

Supporting Information

Stabilization of Ultra-Small Gold Nanoparticles in a Photochromic Organic Cage: Modulating Photocatalytic CO₂ Reduction by Tuning Light Irradiation

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Physical Measurements:

Thermal stability was studied using Mettler Toledo TGA 850 instrument in the temperature range of 30-800 °C with the heating rate of 5 °C/min in N₂ atmosphere. Elemental analysis was performed using Thermo Scientific Flash 2000 CHN analyzer. Powder X-ray diffraction experiment was performed in Bruker D8 discover instrument using Cu-K α radiation. Field Emission Scanning Electron Microscope (FESEM) images were collected using Lica-S440I FESEM instrument. Samples were prepared on a silicon wafer for FESEM studies, and high vacuum with 100 kV accelerating voltage was used for FESEM analysis. Energy dispersive spectroscopy (EDS) analysis was performed with an EDAX genesis instrument attached to the FESEM column. Transmission Electron Microscopic (TEM) images were captured using JEOL JEM-3010 TEM with the accelerating voltage of 300 kV. The organic cage (TAE-DTE) was taken in ethanol and drop cast over carbon-coated copper grid prior to TEM analysis. Whereas, FE-SEM images were taken by drop casting ethanolic dispersion of the material over silicon wafer. UV-Vis studies were performed using the Perkin Elmer Model Lambda 900 spectrophotometer instrument. The lifetime studies were carried out using Edinburgh instrument (FLS 1000). For the lifetime measurement, a nano-LED source with 510 nm was used. ICP analysis was performed using a PerkinElmer Optima 7000 DV instrument. ¹H-NMR spectra were recorded at 600 MHz frequency using a JEOL Varian Inova 600 MHz spectrometer. ¹³C-spectrum was recorded in the same NMR spectrometer at the frequency of 150 MHz. Tetramethyl silane (TMS) was used as an internal reference, and chemical shifts were given in ppm.

***In-situ* Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) measurements:** The IR experiment and *in-situ* DRIFTS measurements were carried out using FT-IR spectrophotometer (BRUKER, VORTEX 70B) within a photoreactor. The 10 mg of photocatalyst (Au@TAE-DTE-O) was evenly coated on the glass disc of 1 cm diameter and placed inside the photoreactor for monitoring reaction progress of photocatalytic CO₂ reduction. Next, the vacuum was applied to remove the air inside the photoreactor and then 99.99 % CO₂ gas along with water vapour was passed for 15 minutes inside the photoreactor. At last, the visible light was irradiated on catalyst by 150 W white LED light (> 400 nm). In situ FT-IR signal was collected through MCT detector at a regular time interval.

Computational Details:

The density functional theoretical (DFT) calculations were performed to obtain the free energy change associated with the open-to-closed transformation of DTE embedded cage. The DFT method was also utilized to determine the stabilization energy of gold within the cage cavity. Time-dependant DFT (TD-DFT) calculations were also performed to gain insight about electronic transitions. In computations, we utilized the B3LYP hybrid density functional method in conjunction with 6-31G(d) basis set.¹ The LANL2DZ was used as basis set and effective core potential (ECP) of Au atoms. The weakly interactive dispersive interactions were tackled in computations by Grimme's d3 (GD3) method.² Verification of the optimized structures was carried out by analytical vibrational frequency analysis which showed the presence of no imaginary frequency in all the optimized structures. All calculations were carried out in Gaussian09 program.³ Free energy changes at 25 °C are presented in kcal mol⁻¹. Moreover, the Schrodinger suite was utilized to measure the cavity volume of TAE-DTE-O and TAE-DTE-C.⁴

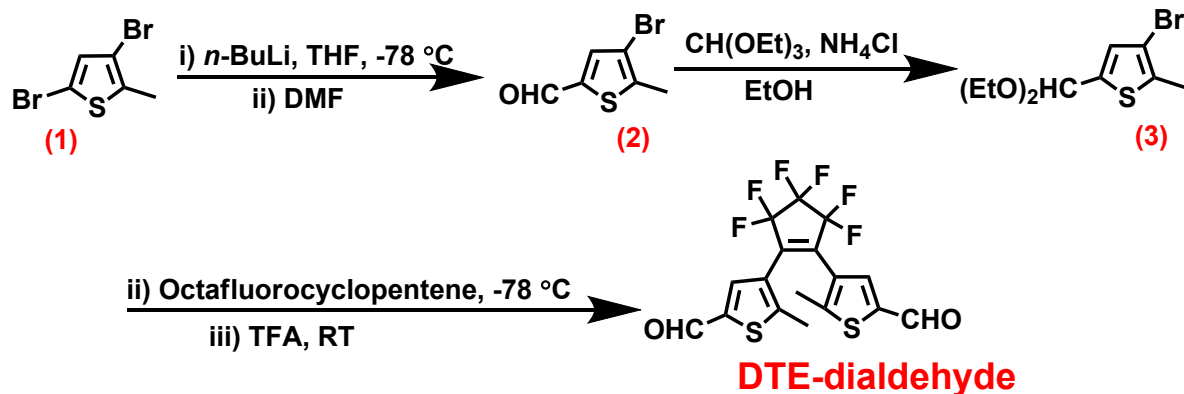
Experimental Section:

Materials and method: Chemicals used for the synthesis of *4,4'-(perfluorocyclopent-1-ene-1,2-diyl)bis(5-methylthiophene-2-carbaldehyde)* (DTE-dialdehyde) were procured from Sigma-Aldrich Chemical Co. Ltd and used as such. 2,2',2''-Triaminotriethylamine (TAE) and hydrated gold salt (AuCl₃.6H₂O) were obtained from Sigma-Aldrich Chemical Co. Ltd and used as such. All solvents were purchased from Spectrochem Pvt. Ltd. India. All the solvents used for the synthesis of DTE-aldehyde were dried using reported procedure before using in the reactions.⁵ HPLC grade anhydrous acetonitrile was purchased from Sigma-Aldrich Chemical Co. Ltd and used as such for photochemical CO₂ reduction. For column chromatography, solvents were purchased from Finar Ltd, India and used as such. Deuterated chloroform (CDCl₃) was purchased from Sigma-Aldrich Chemical Co. Ltd and used for ¹H and ¹³C-NMR as such.

Synthesis:

Synthesis of 4,4'-(perfluorocyclopent-1-ene-1,2-diyl)bis(5-methylthiophene-2-carbaldehyde) (DTE-dialdehyde): DTE-dialdehyde has been synthesized and reported earlier by our group.⁶ Similar synthetic procedure was applied here, and characterization data was found to be similar to the reported one. ¹H-NMR (600 MHz,

CDCl₃): 2.03 (s, 6H, CH₃), 7.73 (s, 2H, ArH), 9.84 (s, 2H, CHO). ¹³C NMR (150 MHz, CDCl₃): 15.4, 125.8, 135.6, 142.2, 151.6, 181.8. ESI-MS⁺ m/z Calcd. for C₁₇H₁₀F₆S₂O₂: 425.0105 [M+H]⁺, found 425.0118.

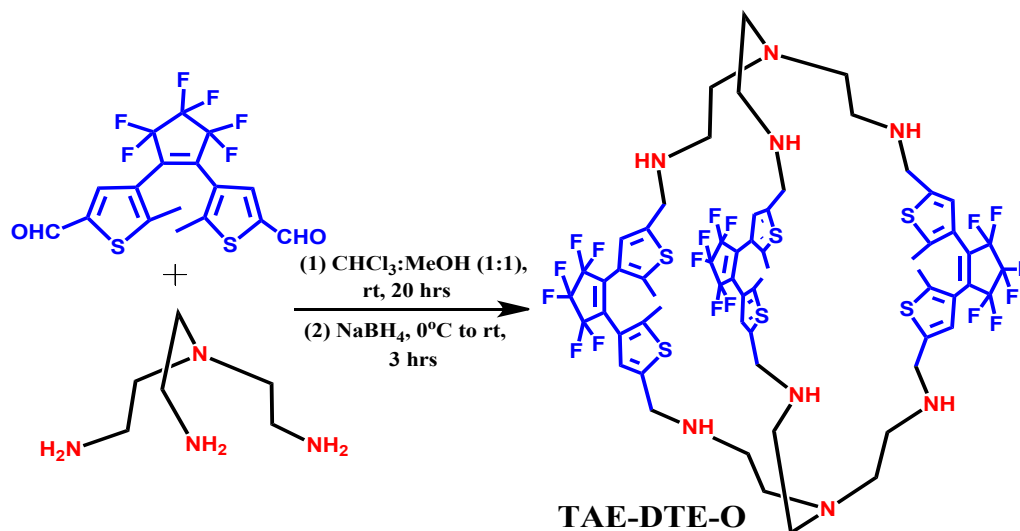


Scheme S1: Synthetic scheme for DTE-dialdehyde.

Synthesis of a photochromic organic cage (TAE-DTE-O):

Synthesis and characterization of the photochromic organic cage (POC) have been recently reported by the Schiff base condensation reaction between DTE-dialdehyde and commercially available 2,2',2''-Triaminotriethylamine (TAE) (Scheme S1).⁷ We have followed a similar procedure with subtle modification. In brief, DTE-dialdehyde (50 mg, 3-equiv) was dissolved in a mixture of chloroform (4 ml) and methanol (16). And, 12 μ l of TAE (2 equiv.) was separately taken in the methanol (10 ml). Now, the TEA solution was added slowly to the solution of DTE-aldehyde in 2 hrs under the stirring condition at room temperature, and the reaction mixture was left to stir for 24 hrs. Now, the pale-yellow coloured reaction mixture was cooled to 0 °C, and anhydrous NaBH₄ (60 equiv., 268 mg) was added into it and allowed to warm to the room temp upon stirring for 3 hrs. The solvents were then removed under vacuum. The residue was dissolved in CHCl₃ (50 ml) and washed thrice with 10% aqueous NaOH (50 ml). The organic layer was dried over anhydrous Na₂SO₄, and the organic solvent was removed under vacuum to afford the TAE-DTE-O cage. The yield of TAE-DTE-O was calculated to be 73%. Characterization data for TAE-DTE-O; IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$ = 615, 738, 893, 982, 1049, 1111, 1184, 1275, 1335, 1445, 1661, 2848, 2922, 3312; ¹H NMR (CDCl₃, 600 MHz): δ : 1.79 (s, 18H (-CH₃)), 2.22 – 2.75 (m, 36H (-N-CH₂)), 3.87 (broad, 6H(-NH)), 6.86 (s, 6H(H-C=)).

^{13}C NMR (CDCl_3 , 150 MHz): 14.3, 46.7, 48.4, 53.9, 116.1, 124.0, 124.3, 126.4, 128.8, 140.6, 142.6. ESI-MS+ m/z Calcd. For $\text{C}_{63}\text{H}_{67}\text{F}_{18}\text{N}_8\text{S}_6$: 1470.6209 $[\text{M}+\text{H}]^+$, found 1470.6211.



Scheme S2: Synthetic scheme for the photochromic organic cage (TAE-DTE-O).

Calculation of photocyclization (Φ_C) and photocycloreversion (Φ_O) for TAE-DTE:

The photoreaction quantum yields of TAE-DTE photochromic cage at 365 nm and >400 nm was calculated. The quantum yields for photocyclization and photocycloreversion were calculated based on the following equation [1]⁸;

$$\Phi_x = \frac{\Delta A / \Delta t}{(Nh\nu / t) \times \epsilon_x \times F_x} \dots\dots\dots (1)$$

where $\Delta A / \Delta t$ is the change of absorbance upon irradiation at detective wavelength, ϵ_x is the molar extinction coefficient at detective wavelength, and F_x is the mean fraction of light absorbed, the value of which is $1-10^{-A}$. For photocyclization quantum yields, it should be the absolute value of Φ_c . For photocycloreversion quantum yields, it should be the absolute value of Φ_o . $Nh\nu$ is the light intensity used for photocyclization and photocycloreversion. Slope for photocyclization ($\Delta A / \Delta t = 0.0093$) and for photocycloreversion ($\Delta A / \Delta t = 0.0051$) from figure S12.

Photoreaction	Quantum Yield (Φ_x) (%)
TAE-DTE-O to TAE-DTE-C	$\Phi_C = 62$
TAE-DTE-C to TAE-DTE-O	$\Phi_O = 53$

Photocyclization conversion ratio measurement: The ratio of the equilibrium concentrations of the open form (Co) and closed forms (Cc) at a given photostationary state (PSS) is expressed as follows⁸:

$$\frac{C_o}{C_c} = \frac{\varphi_{c \rightarrow o} \times \varepsilon_c}{\varphi_{o \rightarrow c} \times \varepsilon_o}$$

where ε_o and ε_c are the molar absorption coefficients of the open and closed forms, $\Phi_{c \rightarrow o}$ and $\Phi_{o \rightarrow c}$ is quantum yields of cycloreversion and cyclization, respectively.

Therefore, the conversion ratio at the photostationary state (PSS) was calculated to be ~77%.

Lifetime calculations: Lifetime data for TAE-DTE and Au@TAE-DTE-C were collected at 650 nm upon exciting at 510 nm. The average lifetime is calculated using the following formula:

$$\text{Average life time, } \tau_{\text{avg}}(\text{ns}) = (\Sigma A_i \tau_i^2 / \Sigma A_i \tau_i)$$

Where, τ_{avg} = average lifetime in nano-seconds, ΣA_i = sum of the percentage of all the components exists in the excited state, $\Sigma \tau_i$ = sum of excited-state lifetimes of all the component.

Table S1: Lifetime data:

Catalyst	τ_1 (ns)	A_1	τ_2 (ns)	A_2	τ_{av} (ns)
TAE-DTE-C	0.61	53.47 %	10.2	2.06 %	1.29
Au@TAE-DTE-C	0.45	100 %	-	-	0.45

Electrochemical characterizations:

(a) Mott–Schottky measurement:

The energy band structure for TAE-DTE-O was depicted by the Mott Schottky (MS) analysis at different frequencies ranging from -2.0 V to +2.0 V using ITO as a working electrode (WE) in N₂-purged aqueous solution of 0.5 M Na₂SO₄ at pH=7, Pt as a counter electrode (CE) and Ag/AgCl as a reference electrode (RE). The curve was fitted by Eq. 1.⁹ An electrochemical ink prepared by making a dispersion of a mixture of catalyst (2.0 mg) in the solvent mixture of isopropanol (500 μ l), water (500 μ l) and Nafion (14 μ l). Upon sonication for 20 minutes, a

well-dispersed ink (3.5 μl) dropped cast over the ITO electrode and allowed to dry for 3 h under ambient condition.

$$1/C^2 = (2/ \epsilon \epsilon_0 A^2 e N_D) (E-E_{\text{FB}} - k_B T/e) \dots\dots\dots \text{Eq.1}$$

Where, C and A are the interfacial capacitance and area, respectively. ϵ is the dielectric constant of the semiconductor, and ϵ_0 is the permittivity of free space. k_B Boltzmann constant, T the absolute temperature and e is the electronic charge. N_D the number of donors, V the applied voltage. Therefore, a plot of $1/C^2$ against V should yield a straight line from which V_{fb} can be determined from the intercept on the V axis.

Calculation of Conduction Band (E_{CB}) and Valance Band (E_{VB}) versus RHE (at pH=7):

The conduction band edge (CB_{Edge}) potentials for TAE-DTE-O and Au@TAE-DTE-O was assigned based on flat band potentials, and valance band (VB) position was calculated by using equation 2.

$$E_{\text{VB}} = E_{\text{CB Edge}} + \text{Band Gap} \dots\dots\dots \text{Eq. 2}$$

For TAE-DTE-O

$$E_{\text{CB Edge (TAE-DTE-O)}} = V_{\text{fb}} = -0.92 \text{ V}$$

$$E_{\text{VB (TAE-DTE-O)}} = -0.92 + \text{Optical Band Gap (TAE-DTE-O)} = -0.60 + 2.09 = 1.49 \text{ V}$$

(b) Photocurrent Measurement:

The similar set up was used for photocurrent measurements as employed for Mott-Schottky analysis. Here, the photocurrent study was performed for TAE-DTE-O and Au@TAE-DTE-O upon consecutive light “ON–OFF” cycles for 30 s over 10 cycles.

(c) Impedance analysis:

Electrochemical impedance spectroscopy (EIS) was performed in a three-electrode cell configuration with a glassy carbon electrode as the working electrode (WE), platinum as a counter electrode (CE) and Ag/AgCl as a reference electrode (RE). 0.5 M Na_2SO_4 was used as an electrolyte at pH = 7. An electrochemical ink prepared by making a dispersion of a mixture of catalyst (2.0 mg) in the solvent mixture of isopropanol (500 μl) and water (500 μl). Upon sonication for 30 minutes, a well-dispersed ink (3.5 μl) dropped cast over the GC electrode and

allowed to dry for 3 h under ambient condition. EIS was recorded at $-1.2 V_{RHE}$ applied bias from 0.1 Hz to 100 kHz (under the dark condition and visible light irradiation).

