78(7)	65(6)	72(9)	-9(6)	36(7)	-6(5)
C(22)	76(8)	102(9)	63(9)	10(6)	34(7)	-16(6)
C(46)	102(9)	63(6)	62(8)	1(5)	45(7)	7(6)

C(43)	73(8)	99(9)	68(10)	22(7)	-1(7)	9(7)
C(15)	46(6)	77(7)	76(9)	-5(6)	18(6)	14(5)
C(4)	69(7)	105(9)	85(9)	34(7)	52(7)	23(6)
C(23)	103(9)	91(8)	48(7)	-4(5)	41(7)	-20(6)
C(42)	86(8)	62(7)	66(9)	2(6)	21(7)	4(6)
C(37)	87(8)	107(9)	81(9)	-5(7)	53(8)	-42(7)
C(10)	76(8)	72(7)	92(10)	-23(7)	35(8)	5(6)
C(11)	104(9)	99(9)	77(10)	-20(7)	40(8)	-14(7)
C(45)	94(10)	86(9)	94(12)	20(7)	36(9)	29(7)
C(6)	75(6)	76(7)	58(7)	20(5)	45(6)	26(5)
C(35)	48(6)	140(11)	61(9)	-4(7)	17(6)	-23(6)
C(3)	81(8)	181(15)	104(12)	66(11)	69(9)	34(10)
C(48)	72(9)	177(15)	152(17)	31(12)	27(10)	19(9)
C(16)	118(9)	80(7)	114(11)	41(7)	78(9)	24(7)
C(17)	121(10)	96(8)	100(10)	-27(7)	83(9)	-21(7)
C(47)	119(10)	83(8)	107(12)	2(7)	53(9)	39(7)
C(8)	93(9)	108(10)	148(14)	38(9)	73(10)	-12(7)
C(9)	76(8)	114(10)	162(15)	-65(10)	41(9)	10(7)
C(32)	78(8)	152(12)	98(11)	-54(9)	23(8)	13(8)
C(36)	76(8)	128(10)	78(10)	-21(8)	37(8)	-47(7)
C(7)	128(10)	114(9)	81(9)	22(7)	75(9)	55(8)
C(40)	116(11)	250(18)	132(15)	2(12)	78(11)	-97(11)
C(24)	92(9)	160(12)	85(11)	-15(9)	31(8)	-63(9)
C(44)	104(11)	97(10)	116(14)	18(9)	54(11)	11(8)
C(2)	151(13)	162(13)	110(12)	52(11)	112(12)	59(11)
C(1B)	122(13)	157(15)	116(12)	22(9)	96(10)	1(10)
C(1A)	122(13)	158(15)	117(12)	21(9)	96(10)	2(10)