Characterization data:

^1H & ^{13}C -NMR spectra for TAE-DTE-O:

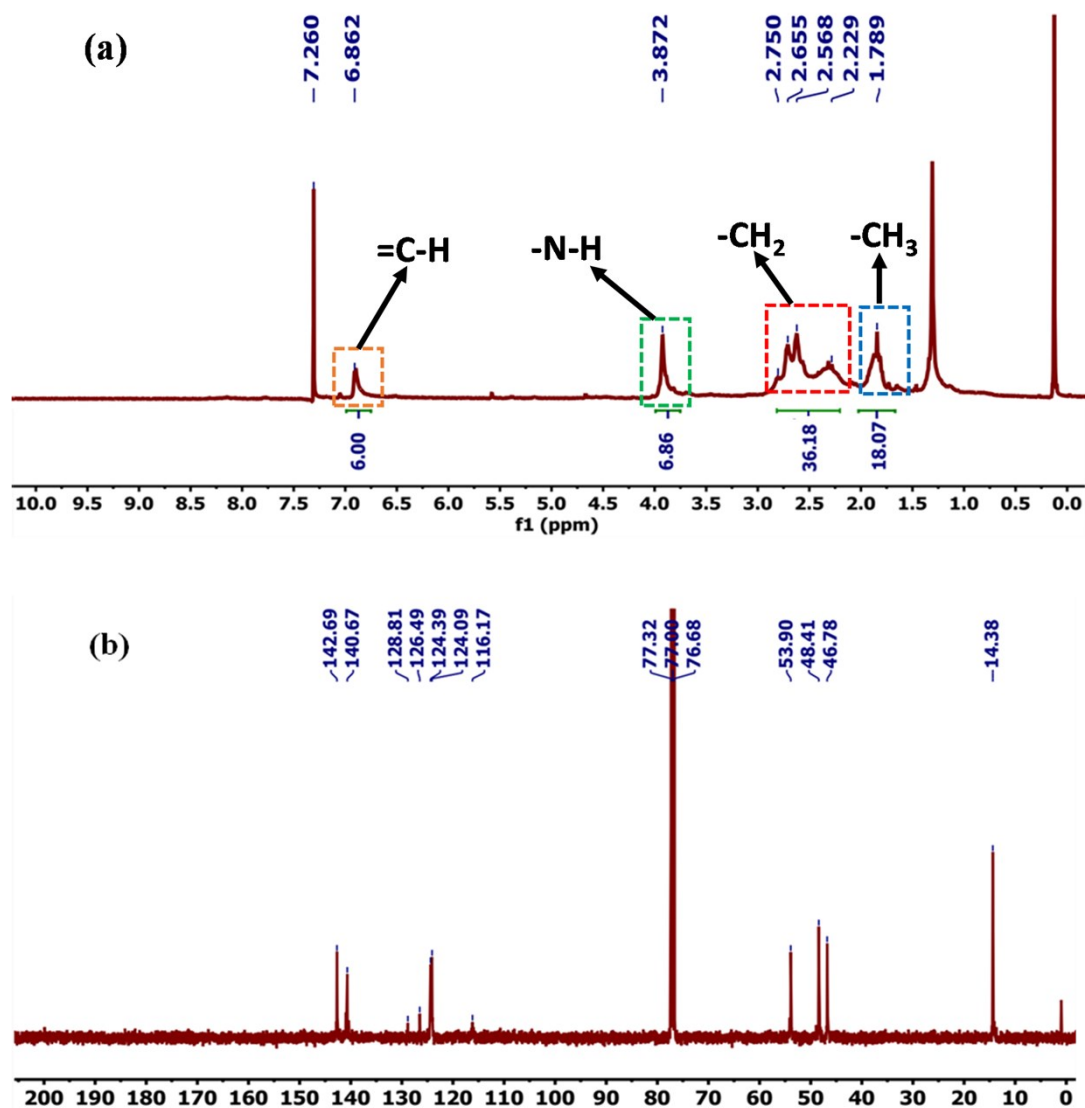


Figure S1: (a) ^1H -NMR (600 MHz) and (b) ^{13}C -NMR (150 MHz) spectra for TAE-DTE-O in CDCl_3 .

IR-spectrum for TAE-DTE-O:

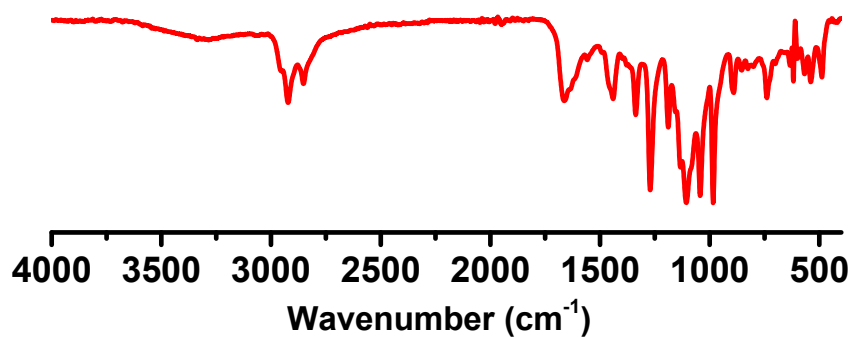


Figure S2: AT-IR spectrum for TAE-DTE-O.

High Resolution Mass Spectrum (HR-MS) for TAE-DTE-O:

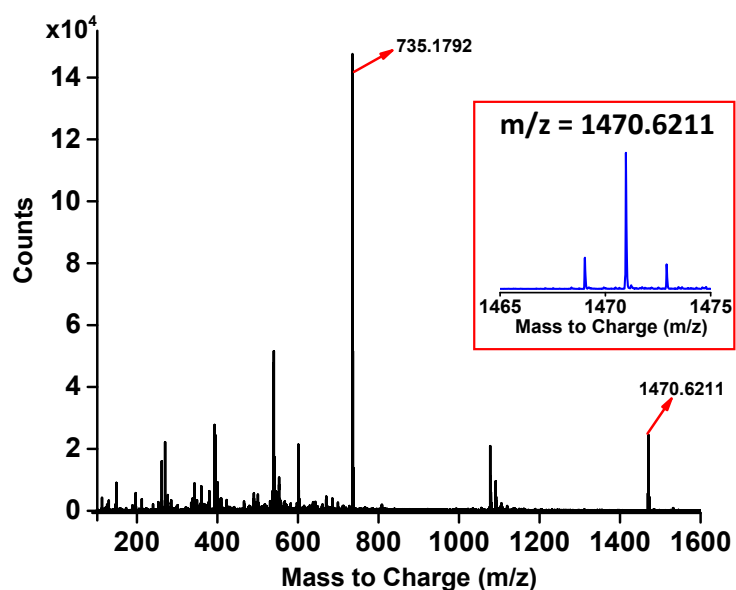


Figure S3: HR-MS spectrum for TAE-DTE-O (reduced cage)

HR-MS for unreduced TAE-DTE-O (reaction aliquot):

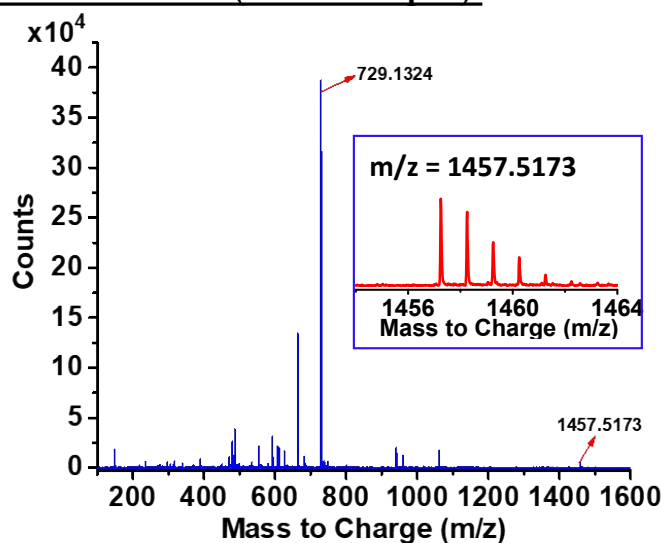


Figure S4: HR-MS spectrum for TAE-DTE-O before reduction.

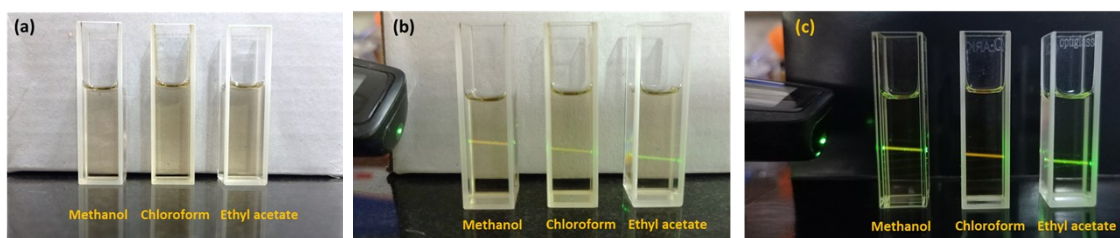


Figure S5: (a) Day light photograph showing a stable dispersion of TAE-DTE-O in different solvents. Photograph showing Tyndall effect with (b) White background and (c) Black background.

PXRD plot:

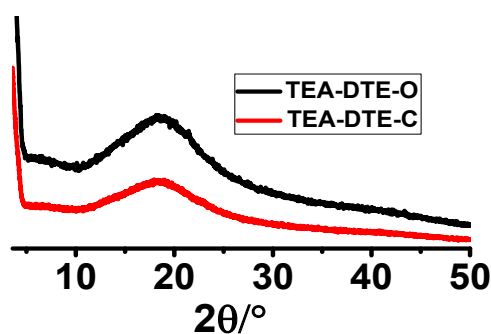


Figure S6: PXRD pattern for TAE-DTE-O and TAE-DTE-C.

Optical band gap:

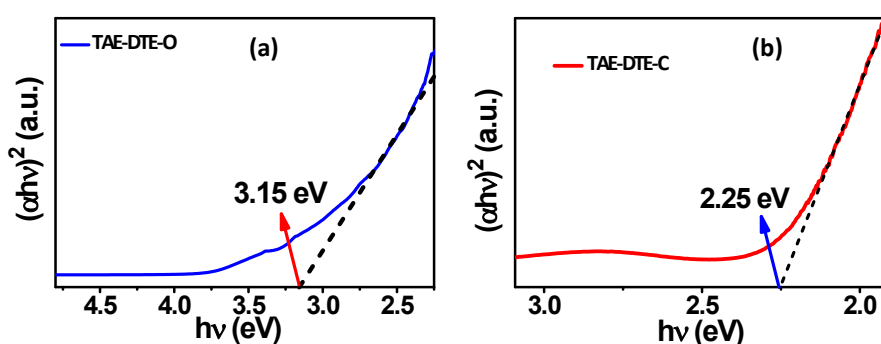


Figure S7: band-gap calculated for (a) TAE-DTE-O and (b) TAE-DTE-C, by the Tauc plot derived from the absorption spectra given in figure 1b.

Reaction kinetics of photoisomerization:

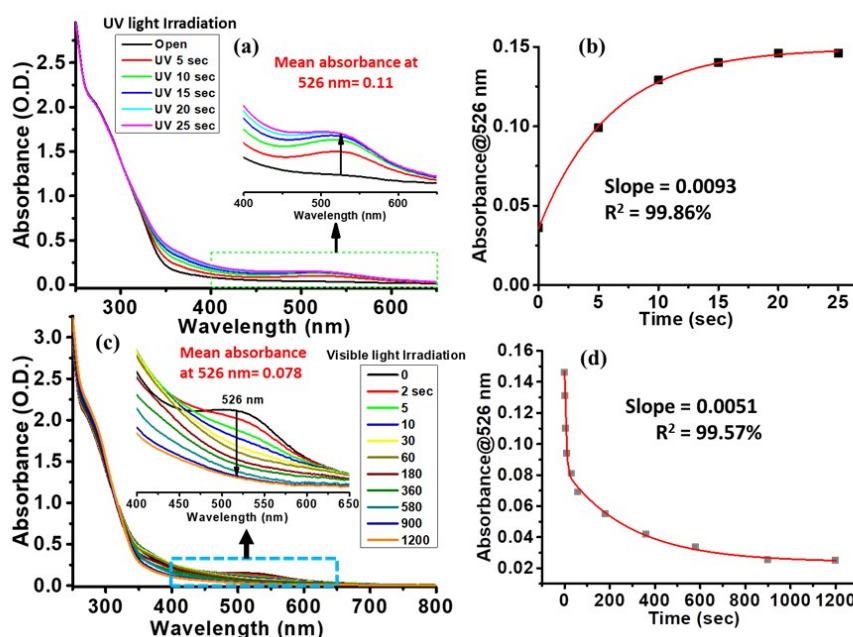


Figure S8: Time dependent UV-Vis absorption spectra in acetonitrile (10^{-5} M) upon (a) UV light irradiation and (b) corresponding change at 526 nm. Time dependent UV-Vis absorption spectra in acetonitrile (10^{-5} M) upon (c) visible light irradiation and (d) corresponding change at 526 nm.

Percentage conversion from TAE-DTE-O to TAE-DTE-C:

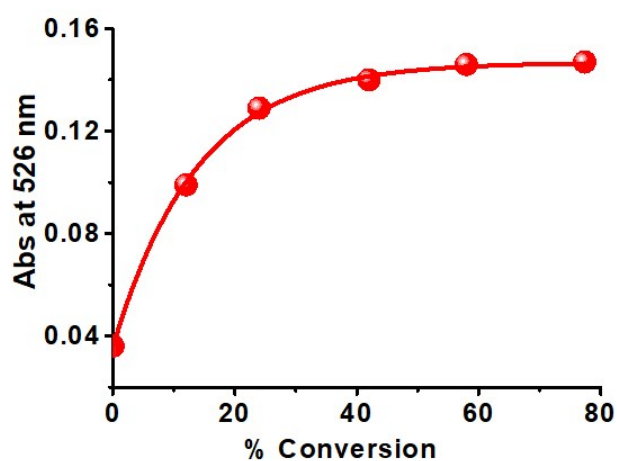


Figure S9: Percentage conversion from TAE-DTE-O to TAE-DTE-C derived from figure S12a and were plotted as the function of absorbance at 526 nm.

FESEM and TEM image for TAE-DTE-C:

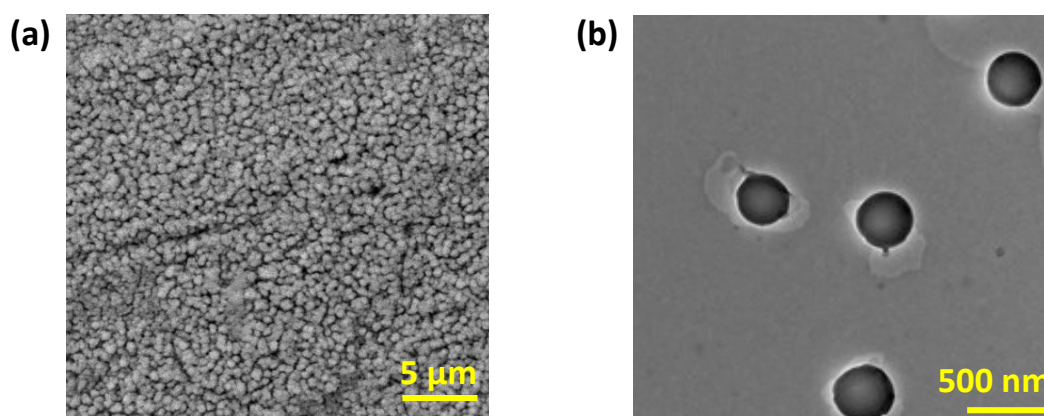


Figure S10: (a) FE-SEM and (b) TEM image for TAE-DTE-C

Optimized structure and plausible electronic transition in TAE-DTE-O:

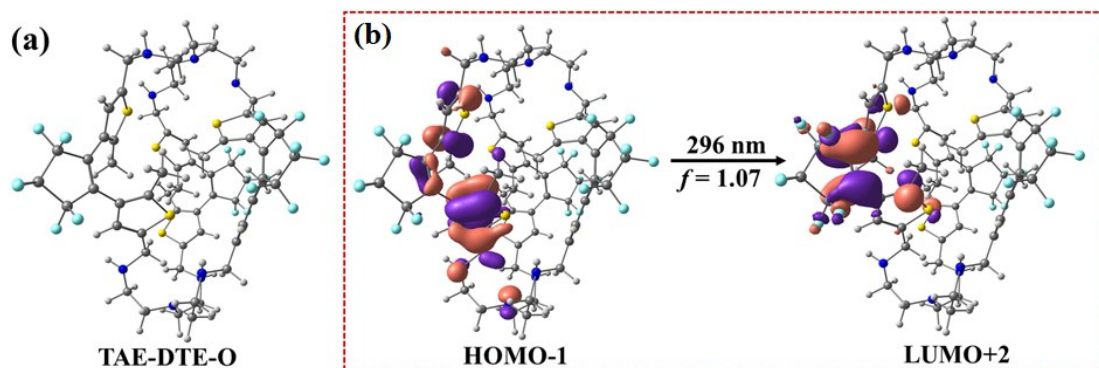


Figure S11: (a) Optimized structure for TAE-DTE-O; (b) Possible electronic transition in TAE-DTE-O.

Optimized structure and plausible electronic transition in TAE-DTE-C:

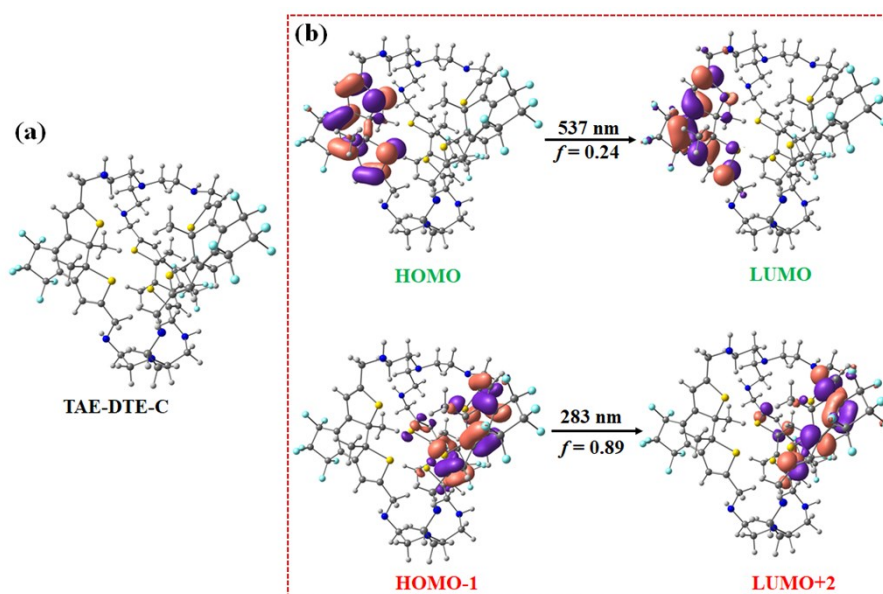


Figure S12: (a) Optimized structure for TAE-DTE-C; (b) Possible electronic transitions in TAE-DTE-O.

The theoretical band gap for TAE-DTE-O and TAE-DTE-C:

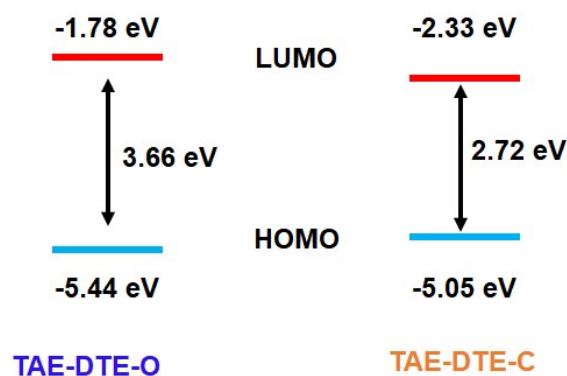


Figure S13: Theoretical band gap for TAE-DTE-O and TAE-DTE-C.

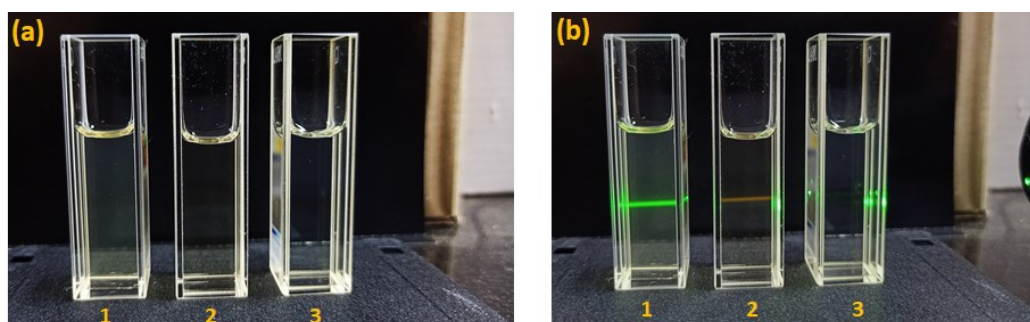


Figure S14: (a) Day light photograph of ultra-fine dispersion of Au@TAE-DTE-O (1), TAE-DTE-O (2) and solution of DTE-dialdehyde (3) in acetonitrile. (b) Photograph showing Tyndall effect in the same solvent, illustrating that the 1 and 2 are in dispersed state while 3 is completely soluble.

PXRD for Au@TAE-DTE-O:

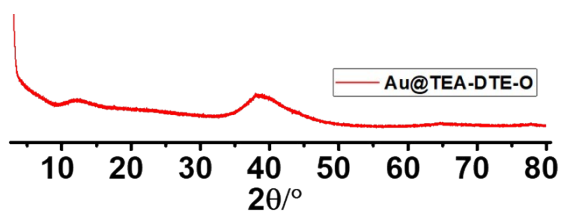


Figure S15: PXRD pattern for Au@TAE-DTE-O.

AT-IR spectrum for Au@TAE-DTE-O:

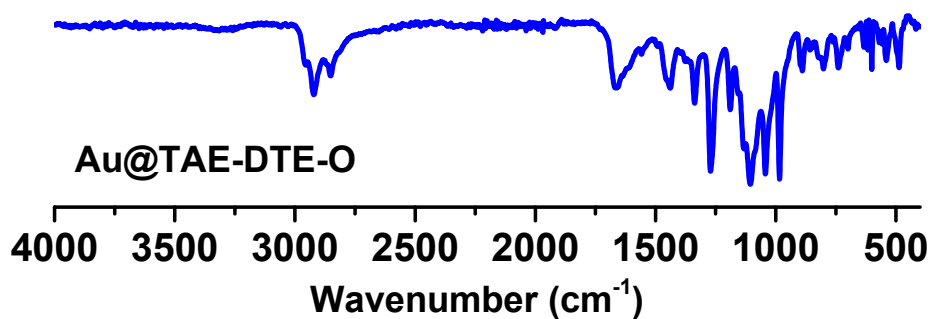


Figure S16: AT-IR spectrum for Au@TAE-DTE-O.

Elemental Mapping for Au@TAE-DTE-O:

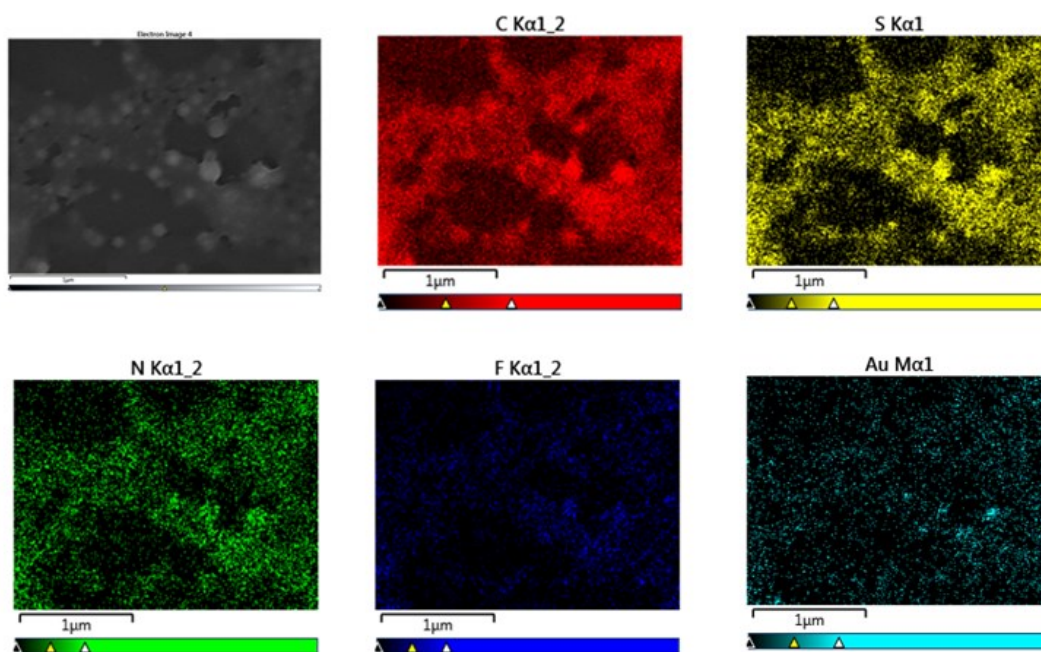


Figure S17: Elemental mapping for Au@TAE-DTE-O.

EDAX analysis for Au@TAE-DTE-O:

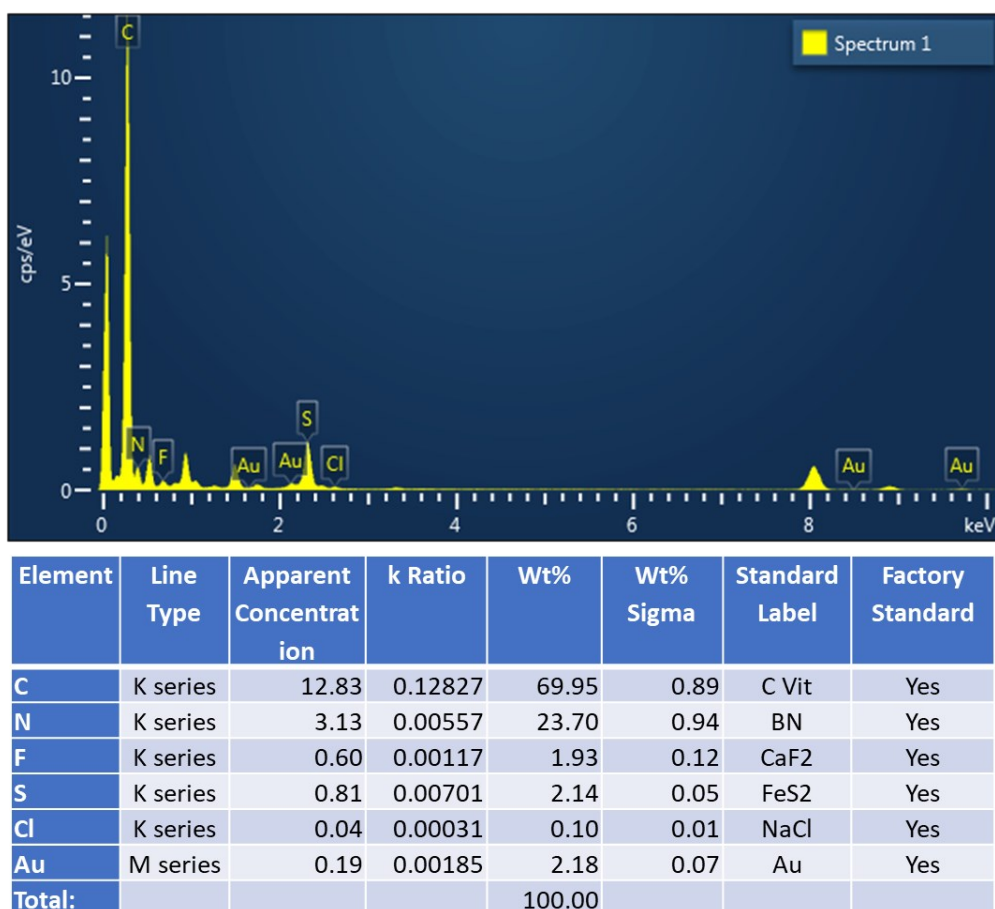


Figure S18: EDAX analysis for Au@TAE-DTE-O.

XPS analysis of Au@TAE-DTE-O:

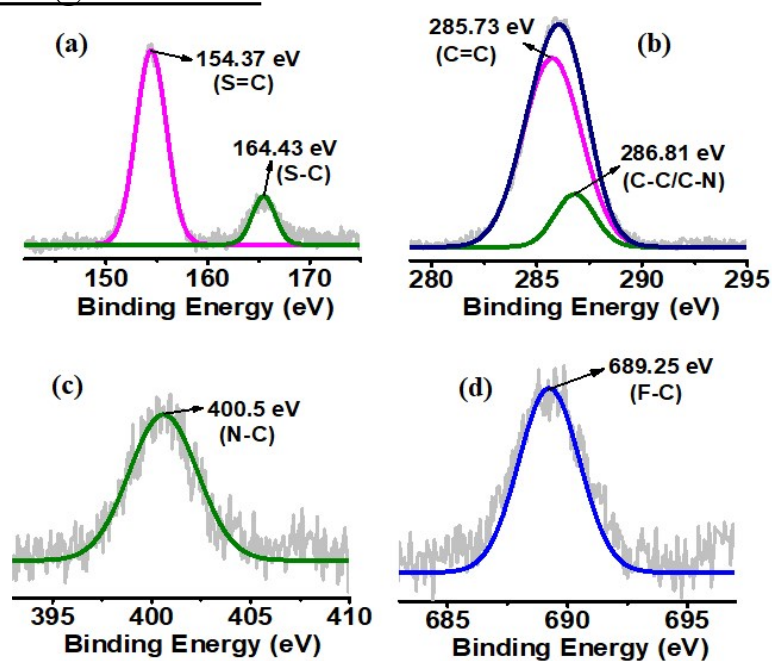


Figure S19: XPS analysis for Au@TAE-DTE-O; Deconvolution spectra for (a) sulphur; (b) carbon; (c) nitrogen and (d) fluorine.

UV-absorption spectra for Au@TAE-DTE:

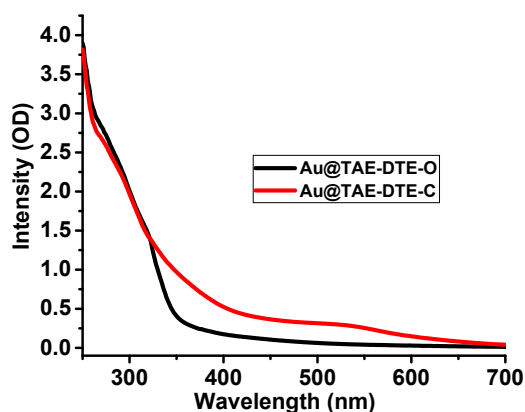


Figure S20: UV absorption spectra in dispersed state in acetonitrile (10^{-5} M) for gold NPs established photochromic cage (Au@TAE-DTE-C).

Absorbance and photoisomerization of Au@TAE-DTE in full-range light (250-750 nm):

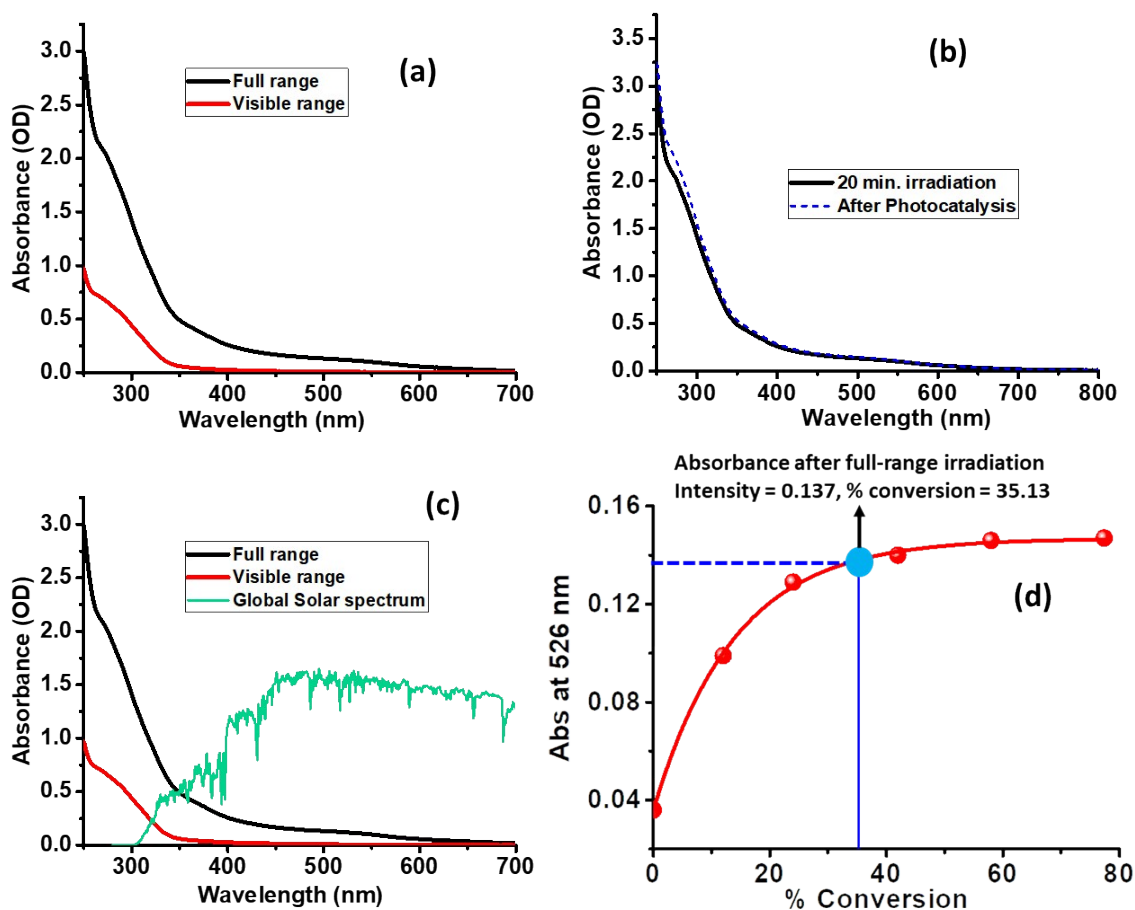


Figure S21: (a) Comparison of UV-Vis absorption spectra of Au@TAE-DTE before and after full-range light irradiation (250-750 nm) for 20 minutes (b) Comparison of UV-Vis absorption spectra of Au@TAE-DTE upon full-range light irradiation for 20 min. and after photocatalysis. (c) Comparison of absorption spectra of Au@TAE-DTE with global solar spectrum. (d) Calculation of photoisomers based on absorbance at 526 nm upon full-range light irradiation (% of Au@TAE-DTE-O and Au@TAE-DTE-C was calculated to be 65% and 35%, respectively).

Isotopic labelling experiment:

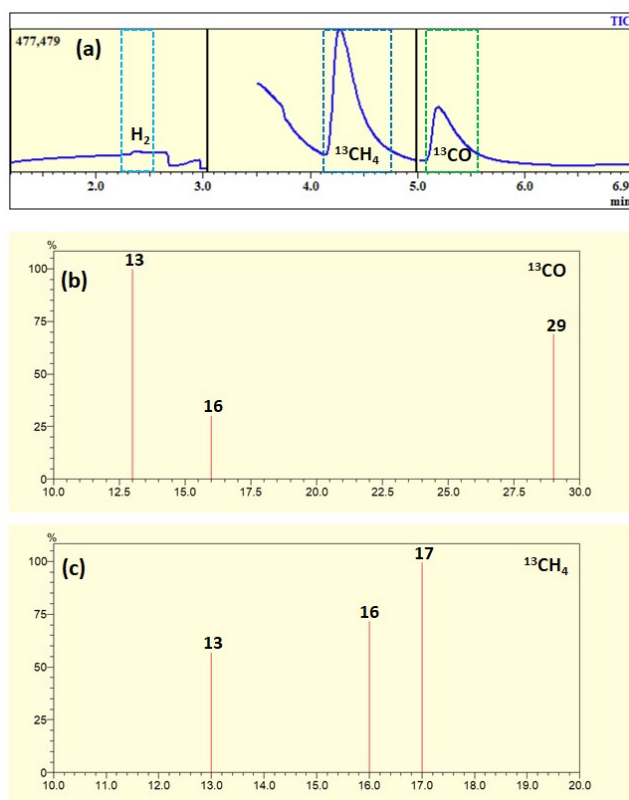


Figure S22: Chromatogram for photocatalysis performed with isotope $^{13}\text{CO}_2$ using Au@TAE-DTE-O under visible light irradiation.

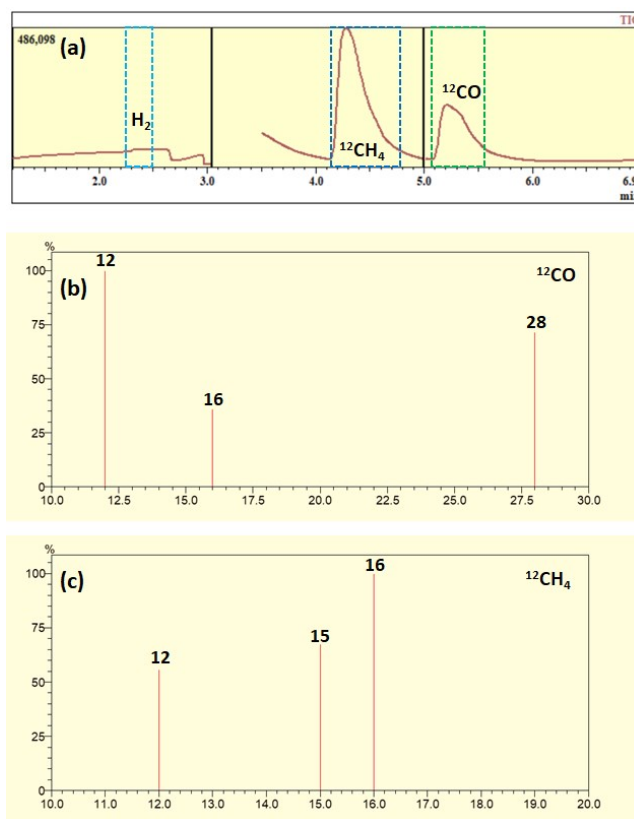


Figure S23: Chromatogram for photocatalysis performed with $^{12}\text{CO}_2$ using Au@TAE-DTE-O under visible light irradiation.

Control experiments for photocatalytic CO₂ reduction using Au@TAE-DTE-O:

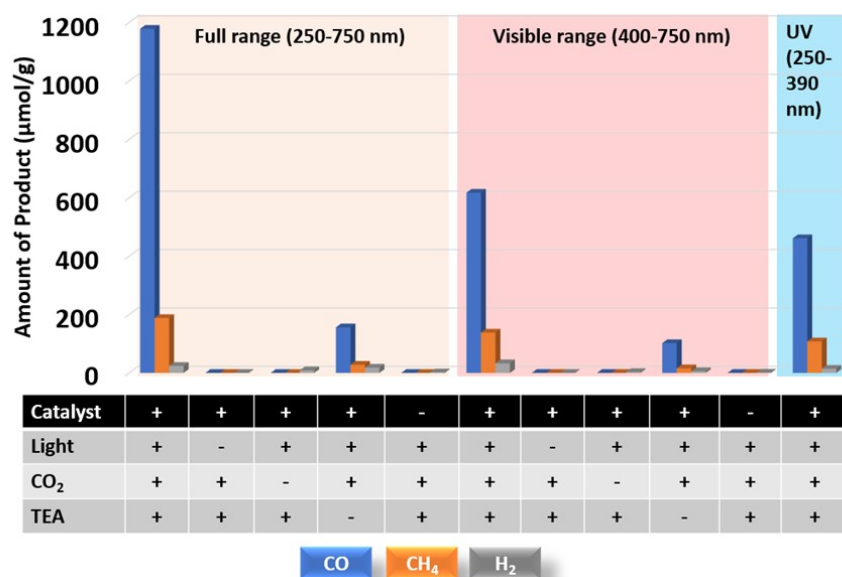


Figure S24: Photocatalytic CO₂ reduction using Au@TAE-DTE-O under various conditions.

Recyclability test:

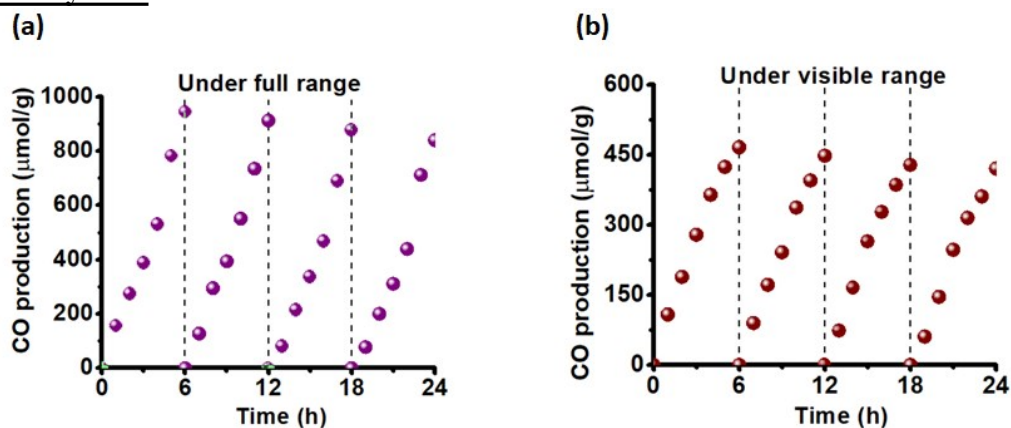


Figure S25: Photocatalytic CO₂ reduction performed with Au@TAE-DTE-O for four cycles under (a) Full range irradiation and (b) Visible light irradiation.

TEM image of Au@TAE-DTE-O after photocatalysis:

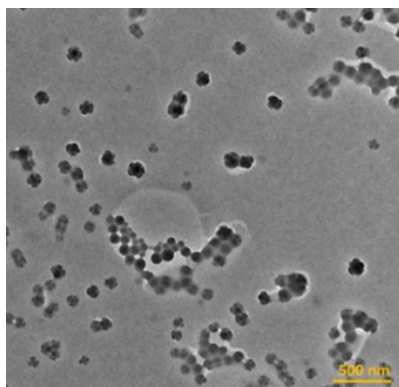


Figure S26: TEM for the recycled Au@TAE-DTE-O after photocatalysis.

Photocatalytic activity of photochromic organic cage (TAE-DTE):

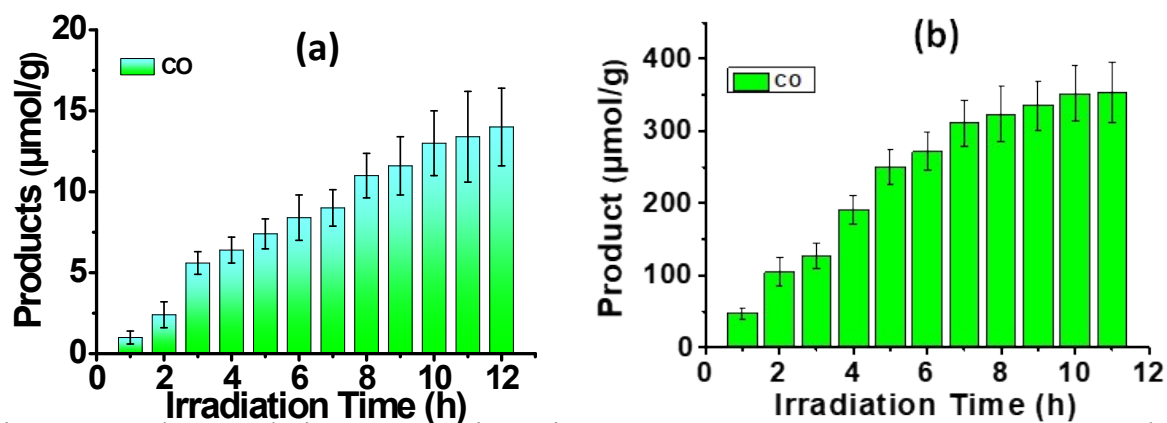


Figure S27: Photocatalytic CO_2 reduction using TAE-DTE under (a) Visible light and (b) full range irradiation.

Excited state lifetime:

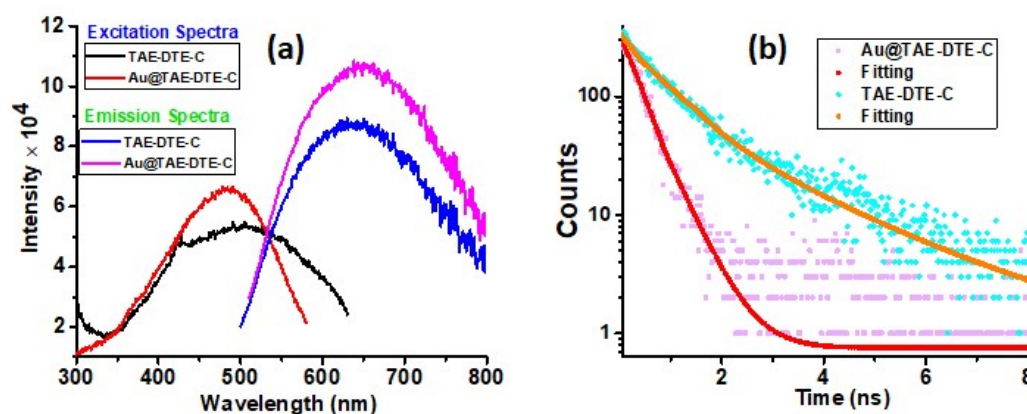


Figure S28: (a) Excitation and emission spectra for TAE-DTE-C and Au@TAE-DTE-C. (b) Excited state lifetime upon exciting at 510 nm and decay was collected at 650 nm.

Optimized structure for the Au NPs stabilized POCs:

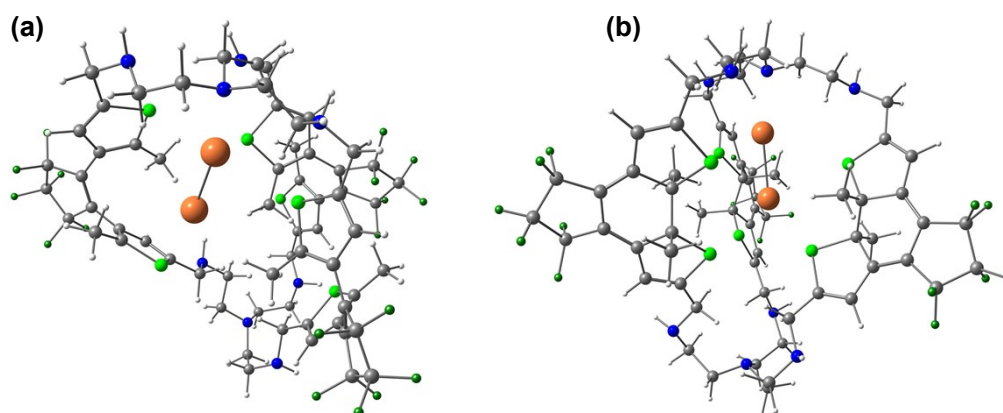


Figure S29: Optimized structure for the Au NPs stabilized (a) Au@TAE-DTE-O and (b) Au@TAE-DTE-C.

Thermodynamic feasibility for electron transfer from cage to Au NPs:

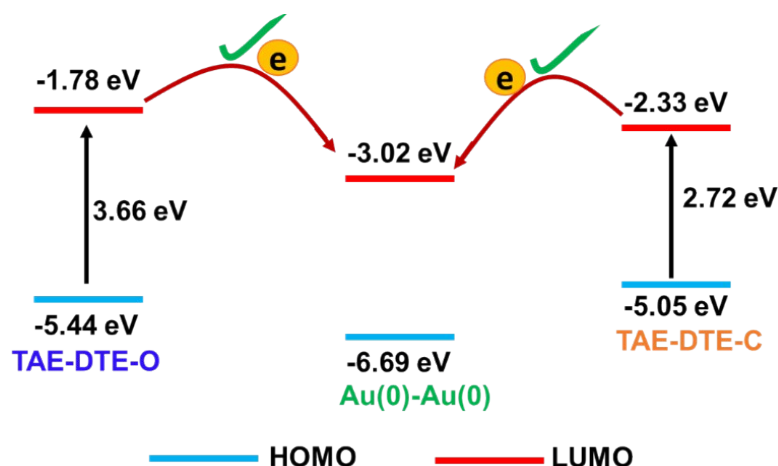


Figure S30: Thermodynamic feasibility of electron transfer from the LUMO of POC (TAE-DTE-O/TAE-DTE-C) to the LUMO of gold NPs.

Plausible CO₂ binding site in TAE-DTE-C:

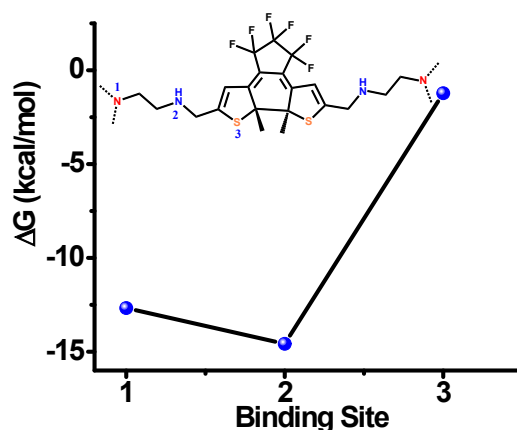


Figure S31: Different CO₂ adsorption sites on TEA-DTE-C and corresponding adsorption energies of COOH* (relative to the least stable binding site).

XYZ Coordinates:

Coordinates of the optimized structures

TAE-DTE-O

TAE-DTE-O			TAE-DTE-C		
Charge 0, Multiplicity 1, HF = -7064.8108411			Charge 0, Multiplicity 1, HF = -7064.8108411		
N	-2.627058203	-5.895957439	-0.944738074	H	-5.618131446
C	-4.008175305	-6.346434495	-0.759995057	C	-5.245808403
C	-4.739859363	-5.507369409	0.294990023	C	-3.906114296
H	-4.550200348	-6.272700472	-1.709020133	H	-5.831216466
H	-4.045981310	-7.413247574	-0.472359036	C	-3.490683268
N	-5.096467392	-4.189769320	-0.232733018	S	-2.659566202
H	-4.067966312	-5.353449421	1.146582088	C	-2.179317168
				H	-4.101071312
				C	-1.487247113
				C	-0.239744018
					-6.059400447
					-3.149062243
					-2.659161201
					-3.464686266
					-2.340011180
					0.080574006
					2.546412194
					3.400050261
					3.756285288
					0.949506072

C	-0.871647064	-0.124431009	4.021446308	S	-0.982336075	4.609650353	-3.852281296
C	-1.230882093	-2.316671177	4.846622370	C	-2.777866210	2.619818201	-4.723994359
H	0.163758012	-1.652202128	0.052612004	C	-0.989065077	5.113983391	-2.173516168
H	-0.254637019	-0.090918007	0.781768060	H	-2.120308163	4.575970348	-0.421721032
H	0.445641034	-1.356110106	1.779255136	H	-3.806390288	2.303101178	-4.529106348
C	-0.012424001	-0.261044020	5.256436404	H	-2.759672213	3.165334242	-5.673052424
C	-0.881001066	1.156557090	3.317767252	H	-2.175734167	1.709885131	-4.839982371
C	-0.550442041	-1.517064118	5.981267479	C	0.002809000	6.133809489	-1.690275129
F	-0.395970030	-3.308970252	4.415658339	H	1.009825076	5.713075422	-1.781191136
F	-2.374582181	-2.921858224	5.283203401	N	-0.199211015	6.485907520	-0.286744022
F	-0.032883002	0.824431065	6.071550463	C	0.556665044	7.677157581	0.118276009
F	1.305250097	-0.464307036	4.902844373	H	0.193339015	8.594173652	-0.385582030
C	0.224181017	2.081250157	3.416009262	H	0.383539029	7.822299576	1.190699093
F	0.417974032	-2.213384171	6.611068523	C	2.060697156	7.612243567	-0.183316014
F	-1.480971113	-1.134355088	6.891108541	H	2.511068191	8.557026679	0.184595014
S	-1.536899115	3.259877251	1.990522151	H	2.193540167	7.629903588	-1.269321094
C	-3.301250254	1.115452083	2.317348175	C	-1.718151129	-6.642537530	-0.086297007
C	0.029555002	3.256757248	2.752477212	C	-0.293850022	-6.088801482	0.043255003
H	1.125649085	1.852085139	3.971527304	H	-2.157092163	-6.637344502	0.918301071
H	-3.635194278	0.512633039	3.166361243	H	-1.652440126	-7.716370568	-0.377831029
H	-4.033301307	1.906168144	2.142566163	N	0.554524040	-6.491037470	-1.084965081
H	-3.305122255	0.460085035	1.441738113	H	0.123680009	-6.448845480	1.001968074
C	0.914143072	4.473335341	2.672004206	H	-0.334952026	-4.994899381	0.098438007
H	0.917329068	4.968529378	3.664452281	C	1.990618155	-6.348668470	-0.874643065
N	2.268294174	4.148496315	2.220320171	C	2.478723190	-4.941323375	-1.091709085
C	3.255147247	5.191925395	2.482558190	H	2.489061191	-7.003690524	-1.601587123
H	3.352745254	5.425452400	3.561778274	C	3.672277278	-4.400748336	-0.716557055
H	4.227088323	4.806766364	2.153818164	S	1.559546118	-3.812468291	-2.059090156
C	2.941534224	6.523171494	1.787431136	C	3.876190297	-3.060403236	-1.198311090
H	3.735430286	7.245970571	2.063030155	H	4.409739338	-4.928758379	-0.122287010
H	2.016492154	6.920709552	2.214279168	C	5.128738393	-2.343010181	-0.969357071
C	-2.210325166	-5.713851461	-2.333574178	C	2.643297203	-1.281319098	-2.642095203
C	-2.930441225	-4.523792344	-2.976079227	C	5.355512419	-1.036780079	-0.678615052
H	-1.141407089	-5.498425413	-2.342783180	C	6.431128467	-3.102298236	-1.030454077
H	-2.355029182	-6.632084533	-2.942299224	H	2.187578165	-0.530354039	-1.985261150
N	-2.189659165	-4.010519306	-4.131453315	H	3.619506278	-0.887836067	-2.940504223
H	-2.986307229	-3.731483285	-2.230140171	H	2.019136157	-1.375583103	-3.535301271
H	-3.976030306	-4.775900366	-3.237199248	C	6.831418511	-0.736744056	-0.630473046
C	-2.805779215	-2.812185217	-4.699510360	C	4.375156335	-0.010166001	-0.331314025
C	-2.627184200	-1.617123122	-3.803644292	C	7.511034555	-2.006016154	-1.201840094
H	-3.892236295	-2.919612221	-4.885482375	F	6.481982506	-4.013376307	-2.035341157
C	-3.581061276	-0.783368059	-3.301641253	F	6.654791529	-3.786338291	0.140486011
S	-1.041675080	-1.127374086	-3.255721251	F	7.254362528	-0.520240040	0.649171048
C	-3.056624233	0.297210023	-2.504304189	F	7.172693545	0.369289028	-1.355553104
H	-4.637215354	-0.917755072	-3.495367265	C	4.330301329	1.293406099	-0.938321069
C	-3.915168297	1.294306098	-1.862322142	F	7.753430597	-1.831503139	-2.525767195
C	-0.736179054	1.144710087	-1.647697126	F	8.669942679	-2.306502174	-0.580888042
C	-3.719333286	2.631064202	-1.709597132	S	2.364960183	1.204606093	0.706489056
C	-5.202396395	0.859812068	-1.201278092	C	3.172874240	-1.389058105	1.507210113
H	0.158457012	0.608273044	-1.324443102	C	3.287269254	2.061900156	-0.511736039
H	-0.410820031	1.988274153	-2.267637174	H	5.061704389	1.629730124	-1.661132127
H	-1.216269091	1.565611119	-0.759432060	H	4.134070313	-1.872458145	1.708919129
C	-4.766878365	3.250919248	-0.825495061	H	2.730580206	-1.093605085	2.464842188
C	-2.677717204	3.488113266	-2.275284171	H	2.524542192	-2.144775166	1.049677081
C	-5.853460431	2.156872163	-0.636736049	C	2.895597220	3.450510264	-0.948242074
F	-4.983314378	-0.031908002	-0.187313014	H	2.601955199	4.029962310	-0.068768005
F	-6.061765446	0.246549019	-2.070923157	N	4.023503305	4.108910311	-1.608029121
F	-5.297665408	4.381519337	-1.357631104	C	3.948452302	5.563716414	-1.722917132
F	-4.248718327	3.606991273	0.399508031	H	4.805280366	5.871453463	-2.334332177
C	-1.950325149	4.444797341	-1.480216114	H	3.045727235	5.919310454	-2.253728173
F	-6.206364452	2.011174156	0.660512052	C	4.057060307	6.269945469	-0.361065027
F	-6.954766553	2.476335187	-1.353291104	H	4.559105348	7.248117549	-0.489952037

H	4.718519359	5.657553457	0.257019020	H	2.426973184	-4.800896365	2.202346168
N	2.770996214	6.442610502	0.335330026	H	1.608342124	-5.049001383	0.643071047
C	3.380625259	-0.208549016	0.604079045	C	1.319045102	-1.194041090	4.188058321
C	2.807121213	-2.597921196	-1.945034149	H	0.547025043	-1.891377142	4.528736347
C	-1.938897148	1.676574127	2.585498199	N	2.139289164	-0.823864063	5.331750402
C	-1.600052123	-1.681050131	1.295029097	C	1.421442107	0.005469000	6.312153493
C	-2.275522174	3.464724267	-3.593639274	H	2.139969162	0.238962018	7.105394529
C	-1.676242127	0.246356019	-2.392470182	H	1.098545081	0.969981072	5.882764468
H	-5.784486463	-2.312169175	0.322809025	C	0.204248015	-0.701705056	6.941709528
H	-5.946934459	-4.256116325	-0.785921059	H	0.158375012	-0.460152035	8.020173608
H	-2.126185164	-4.726302360	-4.853362369	H	0.374996029	-1.780943137	6.880023548
H	-2.332394176	-2.621673200	-5.671520456	C	-0.145738011	0.689879050	-6.078025475
H	0.351849027	-7.460356573	-1.316436100	C	-1.536480118	0.196431015	-5.636352447
H	2.317702178	-6.681738504	0.129023010	H	-0.043511003	1.719853132	-5.723228429
H	0.484099037	5.184024398	1.957307151	H	-0.078794006	0.720436057	-7.185538529
H	2.580623196	3.281875249	2.649268201	N	-2.373954180	1.338087101	-5.251364399
H	4.158659318	3.709764285	-2.534057196	H	-1.417069107	-0.435135033	-4.751312362
H	1.990699150	3.396217260	-1.587588120	H	-2.006458155	-0.420671032	-6.424156504
H	-1.187794089	6.683979517	-0.138628010	C	-3.762847287	1.001145077	-4.959326377
H	-0.031079002	7.016167519	-2.361414182	C	-3.914099300	0.200040015	-3.693650282

TAE-DTE-C

Charge 0, Multiplicity 1, HF = -7064.7247717

N	0.945883070	-0.085884006	-5.491752435	C	-4.870906372	-1.236465093	-2.108647161
C	0.938463074	-1.482313111	-5.930065453	H	-5.727146457	-0.879838066	-4.118857314
C	1.968389149	-2.326283179	-5.166035393	C	-3.505604268	-1.014952079	-1.441207110
H	-0.048887004	-1.899339143	-5.708614458	C	-5.795135467	-1.955264151	-1.423275108
H	1.095014083	-1.573788120	-7.025533533	C	-2.636898201	-2.261357173	-1.754505135
N	1.474144112	-3.684117281	-4.926883377	C	-5.583769427	-2.363892182	-0.047379004
H	2.118278160	-1.858427143	-4.188125320	C	-7.107103560	-2.485509189	-1.913659145
H	2.945256224	-2.324854178	-5.684463443	H	-1.604730124	-2.125790164	-1.426699107
C	2.465795188	-4.534631344	-4.266901328	H	-3.053487233	-3.143302238	-1.257371097
C	2.829839216	-4.000584305	-2.908815221	H	-2.637157202	-2.437152184	-2.833422217
H	2.027310157	-5.536052403	-4.158744319	C	-6.679048484	-3.297838252	0.361384028
C	4.090602313	-3.835124295	-2.430910184	C	-4.552287349	-1.887009144	0.691918055
S	1.541256117	-3.521656267	-1.791496138	C	-7.835144613	-2.932114224	-0.612868049
C	4.153332318	-3.309336252	-1.100569084	F	-6.950549540	-3.579367274	-2.724007206
H	4.976595378	-4.113774313	-2.990909229	F	-7.843185620	-1.577760119	-2.616199200
C	2.801261216	-2.750779209	-0.631888050	F	-7.058082537	-3.175253241	1.663503126
C	5.202057398	-3.191131241	-0.247987019	F	-6.347263504	-4.612836354	0.159907012
C	2.803914214	-1.224861093	-0.909294067	C	-3.704345282	-0.762450058	0.071258006
C	5.031393386	-2.719699206	1.113883083	C	-4.126791316	-2.215610171	2.023395155
C	6.652527497	-3.446308263	-0.519907040	F	-8.702109671	-3.943287299	-0.812040063
H	1.829276139	-0.780389061	-0.700784054	F	-8.505928636	-1.865840144	-0.101771008
H	3.555423273	-0.727643054	-0.288485022	S	-2.113880163	-0.810711060	1.046510082
H	3.049159235	-1.039175077	-1.957938152	C	-4.422529335	0.574140043	0.385896030
C	6.377540486	-2.485305192	1.722643129	C	-2.888548220	-1.754054133	2.334248180
C	3.803716292	-2.585561198	1.674548130	H	-4.724998362	-2.814814218	2.698592204
C	7.305900582	-3.418182260	0.892789066	H	-5.382273389	0.613685046	-0.139047011
F	7.214662540	-2.456926188	-1.282507096	H	-4.610650350	0.634593051	1.461146111
F	6.895530505	-4.624159351	-1.163180087	H	-3.819645289	1.431560108	0.081647006
F	6.443198471	-2.760354211	3.054113234	C	-2.088703158	-1.986378154	3.581159274
F	6.806766525	-1.193811089	1.555092118	H	-1.726742131	-1.031046079	3.969412304
C	2.605844202	-3.106901236	0.858959066	N	-2.838903218	-2.636003204	4.648947357
C	3.411192262	-2.064608157	2.953213224	C	-2.097849161	-2.707296206	5.915597429
F	8.589073653	-3.009760232	0.872667069	H	-2.606857200	-3.453730265	6.535454492
F	7.245072557	-4.667226356	1.425487111	H	-1.059942083	-3.065153237	5.784081431
S	1.129140089	-2.273169172	1.636104122	C	-2.111467162	-1.382960104	6.696038514
C	2.492818191	-4.628597354	1.125059084	H	-2.022047156	-1.601062121	7.777562614
C	2.078691156	-1.830040139	3.065194232	H	-3.103123239	-0.947399073	6.545935482
H	4.126785316	-1.838630141	3.734365285	C	2.245150173	0.558642045	-5.687956437
H	3.379891259	-5.143099390	0.742948056	C	2.343944179	1.909979146	-4.9604896381

H	3.009456230	-0.088204007	-5.250144402
H	2.492467193	0.674065054	-6.763824532
N	3.658785280	2.050462159	-4.327180332
H	1.594258124	1.918973148	-4.163087319
H	2.114554160	2.750051209	-5.642110425
C	3.876230297	3.355856256	-3.707849282
C	2.927028222	3.602785277	-2.568244195
H	4.906081377	3.370352257	-3.324796255
C	2.300648177	4.776893367	-2.298424177
S	2.578306199	2.294153177	-1.425637106
C	1.470226110	4.746669361	-1.132465089
H	2.445808185	5.675258458	-2.888695220
C	1.201355093	3.311574254	-0.651411050
C	0.862264064	5.756326455	-0.461818035
C	-0.129128010	2.847277215	-1.298534097
C	0.113406009	5.520678428	0.757104056
C	0.777634059	7.203471552	-0.838743066
H	-0.323695025	1.794134139	-1.092683083
H	-0.964351076	3.440466263	-0.913078071
H	-0.078617006	2.982736230	-2.381931183
C	-0.624437049	6.767827493	1.127117086
C	0.155792012	4.329292331	1.403504109
C	0.210244016	7.886202598	0.439750034
F	-0.097081008	7.415664591	-1.872148143
F	1.969708149	7.748444583	-1.214330090
F	-0.739192057	6.972937547	2.467942187
F	-1.892376144	6.798305510	0.603980046
C	1.170710089	3.288757252	0.894780069
C	-0.587135043	3.865228295	2.537973192
F	-0.505473039	8.995398699	0.172884013
F	1.246630096	8.212296647	1.256495097
S	0.561160045	1.669760129	1.611634125
C	2.535944195	3.616754276	1.546673120
C	-0.507526039	2.525639193	2.740717210
H	-1.199283094	4.522969347	3.142621240
H	2.896927223	4.587435349	1.192360090
H	2.413774186	3.665258282	2.631763203
C	3.282359251	2.857510217	1.306086102
C	-1.254449097	1.697328131	3.740877287
H	-0.555105040	1.028820079	4.248036323
N	-1.942345151	2.474024191	4.765196364
C	-2.573723196	1.620972124	5.783418425
H	-3.219010246	2.273067173	6.381824494
H	-3.222287245	0.843445065	5.340198400
C	-1.544411120	0.963242074	6.721992488
H	-1.954156149	0.917167071	7.748267573
H	-0.681384051	1.633439122	6.765073496
N	-1.092529082	-0.383884029	6.304756495
H	2.937875223	-0.285304022	4.998970384
H	0.769054058	-0.338303026	3.756824287
H	-2.669311202	3.032784231	4.320618327
H	-1.935237147	1.033360081	3.175858244
H	-3.074067233	-3.582692274	4.356588331
H	-1.181888090	-2.552232196	3.290619253
H	1.205010093	-4.119761313	-5.807694431
H	3.405313262	-4.646593354	-4.840513368
H	-2.360009180	2.039592154	-5.989092476
H	-4.267416328	0.444664034	-5.772155416
H	4.394921338	1.889176146	-5.012456381
H	3.777301288	4.204226321	-4.411394335

Au@TAE-DTE-O (two gold atoms encapsulated)

Charge 0, Multiplicity 1, HF = -7335.7572239

N	1.947738000	-6.698012000	-0.254384000
C	1.350230000	-7.772540000	0.545601000
C	0.481259000	-7.213528000	1.678788000
H	0.738833000	-8.421714000	-0.092624000
H	2.128739000	-8.426117000	0.974068000
N	-0.767887000	-6.660879000	1.158549000
H	1.030153000	-6.397192000	2.161604000
H	0.313556000	-7.989906000	2.449218000
C	-1.419615000	-5.686963000	2.033073000
C	-0.682878000	-4.378216000	2.023736000
H	-1.510315000	-6.018914000	3.084744000
C	-0.355432000	-3.569585000	3.074143000
S	-0.171995000	-3.670019000	0.512904000
C	0.278504000	-2.343846000	2.674500000
H	-0.568049000	-3.818116000	4.108107000
C	0.849019000	-1.378095000	3.625512000
C	1.242676000	-1.238252000	0.552464000
C	0.540173000	-0.087769000	3.925894000
C	2.118674000	-1.813303000	4.311338000
H	2.194286000	-1.651637000	0.202266000
H	0.700617000	-0.877076000	-0.326592000
H	1.458396000	-0.380414000	1.192945000
C	1.610556000	0.479472000	4.842036000
C	-0.544111000	0.810891000	3.529511000
C	2.383254000	-0.742669000	5.383400000
F	3.164102000	-1.839220000	3.420685000
F	2.034047000	-3.057614000	4.855666000
F	1.121531000	1.235949000	5.855629000
F	2.488504000	1.280183000	4.140260000
C	-0.361619000	2.242734000	3.588852000
F	3.694937000	-0.487776000	5.571710000
F	1.835366000	-1.131140000	6.560615000
S	-2.794594000	1.901190000	2.880140000
C	-2.472438000	-0.869549000	2.969985000
C	-1.468354000	2.967045000	3.268082000
H	0.577167000	2.711841000	3.850523000
H	-2.157717000	-1.556707000	3.760686000
H	-3.563121000	-0.811384000	2.978283000
H	-2.171034000	-1.318957000	2.019553000
C	-1.576300000	4.462913000	3.240069000
H	-0.547253000	4.856678000	3.351489000
N	-2.241831000	4.957453000	2.035800000
C	-2.029711000	6.383692000	1.829692000
H	-2.449346000	6.936940000	2.681000000
H	-0.953478000	6.646382000	1.796593000
C	-2.728868000	6.856135000	0.550398000
H	-2.531451000	7.932484000	0.389593000
H	-3.805334000	6.755115000	0.706856000
C	1.686728000	-6.764777000	-1.689809000
C	0.202262000	-6.573050000	-2.007244000
H	2.224188000	-5.945317000	-2.169931000
H	2.058883000	-7.711498000	-2.141217000
N	0.005083000	-6.240562000	-3.419752000
H	-0.159556000	-5.740132000	-1.404203000
H	-0.396255000	-7.452264000	-1.703697000
C	-1.393312000	-5.947069000	-3.730140000
C	-1.838150000	-4.671865000	-3.070031000
H	-2.095606000	-6.741239000	-3.408298000
C	-2.905455000	-4.474511000	-2.244095000
S	-0.928574000	-3.190927000	-3.260089000
C	-3.043045000	-3.115723000	-1.789879000

H	-3.590748000	-5.265193000	-1.964714000	C	3.578034000	3.684851000	-0.738287000
C	-4.113838000	-2.674660000	-0.896738000	F	7.467789000	2.775015000	-3.448042000
C	-1.780840000	-0.844616000	-1.969005000	F	8.971033000	2.646845000	-1.844450000
C	-4.891834000	-1.563840000	-0.973522000	S	2.315715000	2.584361000	1.205423000
C	-4.394978000	-3.426752000	0.382490000	C	4.284718000	0.551784000	1.319715000
H	-0.719312000	-0.592049000	-2.039288000	C	2.452980000	3.862721000	0.009687000
H	-2.315081000	-0.181714000	-2.659815000	H	3.878488000	4.360742000	-1.529116000
H	-2.108843000	-0.578272000	-0.960690000	H	5.379602000	0.566310000	1.339761000
C	-5.701699000	-1.385434000	0.284159000	H	3.917980000	0.453491000	2.343513000
C	-4.965700000	-0.539398000	-2.011500000	H	3.986356000	-0.346527000	0.768421000
C	-5.668737000	-2.771279000	0.969260000	C	1.400985000	4.932538000	-0.125636000
F	-3.368925000	-3.292703000	1.275436000	H	1.737303000	5.837854000	0.401630000
F	-4.574248000	-4.769009000	0.197528000	N	1.133430000	5.265892000	-1.543391000
F	-6.971982000	-0.968571000	0.051797000	C	-0.296626000	5.319154000	-1.876958000
F	-5.128390000	-0.451029000	1.119101000	H	-0.368861000	5.451321000	-2.963545000
C	-5.026215000	0.850540000	-1.653940000	H	-0.808890000	4.378515000	-1.619989000
F	-5.637032000	-2.688406000	2.315826000	C	-1.024223000	6.459982000	-1.137418000
F	-6.760645000	-3.480022000	0.594960000	H	-1.115556000	7.357284000	-1.777298000
S	-4.908320000	0.794231000	-4.213247000	H	-0.412348000	6.765576000	-0.286297000
C	-4.893825000	-2.022868000	-4.147191000	N	-2.332694000	6.049517000	-0.608336000
C	-4.969985000	1.698602000	-2.719825000	C	3.772945000	1.794101000	0.653302000
H	-5.040415000	1.167319000	-0.619808000	C	3.801620000	-0.477541000	-2.176703000
H	-5.305245000	-2.834532000	-3.541179000	C	-1.838216000	0.474427000	3.152020000
H	-5.476742000	-1.951458000	-5.071433000	C	0.461499000	-2.260907000	1.311855000
H	-3.866133000	-2.302895000	-4.409330000	C	-4.928786000	-0.739282000	-3.375880000
C	-4.899284000	3.200891000	-2.698341000	C	-2.033919000	-2.292189000	-2.260203000
H	-4.151276000	3.557214000	-3.413998000	H	-2.436596000	-5.535230000	1.653893000
N	-4.507094000	3.695367000	-1.355842000	H	-1.415866000	-7.411776000	0.934811000
C	-4.606544000	5.175471000	-1.225402000	H	0.325419000	-7.006307000	-4.010182000
H	-5.465192000	5.530727000	-1.813847000	H	-1.484037000	-5.861045000	-4.821013000
H	-4.828820000	5.372223000	-0.175350000	H	4.575963000	-6.004008000	-2.023297000
C	-3.353146000	5.959104000	-1.648857000	H	6.271025000	-4.275425000	-1.420573000
H	-3.677028000	6.962912000	-1.989709000	H	-2.139429000	4.826902000	4.112735000
H	-2.906649000	5.464517000	-2.518994000	H	-1.899370000	4.451593000	1.217938000
C	3.331369000	-6.456717000	0.128311000	H	1.546222000	4.535109000	-2.117441000
C	3.940392000	-5.115134000	-0.298041000	H	0.486888000	4.591753000	0.382152000
H	3.364530000	-6.476412000	1.223886000	H	-5.165378000	3.305288000	-0.682426000
H	4.009187000	-7.273853000	-0.211185000	H	-5.866778000	3.640766000	-2.991529000
N	4.297114000	-5.072195000	-1.723202000	Au	-2.531085000	2.717312000	-0.685392000
H	4.833021000	-4.949664000	0.333404000	Au	-0.260607000	1.813891000	0.074512000
H	3.231118000	-4.309727000	-0.075664000				
C	5.373122000	-4.145719000	-2.056002000				
C	4.970295000	-2.700978000	-1.964988000	Au@TAE-DTE-C (two gold atoms encapsulated)			
H	5.678649000	-4.365701000	-3.088063000	Charge 0, Multiplicity 1, HF = -7335.6765781			
C	5.769552000	-1.643617000	-1.652854000	N	0.372345645	-0.584029440	-5.109284885
S	3.374000000	-2.152988000	-2.419594000	C	0.410915469	-2.029820716	-5.462952652
C	5.122698000	-0.361999000	-1.774621000	C	1.607017964	-2.784298862	-4.853282505
H	6.804789000	-1.753391000	-1.352047000	H	-0.499697200	-2.482003305	-5.065671932
C	5.880389000	0.875796000	-1.601712000	H	0.398176509	-2.134905412	-6.561686655
C	2.784827000	0.593897000	-2.433678000	N	1.180119580	-4.093199536	-4.360050960
C	5.536603000	2.091709000	-1.102676000	H	1.976133081	-2.224409293	-3.988279119
C	7.330857000	0.884884000	-2.033609000	H	2.438487483	-2.851243769	-5.579364502
H	2.245967000	0.874523000	-1.519226000	C	2.246373800	-4.864393053	-3.720737595
H	3.271736000	1.499499000	-2.807840000	C	2.712802068	-4.248777552	-2.426557865
H	2.042153000	0.272947000	-3.171322000	H	1.836978393	-5.861164458	-3.506949320
C	6.673766000	3.075737000	-1.234012000	C	3.990967429	-4.276772563	-1.959154926
C	4.318880000	2.496031000	-0.401668000	S	1.542398294	-3.453334134	-1.372029276
C	7.689830000	2.382064000	-2.169285000	C	4.152557359	-3.680456395	-0.669126010
F	7.555330000	0.215059000	-3.192438000	H	4.808365872	-4.755907912	-2.487450111
F	8.131493000	0.310651000	-1.077646000	C	2.930586452	-2.840126305	-0.263246718
F	7.252081000	3.329564000	-0.024979000	C	5.207584882	-3.698152162	0.186417394
F	6.283085000	4.278631000	-1.748417000	C	3.245380805	-1.375198413	-0.664130598
				C	5.131084437	-3.095182580	1.502729410

C	6.586455378	-4.226988600	-0.052830969	F	-8.886239593	-3.969745839	0.821822338
H	2.390061780	-0.721218774	-0.492310802	F	-8.803453623	-1.800020384	1.199804566
H	4.106918049	-1.009971182	-0.096221225	S	-2.424314339	-0.100413025	1.455986977
H	3.486640338	-1.336295683	-1.729803040	C	-4.861023368	0.911409586	0.691289577
C	6.499295228	-3.059263541	2.104151419	C	-2.908861932	-1.051969387	2.876988168
C	3.954393095	-2.672721120	2.031922577	H	-4.572415960	-2.224046568	3.560450875
C	7.243211493	-4.203369726	1.357727086	H	-5.861078096	0.782865690	0.266860852
F	7.312366546	-3.419028689	-0.887933034	H	-4.962161989	1.200243963	1.740742134
F	6.613235027	-5.477121531	-0.598794257	H	-4.351586907	1.712853789	0.151735676
F	6.520244932	-3.240412720	3.453427698	C	-1.925629203	-1.140642656	4.007301252
F	7.152954599	-1.881955850	1.846109870	H	-1.656616922	-0.135051474	4.342089504
C	2.674223692	-3.027039478	1.250968000	N	-2.444622214	-1.870863375	5.156585420
C	3.686201064	-1.953306750	3.243572516	C	-1.547243858	-1.851661067	6.319198218
F	8.577882930	-4.024839705	1.313837432	H	-1.943452899	-2.587525842	7.027312362
F	6.972761278	-5.376842760	1.986437623	H	-0.520939742	-2.175779692	6.069725171
S	1.377876145	-1.882095733	1.961533732	C	-1.510006867	-0.483057375	7.025597034
C	2.278108851	-4.473863735	1.637176548	H	-1.429181895	-0.638021521	8.118446110
C	2.423289899	-1.459386576	3.324928232	H	-2.481344797	-0.011220008	6.851000398
H	4.447641320	-1.777847233	3.993875840	C	1.608310913	0.091494703	-5.586756315
H	3.046357273	-5.175974352	1.298661443	C	1.723862576	1.572447216	-5.180022722
H	2.194817262	-4.545628050	2.724786213	H	2.450849450	-0.433423750	-5.133865565
H	1.323333899	-4.754495262	1.188145162	H	1.683199225	-0.022682704	-6.682180790
C	1.832012107	-0.538749663	4.349631925	N	3.080691066	1.835527474	-4.697080409
H	0.875733588	-0.945099994	4.691923656	H	1.039715521	1.776843162	-4.350436730
N	2.679111157	-0.325146745	5.514825886	H	1.431114091	2.233024807	-6.017057324
C	2.095159507	0.614773542	6.481685373	C	3.328619656	3.216360418	-4.289937885
H	2.865354878	0.802614823	7.237607083	C	2.589533583	3.599669963	-3.034167009
H	1.851106764	1.591409722	6.025596975	H	4.406834615	3.303405704	-4.097850851
C	0.846660934	0.047585764	7.185208216	C	2.160691722	4.855275006	-2.732429623
H	0.857436157	0.341786531	8.251623883	S	2.282547727	2.380825436	-1.794128022
H	0.934631116	-1.042749654	7.167586244	C	1.553894309	4.969594633	-1.442620150
C	-0.827089213	0.068594302	-5.703929758	H	2.310005930	5.708303196	-3.385930790
C	-2.175951294	-0.537568492	-5.269693760	C	1.205338390	3.595689021	-0.846768314
H	-0.817564747	1.109084281	-5.373065016	C	1.197182250	6.069151914	-0.730167431
H	-0.735069893	0.057525203	-6.804165671	C	-0.269515193	3.306204613	-1.228396918
N	-3.156128400	0.539042965	-5.099646996	C	0.652688494	5.963815531	0.608700096
H	-2.054889631	-1.027878879	-4.299187765	C	1.207334669	7.500432489	-1.166331518
H	-2.509258294	-1.305800076	-5.991468694	H	-0.559979588	2.291655270	-0.950959986
C	-4.498288266	0.111546485	-4.706598683	H	-0.931748645	4.025966207	-0.736583626
C	-4.586563948	-0.316755196	-3.260754621	H	-0.387478682	3.407100674	-2.310728003
H	-5.162891974	0.974169531	-4.849152494	C	0.125141083	7.298109558	1.028193501
C	-5.570103901	-1.091893392	-2.720880133	C	0.668453743	4.795933683	1.300163423
S	-3.347454868	0.220831954	-2.130208027	C	0.936597740	8.290410088	0.147232580
C	-5.411648917	-1.337194623	-1.321801423	F	0.207380091	7.777021425	-2.060839039
H	-6.412086500	-1.473597927	-3.289154008	F	2.374925220	7.890901533	-1.754191306
C	-3.992943419	-0.981362209	-0.841835287	F	0.272576230	7.565095568	2.354919669
C	-6.243438981	-1.918866117	-0.416828451	F	-1.205499455	7.450136626	0.733386998
C	-3.180548104	-2.300315409	-0.962107089	C	1.458436502	3.627609818	0.679735363
C	-5.857615637	-2.073632502	0.971068748	C	0.067076378	4.457888176	2.556695663
C	-7.558818996	-2.586915420	-0.661940031	F	0.295544901	9.456555664	-0.063011735
H	-2.126941400	-2.143033966	-0.724555231	F	2.122797170	8.540200218	0.760362771
H	-3.598069985	-3.060468912	-0.294942832	S	0.836557226	2.118515739	1.596748803
H	-3.246259313	-2.665984164	-1.990169963	C	2.948746370	3.817312581	1.055580366
C	-6.816346326	-3.008264412	1.638509296	C	0.042260193	3.124750189	2.815860618
C	-4.763365178	-1.460647182	1.492000500	H	-0.381676555	5.200535268	3.205074009
C	-8.098706793	-2.878220119	0.768615555	H	3.340122398	4.726967388	0.589577064
F	-7.420327172	-3.774573681	-1.331175708	H	3.036073126	3.916412969	2.140726743
F	-8.435920232	-1.833032583	-1.385151925	H	3.550739409	2.967608592	0.727217490
F	-7.059078766	-2.720614942	2.946083159	C	-0.650139998	2.402261046	3.932366991
F	-6.389796549	-4.310188286	1.583855071	H	0.040040025	1.694947643	4.399777862
C	-4.070410899	-0.416320437	0.597996671	N	-1.167677025	3.278004175	4.975101399
C	-4.129985277	-1.633691069	2.766989543	C	-1.801201905	2.541587447	6.077358977

H	-2.325493160	3.284220431	6.688692158	H	-0.832207000	0.578450000	4.418325000
H	-2.565011610	1.823867662	5.724977518	H	-2.021046000	-0.359070000	3.496036000
C	-0.781202105	1.821517099	6.977387240	C	2.002758000	2.768868000	1.914879000
H	-1.146989835	1.825617143	8.021692929	H	1.234391000	3.506434000	2.167113000
H	0.129894330	2.426467915	6.965219391	N	3.245735000	3.152824000	2.562596000
N	-0.443691437	0.437573009	6.575525169	C	3.669971000	4.548558000	2.343966000
H	3.571980049	0.055079851	5.204276667	H	4.614253000	4.659821000	2.886743000
H	1.577239440	0.402436455	3.824721290	H	3.875770000	4.762784000	1.284067000
H	-1.861983886	3.900734252	4.565325175	C	2.646089000	5.571501000	2.877802000
H	-1.440064653	1.778307585	3.469266137	H	3.165916000	6.366794000	3.439715000
H	-2.601841050	-2.840072456	4.885523322	H	2.004693000	5.066596000	3.605650000
H	-0.990172523	-1.575494684	3.603486665	C	-2.319353000	-4.094076000	-3.523405000
H	0.788035328	-4.645200422	-5.120359205	C	-3.760203000	-3.611144000	-3.253869000
H	3.133595286	-5.009638147	-4.365232441	H	-1.736366000	-3.242236000	-3.870980000
H	-3.227003268	1.080212963	-5.958597843	H	-2.305511000	-4.883729000	-4.289901000
H	-4.901110291	-0.706613778	-5.332881519	N	-4.143260000	-2.548438000	-4.174186000
H	3.759569209	1.580740344	-5.411648494	H	-3.805597000	-3.190019000	-2.241341000
H	3.079332689	3.959281576	-5.070830363	H	-4.473538000	-4.455437000	-3.277092000
Au	0.206713426	-0.411956555	-2.781079110	C	-5.420817000	-1.910340000	-3.853364000
Au	-0.397083558	-0.334129164	-0.307700518	C	-5.275865000	-0.866019000	-2.771601000

CO₂@Au@TAE-DTE-C

Charge 0, Multiplicity 1, HF = -7524.1355074

N	-1.643886000	-4.614796000	-2.285869000	C	-6.257654000	-0.342073000	-1.987784000
C	-2.409231000	-5.783964000	-1.715045000	S	-3.685051000	-0.133238000	-2.575836000
C	-2.232828000	-6.029180000	-0.206605000	C	-5.827458000	0.759029000	-1.175800000
H	-3.469659000	-5.616048000	-1.902327000	H	-7.292925000	-0.663654000	-2.029172000
H	-2.122852000	-6.682093000	-2.277147000	C	-4.294764000	0.897200000	-1.145852000
N	-3.131147000	-5.164305000	0.565360000	C	-6.531221000	1.650345000	-0.431294000
H	-1.203191000	-5.819437000	0.105324000	C	-3.810821000	0.211739000	0.158632000
H	-2.409341000	-7.099061000	-0.005655000	C	-5.881804000	2.772823000	0.222307000
C	-2.854925000	-5.062451000	1.997692000	C	-7.987783000	1.625994000	-0.077721000
C	-1.738391000	-4.106275000	2.331727000	H	-2.720939000	0.209998000	0.214717000
H	-3.772159000	-4.693462000	2.475484000	H	-4.213685000	0.724313000	1.037196000
C	-0.762267000	-4.266947000	3.254084000	H	-4.158830000	-0.825138000	0.167573000
S	-1.728219000	-2.455309000	1.588207000	C	-6.845496000	3.390692000	1.187967000
C	0.116150000	-3.142815000	3.425471000	C	-4.606039000	3.135445000	-0.063001000
H	-0.667465000	-5.166071000	3.854781000	C	-8.231849000	3.011223000	0.592088000
C	-0.021157000	-2.108580000	2.294736000	F	-8.272272000	0.641410000	0.829159000
C	1.073741000	-2.898843000	4.350471000	F	-8.806136000	1.429300000	-1.147551000
C	1.074910000	-2.461202000	1.260841000	F	-6.701090000	4.732733000	1.335295000
C	1.820841000	-1.656268000	4.357279000	F	-6.742789000	2.827569000	2.433340000
C	1.603934000	-3.819278000	5.417235000	C	-3.930016000	2.400006000	-1.234102000
H	1.019339000	-1.842617000	0.363868000	C	-3.748490000	4.097834000	0.573435000
H	2.061950000	-2.337253000	1.713435000	F	-9.210413000	2.983104000	1.512953000
H	0.964118000	-3.506269000	0.961238000	F	-8.542923000	3.913006000	-0.372386000
C	2.987929000	-1.795655000	5.291366000	S	-2.107974000	2.772370000	-1.009245000
C	1.438497000	-0.590816000	3.609113000	C	-4.378244000	3.066851000	-2.557049000
C	2.503777000	-2.891383000	6.287844000	C	-2.438016000	3.993609000	0.232087000
F	2.370985000	-4.806860000	4.875472000	H	-4.122385000	4.798061000	1.310949000
F	0.622674000	-4.413455000	6.144289000	H	-5.454856000	2.935895000	-2.699348000
F	3.324742000	-0.643466000	5.919620000	H	-4.162062000	4.137220000	-2.513746000
F	4.094599000	-2.260070000	4.640602000	H	-3.855514000	2.635135000	-3.413353000
C	0.073435000	-0.698651000	2.914802000	C	-1.241330000	4.674308000	0.839517000
C	2.090432000	0.663457000	3.373733000	H	-0.723169000	5.279258000	0.081814000
F	3.511123000	-3.547521000	6.880210000	N	-1.587857000	5.515425000	1.976811000
F	1.724705000	-2.297372000	7.225659000	C	-0.473529000	5.814599000	2.883447000
S	0.032608000	0.743344000	1.714192000	H	-0.921269000	6.288977000	3.762633000
C	-1.031596000	-0.392610000	3.958480000	H	0.017502000	4.894248000	3.247622000
C	1.543141000	1.426828000	2.397834000	C	0.583713000	6.778160000	2.306090000
H	2.971708000	0.980483000	3.917382000	H	0.835114000	7.530780000	3.076408000
H	-1.033415000	-1.151191000	4.745158000	H	0.116323000	7.325360000	1.480236000
				C	-0.246413000	-5.094759000	-2.563564000
				C	0.777422000	-4.049941000	-3.023602000

H	0.120015000	-5.523938000	-1.626339000
H	-0.309662000	-5.909190000	-3.302074000
N	2.127795000	-4.545785000	-2.702892000
H	0.602754000	-3.112967000	-2.493332000
H	0.646890000	-3.828603000	-4.096237000
C	3.232181000	-3.951658000	-3.481730000
C	3.679522000	-2.572659000	-3.061670000
H	4.092660000	-4.621816000	-3.388075000
C	4.966279000	-2.152422000	-2.902798000
S	2.476652000	-1.293644000	-2.898663000
C	5.102907000	-0.744966000	-2.647036000
H	5.818948000	-2.821917000	-2.937704000
C	3.792460000	0.019797000	-2.885748000
C	6.171558000	0.003491000	-2.264865000
C	3.848751000	0.637829000	-4.305101000
C	6.042530000	1.409649000	-1.913489000
C	7.604728000	-0.420315000	-2.135661000
H	2.903016000	1.117123000	-4.565894000
H	4.652287000	1.377597000	-4.363567000
H	4.051954000	-0.153169000	-5.031308000
C	7.410505000	1.986884000	-1.704785000
C	4.834176000	1.998925000	-1.725409000
C	8.260550000	0.738703000	-1.330101000
F	8.221530000	-0.517658000	-3.349722000
F	7.757979000	-1.620116000	-1.509247000
F	7.456877000	2.940116000	-0.735170000
F	7.921161000	2.534120000	-2.846499000
C	3.619790000	1.055460000	-1.757657000
C	4.463703000	3.352225000	-1.393398000
F	9.568574000	0.890578000	-1.592348000
F	8.090486000	0.492767000	-0.003953000
S	2.169446000	2.204262000	-2.002705000
C	3.526327000	0.410894000	-0.351660000
C	3.130589000	3.599629000	-1.487924000
H	5.181765000	4.116257000	-1.122584000
H	4.392904000	-0.232390000	-0.176664000
H	3.530583000	1.196800000	0.403600000
H	2.620936000	-0.185927000	-0.241886000
C	2.351105000	4.847983000	-1.193310000
H	1.822622000	4.713570000	-0.241165000
N	3.188445000	6.025687000	-1.050298000
C	2.481613000	7.166105000	-0.448827000
H	2.944301000	8.083655000	-0.828837000
H	1.416981000	7.202118000	-0.740917000
C	2.620267000	7.179474000	1.074935000
H	2.370109000	8.184004000	1.455586000
H	3.681254000	7.025649000	1.289073000
N	1.822268000	6.153157000	1.796905000
H	3.993442000	2.536683000	2.246551000
H	2.033670000	2.753549000	0.812516000
H	3.565332000	6.285922000	-1.958021000
H	1.558478000	4.965616000	-1.960716000
H	-2.300255000	5.038358000	2.525034000
H	-0.526827000	3.868973000	1.105367000
H	-4.095614000	-5.452875000	0.426410000
H	-2.614141000	-6.030223000	2.469993000
H	-4.155173000	-2.886320000	-5.132507000
H	-6.215447000	-2.622765000	-3.567465000
H	2.161879000	-5.547100000	-2.887954000
H	2.981897000	-3.892663000	-4.558992000
Au	-1.585317000	-3.007344000	-0.729669000
Au	-0.129886000	0.124098000	-0.716566000

C	-0.525399000	-0.293848000	-2.691672000
O	-0.777230000	-1.391280000	-3.144829000
O	-0.512586000	0.759379000	-3.548052000

COOH binding with secondary amine of TAE-DTE-C
Charge 1, Multiplicity 1, HF = -7253.6880097

N	3.462655000	4.117020000	-2.832990000
C	3.248993000	3.281471000	-4.013997000
C	3.925953000	1.913880000	-3.907257000
H	2.175331000	3.103748000	-4.126492000
H	3.586618000	3.791608000	-4.942160000
N	3.577059000	1.087101000	-5.066664000
H	3.585337000	1.427096000	-2.989144000
H	5.020163000	2.026314000	-3.801089000
C	4.407635000	-0.115157000	-5.193734000
C	4.108566000	-1.069749000	-4.070492000
H	4.187598000	-0.580779000	-6.161441000
C	4.860633000	-1.214593000	-2.946607000
S	2.600482000	-1.992704000	-4.070853000
C	4.258412000	-2.023478000	-1.936706000
H	5.821326000	-0.729575000	-2.813564000
C	2.772449000	-2.294436000	-2.231088000
C	4.751310000	-2.459424000	-0.748921000
C	1.965196000	-1.178499000	-1.529582000
C	3.941227000	-3.248606000	0.152129000
C	6.092218000	-2.176150000	-0.148462000
H	0.901753000	-1.248032000	-1.766607000
H	2.086545000	-1.255975000	-0.448396000
H	2.336289000	-0.203876000	-1.849468000
C	4.574918000	-3.262302000	1.505269000
C	2.767480000	-3.805914000	-0.238262000
C	6.076764000	-2.934871000	1.224774000
F	6.314803000	-0.835579000	0.061108000
F	7.126113000	-2.606110000	-0.924086000
F	4.431191000	-4.436820000	2.174424000
F	4.053703000	-2.280094000	2.317760000
C	2.405176000	-3.709743000	-1.733953000
C	1.769047000	-4.473952000	0.543819000
F	6.637355000	-2.211940000	2.211892000
F	6.746197000	-4.104319000	1.088289000
S	0.560441000	-4.079661000	-1.775019000
C	3.128141000	-4.844512000	-2.494156000
C	0.590455000	-4.658943000	-0.102403000
H	1.932648000	-4.727906000	1.585362000
H	4.211325000	-4.702872000	-2.432386000
H	2.876075000	-5.806485000	-2.040944000
H	2.839156000	-4.861917000	-3.546999000
C	-0.693157000	-5.190840000	0.471541000
H	-1.340687000	-5.513931000	-0.359694000
N	-0.546147000	-6.272953000	1.435985000
C	-1.220471000	-6.107888000	2.716458000
H	-0.855290000	-6.902906000	3.374586000
H	-0.980983000	-5.152519000	3.217271000
C	-2.746413000	-6.271184000	2.607212000
H	-3.148583000	-6.670409000	3.554554000
H	-2.926588000	-7.029248000	1.837564000
C	2.606624000	5.306864000	-2.828238000
C	1.112219000	5.081152000	-2.597240000
H	2.963448000	5.962614000	-2.023078000
H	2.717224000	5.885662000	-3.767316000
N	0.811865000	4.521396000	-1.278484000
H	0.686429000	4.423148000	-3.364732000

H	0.629447000	6.066408000	-2.734087000	H	1.078496000	0.572202000	0.028162000
C	-0.536386000	4.796800000	-0.809390000	H	0.517718000	2.101096000	0.695505000
C	-1.534411000	3.796553000	-1.319331000	H	1.959798000	2.080158000	-0.315707000
H	-0.543965000	4.711371000	0.283152000	C	-0.788768000	3.564857000	3.441761000
C	-2.891561000	3.946666000	-1.372032000	C	0.279213000	1.251749000	3.176213000
S	-0.933874000	2.205826000	-1.747450000	C	-0.081061000	4.911547000	3.769326000
C	-3.595501000	2.734865000	-1.608740000	F	1.174334000	5.454617000	1.806522000
H	-3.393780000	4.871131000	-1.111453000	F	2.272067000	5.479429000	3.702551000
C	-2.668034000	1.560279000	-1.980157000	F	-1.680591000	3.204795000	4.398854000
C	-4.922236000	2.445344000	-1.443248000	F	-1.512319000	3.729395000	2.269721000
C	-2.855360000	1.209480000	-3.472711000	C	1.573363000	0.503794000	2.812200000
C	-5.375446000	1.079250000	-1.332763000	C	-0.856299000	0.384437000	3.314146000
C	-6.071353000	3.385701000	-1.245061000	F	-0.802236000	5.984157000	3.390579000
H	-2.158287000	0.426636000	-3.782182000	F	0.138736000	4.965219000	5.105031000
H	-3.875863000	0.866056000	-3.664287000	S	0.974992000	-1.185727000	2.232413000
H	-2.669809000	2.099264000	-4.079189000	C	2.434745000	0.289784000	4.075136000
C	-6.873789000	1.064906000	-1.268772000	C	-0.661395000	-0.865505000	2.824882000
C	-4.508161000	0.051108000	-1.162677000	H	-1.798978000	0.747804000	3.705976000
C	-7.207925000	2.470945000	-0.693814000	H	2.772295000	1.254238000	4.467072000
F	-6.492810000	3.943895000	-2.418878000	H	1.836841000	-0.207826000	4.842891000
F	-5.799253000	4.409837000	-0.388900000	H	3.307954000	-0.327357000	3.853277000
F	-7.381068000	0.061464000	-0.492467000	C	-1.673744000	-1.955271000	2.625412000
F	-7.435816000	0.944202000	-2.506623000	H	-1.223965000	-2.913448000	2.913610000
C	-3.020301000	0.408327000	-1.009675000	N	-2.900315000	-1.766707000	3.390875000
C	-4.750990000	-1.347707000	-0.967730000	C	-3.979548000	-2.680093000	3.033508000
F	-8.439488000	2.892912000	-1.022012000	H	-4.871219000	-2.345290000	3.573004000
F	-7.097728000	2.404526000	0.659247000	H	-4.229847000	-2.633305000	1.951739000
S	-2.128754000	-1.218059000	-1.344789000	C	-3.655892000	-4.145867000	3.412280000
C	-2.764434000	0.767494000	0.476646000	H	-4.425786000	-4.548326000	4.091716000
C	-3.623777000	-2.109535000	-1.001962000	H	-2.725942000	-4.151804000	3.982766000
H	-5.762304000	-1.714184000	-0.822061000	N	-3.491087000	-5.038466000	2.240813000
H	-3.282485000	1.691323000	0.747907000	H	0.424587000	-6.538489000	1.555112000
H	-3.143895000	-0.037817000	1.109519000	H	-1.208329000	-4.343351000	0.946171000
H	-1.701648000	0.895543000	0.678013000	H	-3.230972000	-0.810459000	3.291644000
C	-3.484829000	-3.564326000	-0.691085000	H	-1.855318000	-2.026367000	1.532765000
H	-2.994412000	-3.736277000	0.269607000	H	-2.952145000	-4.119716000	-1.468025000
N	-4.843428000	-4.221439000	-0.559878000	H	3.684373000	1.634946000	-5.919106000
C	-4.811902000	-5.576111000	0.162661000	H	5.492382000	0.100807000	-5.166736000
H	-5.718642000	-6.102581000	-0.146310000	H	1.483141000	4.834979000	-0.583042000
H	-3.937876000	-6.109962000	-0.214234000	H	-0.894762000	5.815054000	-1.048221000
C	-4.800080000	-5.395545000	1.684352000	H	6.450070000	2.590708000	-1.516329000
H	-5.192286000	-6.329949000	2.120931000	H	6.449814000	3.342064000	0.974158000
H	-5.538056000	-4.626689000	1.945819000	H	-5.433927000	-3.595642000	0.003344000
C	4.869085000	4.516273000	-2.635126000	C	-5.495813000	-4.366908000	-1.909122000
C	5.341943000	4.272789000	-1.200366000	O	-6.769279000	-4.020902000	-1.772017000
H	5.519743000	3.969486000	-3.326186000	O	-4.898206000	-4.776754000	-2.853271000
H	5.010863000	5.579774000	-2.884171000	H	-7.226571000	-4.112268000	-2.632197000
N	5.638861000	2.859642000	-0.963589000	COOH binding with tertiary amine of TAE-DTE-C			
H	4.533638000	4.567887000	-0.522489000	Charge 1, Multiplicity 1, HF = -7253.6849743			
H	6.207526000	4.924651000	-0.974955000	N	2.461200000	-4.568100000	2.452100000
C	5.901777000	2.542010000	0.446107000	C	2.358100000	-3.694600000	3.619300000
C	4.594481000	2.296745000	1.155410000	C	3.275200000	-2.471100000	3.529800000
H	6.517125000	1.638438000	0.486652000	H	1.330300000	-3.327500000	3.691100000
C	3.807925000	3.241518000	1.750406000	H	2.572000000	-4.247200000	4.561600000
S	3.926395000	0.671713000	1.160069000	N	3.132900000	-1.645800000	4.735600000
C	2.554106000	2.747158000	2.212279000	H	2.999700000	-1.888600000	2.647300000
H	4.117046000	4.272851000	1.882052000	H	4.323400000	-2.777100000	3.375500000
C	2.277616000	1.321324000	1.707992000	C	4.213700000	-0.667400000	4.926400000
C	1.521813000	3.355482000	2.859195000	C	4.156300000	0.394500000	3.863100000
C	1.405768000	1.522193000	0.442476000	H	4.089200000	-0.225900000	5.921300000
C	0.335051000	2.607209000	3.226100000	C	4.864300000	0.381000000	2.704100000
C	1.292580000	4.818170000	3.034395000				

S	2.972600000	1.710800000	3.975300000	C	-7.678300000	-0.883900000	0.747400000
C	4.441400000	1.357500000	1.747800000	F	-7.278900000	-2.630500000	2.312500000
H	5.639100000	-0.347500000	2.490700000	F	-6.695600000	-3.029600000	0.235100000
C	3.074700000	1.957600000	2.118900000	F	-7.387400000	1.512600000	0.770200000
C	4.975200000	1.702000000	0.549800000	F	-7.614000000	0.470800000	2.694700000
C	1.990300000	1.052700000	1.491100000	C	-3.176700000	0.246700000	1.129100000
C	4.319300000	2.653700000	-0.319600000	C	-4.482200000	2.331500000	1.260200000
C	6.210500000	1.158700000	-0.093400000	F	-8.973400000	-1.089000000	1.056700000
H	0.988500000	1.353400000	1.798400000	F	-7.565100000	-0.721700000	-0.598700000
H	2.050600000	1.104500000	0.403000000	S	-1.949100000	1.604800000	1.530100000
H	2.152100000	0.020300000	1.801400000	C	-3.056800000	-0.040600000	-0.391100000
C	4.866500000	2.532800000	-1.701600000	C	-3.218800000	2.827700000	1.307000000
C	3.294300000	3.433700000	0.116200000	H	-5.349400000	2.969300000	1.149200000
C	6.251300000	1.824900000	-1.516800000	H	-3.790900000	-0.789100000	-0.702100000
F	6.207100000	-0.210800000	-0.206400000	H	-3.253800000	0.882800000	-0.937900000
F	7.344900000	1.466300000	0.601300000	H	-2.061300000	-0.399500000	-0.650400000
F	5.000700000	3.721600000	-2.351300000	C	-2.790400000	4.251200000	1.098100000
F	4.070300000	1.744600000	-2.503000000	H	-2.345400000	4.313900000	0.100400000
C	2.998600000	3.420700000	1.628000000	N	-3.909900000	5.182700000	1.125000000
C	2.402600000	4.270300000	-0.624900000	C	-3.690700000	6.436700000	0.396000000
F	6.490200000	0.916200000	-2.484300000	H	-4.432100000	7.153200000	0.767100000
F	7.226200000	2.764900000	-1.545400000	H	-2.696900000	6.881200000	0.585400000
S	1.287300000	4.177600000	1.766700000	C	-3.916700000	6.271000000	-1.115000000
C	3.995300000	4.369300000	2.332600000	H	-4.245000000	7.233100000	-1.549900000
C	1.319300000	4.696900000	0.079600000	H	-4.754000000	5.576800000	-1.226300000
H	2.541600000	4.458000000	-1.683700000	C	3.786700000	-5.193500000	2.287900000
H	5.015700000	3.990800000	2.219000000	C	4.330600000	-5.026800000	0.866300000
H	3.936600000	5.361300000	1.877500000	H	4.502000000	-4.767900000	3.000200000
H	3.772800000	4.455700000	3.398400000	H	3.740900000	-6.267300000	2.530400000
C	0.129300000	5.450200000	-0.442600000	N	4.896300000	-3.694500000	0.653600000
H	-0.405300000	5.911100000	0.399100000	H	3.494700000	-5.153500000	0.170600000
N	0.435500000	6.463000000	-1.450600000	H	5.060200000	-5.830000000	0.645300000
C	-0.435800000	6.468700000	-2.624100000	C	5.165700000	-3.389700000	-0.759000000
H	-0.030900000	7.219000000	-3.312600000	C	3.909000000	-2.876200000	-1.412500000
H	-0.433900000	5.506600000	-3.168100000	H	5.946000000	-2.624200000	-0.803700000
C	-1.883400000	6.865800000	-2.285700000	C	2.953300000	-3.633600000	-2.023500000
H	-2.332500000	7.390500000	-3.150300000	S	3.541600000	-1.158700000	-1.321300000
H	-1.832900000	7.593100000	-1.469100000	C	1.795300000	-2.900800000	-2.421600000
C	1.428800000	-5.610400000	2.428300000	H	3.069100000	-4.696000000	-2.210200000
C	-0.018600000	-5.167900000	2.215100000	C	1.785500000	-1.478400000	-1.837600000
H	1.682900000	-6.294700000	1.607600000	C	0.668200000	-3.282100000	-3.080000000
H	1.457500000	-6.219300000	3.355500000	C	0.932700000	-1.586500000	-0.549300000
N	-0.244000000	-4.540900000	0.917200000	C	-0.378100000	-2.325400000	-3.388800000
H	-0.341200000	-4.473100000	2.999900000	C	0.202100000	-4.668500000	-3.364700000
H	-0.635600000	-6.078900000	2.341300000	H	0.080800000	-0.911500000	-0.571800000
C	-1.638000000	-4.525300000	0.493700000	H	0.551300000	-2.601600000	-0.442500000
C	-2.411400000	-3.392600000	1.112600000	H	1.545000000	-1.371100000	0.329200000
H	-1.654200000	-4.369900000	-0.590600000	C	-1.634100000	-3.065400000	-3.704600000
C	-3.763700000	-3.273200000	1.207800000	C	-0.204100000	-0.985400000	-3.247400000
S	-1.491100000	-1.988100000	1.634400000	C	-1.135100000	-4.473900000	-4.140400000
C	-4.205700000	-1.959300000	1.563500000	F	-0.070300000	-5.360900000	-2.194000000
H	-4.450700000	-4.052400000	0.897300000	F	1.083300000	-5.441600000	-4.055900000
C	-3.052100000	-1.030500000	1.989400000	F	-2.418600000	-2.487900000	-4.651800000
C	-5.436000000	-1.387200000	1.452100000	F	-2.421500000	-3.216700000	-2.578300000
C	-3.128200000	-0.770700000	3.509100000	C	1.205700000	-0.492900000	-2.876600000
C	-5.609600000	0.057400000	1.472200000	C	-1.170300000	0.071200000	-3.314200000
C	-6.749900000	-2.052600000	1.188400000	F	-2.030800000	-5.450000000	-3.893100000
H	-2.273000000	-0.180600000	3.844800000	F	-0.866200000	-4.442800000	-5.470500000
H	-4.049300000	-0.237300000	3.760800000	S	0.923000000	1.237300000	-2.202400000
H	-3.122500000	-1.726600000	4.039300000	C	2.058100000	-0.368700000	-4.159500000
C	-7.072000000	0.369500000	1.439800000	C	-0.755000000	1.239700000	-2.760100000
C	-4.552800000	0.900500000	1.354600000	H	-2.170000000	-0.095100000	-3.696400000

H	2.208900000	-1.355700000	-4.607900000
H	1.535500000	0.265700000	-4.880100000
H	3.031800000	0.073800000	-3.941800000
C	-1.559100000	2.472700000	-2.469600000
H	-0.984000000	3.353100000	-2.781800000
N	-2.853800000	2.498100000	-3.140400000
C	-3.741700000	3.569700000	-2.664800000
H	-4.712600000	3.399100000	-3.141600000
H	-3.907200000	3.520500000	-1.574800000
C	-3.219200000	4.976100000	-3.035400000
H	-3.997000000	5.541100000	-3.581200000
H	-2.390900000	4.857100000	-3.739100000
N	-2.754300000	5.749400000	-1.867900000
H	1.410000000	6.423600000	-1.728500000
H	-0.567200000	4.703500000	-0.849600000
H	-3.328400000	1.612000000	-2.979700000
H	-1.637800000	2.545400000	-1.365900000
H	-4.176700000	5.374800000	2.086600000
H	-1.981200000	4.509000000	1.808200000
H	3.108700000	-2.245300000	5.559300000
H	5.216200000	-1.131500000	4.884900000
H	0.324800000	-4.970600000	0.193100000
H	-2.170600000	-5.475600000	0.687200000
H	5.762900000	-3.609600000	1.180200000
H	5.528700000	-4.266300000	-1.324800000
C	2.239500000	-3.661100000	1.258800000
O	2.243900000	-4.425800000	0.174600000
O	2.098200000	-2.485800000	1.382500000
H	2.113400000	-3.878800000	-0.603400000

COOH binding with sulphur of TAE-DTE-C

Charge 1, Multiplicity 1, HF = -7253.6667244

N	2.018020000	5.147872000	-2.124211000
C	2.351392000	4.474778000	-3.383496000
C	3.539845000	3.519721000	-3.269220000
H	1.487343000	3.887893000	-3.709473000
H	2.553566000	5.214630000	-4.188208000
N	3.776482000	2.849670000	-4.550769000
H	3.325029000	2.777180000	-2.495785000
H	4.439798000	4.057749000	-2.925252000
C	5.036095000	2.100457000	-4.578617000
C	4.927595000	0.888876000	-3.694017000
H	5.231917000	1.797571000	-5.613843000
C	5.472303000	0.758215000	-2.453774000
S	3.895649000	-0.455141000	-4.191628000
C	5.046903000	-0.406617000	-1.746542000
H	6.142908000	1.493169000	-2.022818000
C	3.851997000	-1.086888000	-2.433989000
C	5.434399000	-0.905562000	-0.544117000
C	2.574047000	-0.500736000	-1.792146000
C	4.824157000	-2.098918000	0.000264000
C	6.466488000	-0.360220000	0.391751000
H	1.689656000	-0.783360000	-2.358621000
H	2.471593000	-0.834065000	-0.756163000
H	2.636039000	0.588641000	-1.795084000
C	5.135167000	-2.181065000	1.461979000
C	4.066004000	-2.928481000	-0.758339000
C	6.436649000	-1.330714000	1.626969000
F	6.205188000	0.926378000	0.796425000
F	7.710434000	-0.329128000	-0.161460000
F	5.295516000	-3.444977000	1.930524000
F	4.133766000	-1.600312000	2.205566000

C	3.987067000	-2.613654000	-2.262284000
C	3.356128000	-4.123639000	-0.398151000
F	6.462844000	-0.661630000	2.793916000
F	7.499644000	-2.165051000	1.560963000
S	2.505749000	-3.626923000	-2.852018000
C	5.227078000	-3.210890000	-2.966740000
C	2.547663000	-4.625916000	-1.359688000
H	3.464014000	-4.577803000	0.579735000
H	6.132737000	-2.725775000	-2.591506000
H	5.293210000	-4.280219000	-2.750930000
H	5.176992000	-3.067942000	-4.047801000
C	1.752283000	-5.914548000	-1.332153000
H	2.196165000	-6.602462000	-2.066546000
N	1.665769000	-6.569031000	-0.045499000
C	0.757150000	-5.946445000	0.923521000
H	1.239929000	-5.914409000	1.904671000
H	0.535129000	-4.901322000	0.657022000
C	-0.550006000	-6.753603000	0.973810000
H	-0.334208000	-7.764433000	1.365586000
H	-0.871098000	-6.891783000	-0.062554000
C	0.766895000	5.910484000	-2.242666000
C	-0.533634000	5.099918000	-2.269703000
H	0.705178000	6.588759000	-1.382661000
H	0.778685000	6.554190000	-3.144337000
N	-0.870933000	4.480162000	-0.980221000
H	-0.500279000	4.327895000	-3.048129000
H	-1.325673000	5.806128000	-2.570043000
C	-2.287428000	4.474320000	-0.646092000
C	-2.975598000	3.250576000	-1.183325000
H	-2.381781000	4.418434000	0.445113000
C	-4.317050000	3.028559000	-1.355955000
S	-1.930402000	1.886280000	-1.503046000
C	-4.641804000	1.671000000	-1.612243000
H	-5.073458000	3.785693000	-1.183937000
C	-3.390806000	0.794272000	-1.842777000
C	-5.844950000	1.010037000	-1.592071000
C	-3.382046000	0.375124000	-3.332011000
C	-5.897336000	-0.425754000	-1.494927000
C	-7.230292000	1.582995000	-1.583753000
H	-2.497101000	-0.206322000	-3.581682000
H	-4.277982000	-0.196085000	-3.584596000
H	-3.372051000	1.279623000	-3.945264000
C	-7.326260000	-0.870663000	-1.651496000
C	-4.800994000	-1.169692000	-1.183431000
C	-8.125245000	0.375199000	-1.167339000
F	-7.615430000	2.012742000	-2.819842000
F	-7.371383000	2.632815000	-0.727748000
F	-7.630736000	-1.988189000	-0.944627000
F	-7.623090000	-1.103963000	-2.961212000
C	-3.557735000	-0.352330000	-0.816928000
C	-4.626713000	-2.579493000	-1.053438000
F	-9.363883000	0.432511000	-1.676559000
F	-8.187792000	0.328987000	0.188296000
S	-2.213057000	-1.679890000	-0.615490000
C	-3.682575000	0.140838000	0.648260000
C	-3.367636000	-3.040522000	-0.834434000
H	-5.467372000	-3.261923000	-1.109427000
H	-4.551777000	0.793455000	0.738708000
H	-3.830922000	-0.708495000	1.320170000
H	-2.799143000	0.694456000	0.962863000
C	-2.862615000	-4.439507000	-0.636880000
H	-2.179596000	-4.474862000	0.218399000

N	-3.956873000	-5.358180000	-0.351551000	C	-1.390493000	-0.447337000	3.058184000
C	-3.500416000	-6.693916000	0.059437000	F	-2.921657000	4.933434000	3.670568000
H	-4.383706000	-7.341427000	0.051998000	F	-1.773028000	3.971364000	5.289399000
H	-2.790212000	-7.134125000	-0.661309000	S	0.838050000	-1.338899000	1.958829000
C	-2.934104000	-6.751948000	1.483287000	C	1.662884000	0.262529000	4.062695000
H	-2.874447000	-7.819414000	1.771910000	C	-0.810991000	-1.569463000	2.560123000
H	-3.668716000	-6.281281000	2.143640000	H	-2.408139000	-0.423234000	3.432669000
C	3.110781000	6.011962000	-1.625347000	H	1.685921000	1.229797000	4.574466000
C	3.582499000	5.624538000	-0.222153000	H	1.145015000	-0.457523000	4.701232000
H	3.959704000	6.003718000	-2.320496000	H	2.687487000	-0.080691000	3.905860000
H	2.781144000	7.059405000	-1.590892000	C	-1.453946000	-2.927948000	2.529546000
N	4.362668000	4.385351000	-0.204100000	H	-1.055771000	-3.522264000	1.703654000
H	2.687303000	5.471747000	0.386551000	N	-1.202278000	-3.651080000	3.774934000
H	4.137415000	6.471868000	0.224175000	C	-1.974917000	-4.891059000	3.920125000
C	4.664252000	3.892493000	1.149760000	H	-1.971612000	-5.142621000	4.986328000
C	3.462207000	3.151039000	1.676811000	H	-3.033013000	-4.764899000	3.624167000
H	5.526466000	3.223832000	1.089204000	C	-1.351717000	-6.070589000	3.167125000
C	2.368123000	3.743959000	2.236636000	H	-1.684977000	-7.017239000	3.629368000
S	3.323558000	1.409388000	1.469895000	H	-0.273350000	-6.006151000	3.325448000
C	1.271471000	2.866083000	2.445606000	N	-1.631770000	-6.092423000	1.714533000
H	2.334286000	4.793055000	2.507639000	H	2.584945000	-6.752772000	0.340806000
C	1.491936000	1.489124000	1.795533000	H	0.730618000	-5.722781000	-1.690973000
C	0.042089000	3.101427000	2.977739000	H	-1.421970000	-3.030689000	4.551243000
C	0.791761000	1.573896000	0.419543000	H	-2.536960000	-2.796421000	2.324871000
C	-0.911927000	2.029861000	3.147411000	H	-4.530312000	-5.468109000	-1.186563000
C	-0.585284000	4.417706000	3.284781000	H	-2.255702000	-4.726442000	-1.519022000
H	0.875187000	0.637158000	-0.130264000	H	3.800113000	3.540651000	-5.299001000
H	-0.264487000	1.795054000	0.563012000	H	5.904798000	2.692729000	-4.234747000
H	1.224822000	2.382014000	-0.175952000	H	-0.332918000	4.877646000	-0.217171000
C	-2.258227000	2.621812000	3.409223000	H	-2.831591000	5.378584000	-0.971082000
C	-0.568317000	0.724491000	2.997378000	H	5.241936000	4.538497000	-0.693853000
C	-1.946179000	4.047945000	3.948877000	H	4.918216000	4.701840000	1.857170000
F	-0.848308000	5.132602000	2.122560000	C	-0.876499000	-1.727743000	-1.973345000
F	0.158843000	5.239723000	4.066270000	O	-0.317184000	-2.906081000	-1.853921000
F	-3.048581000	1.909987000	4.249012000	O	-0.573216000	-0.770455000	-2.618797000
F	-2.967772000	2.767145000	2.224473000	H	0.591734000	-2.946745000	-2.316894000
C	0.910927000	0.391955000	2.717510000				

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