

*Supporting Information for*

**Electronic Transport in Radial  $\pi$ -Conjugated Macrocyclic Molecules: A Density Functional Theory Study**

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## **1. Computational procedure protocol**

In this study, we have designed a computational approach to accurately understand electronic and transport properties across thiophene-based macrocycles while maintaining computational efficiency. In the first step, we have designed thiophene-based macrocycles by incorporating D-A moieties such as DPP and BT to assess their effects on transport efficiency across the macrocycles. Further, we have optimized the structures utilizing density functional theory (DFT) with the Gaussian Software package. In this DFT theory, the PBE0 hybrid function is used to predict accurate HOMO- LUMO gaps and orbital delocalization in aromatic systems. As reported in studies of gold thiophene systems, charge-transport calculations across molecular junctions use the PBE0 functional within the Generalized Gradient Approximation (GGA). The basis set for this study is 6-31G\*\*, which includes the contribution of d orbitals on S, C, and N atoms in the macrocyclic molecular systems. Since heavy Au atoms are used as electrodes in macrocyclic molecular junctions, the LANL2DZ basis set with effective core potentials is used. Thus, for thiophene-functionalized aromatic molecular junctions, the GENECP basis set is used, with 6-31G\*\* for lighter atoms and LANL2DZ for heavy atoms, which provides accurate results while lowering computational cost. The molecular junctions are designed by anchoring Marksüf Decahedron Au clusters that mimic the properties of the Au (111) surface. For the transport calculations, a single zeta potential (SZP) is used for the valence electrons of Au, and a double zeta potential (DZP) is used for other atoms in the system.

## **2. Comparison of the SZP and DZP basis sets for modelling metal contacts**

We investigated the charge transport and electronic properties of the thiophene-based D-A macrocyclic structure connected to the gold electrodes, using basis-set approaches that balance accuracy and computational cost, particularly at the metal-molecule interface. The macrocyclic system consists of alternating thiophene donor units and DPP or BT as acceptor units. It has

been designed to improve the charge transport by tuning the frontier orbital energies and radial  $\pi$ -conjugation. The macrocyclic molecules are attached to the Au<sub>18</sub> clusters on both sides through sulphur linkers, which is effective for anchoring geometry and electrode spacing. [1,2]

The gold electrodes were modelled in the Single-zeta Polarized (SZP) basis set using the LANL2DZ pseudopotential. This basis set helps gold atoms to delocalize the electronic states.[3] Especially, it reduces the computational cost compared to Double Zeta Polarization (DZP). For the organic molecules, we have used the Double Zeta Polarized basis set (6-316\*\*). It studied the molecular orbital energies,  $\pi$ -conjugation, and D-A interactions.[4] This level was critical for describing the radial  $\pi$ -conjugation, HOMO-LUMO gap, and orbital localization. Even though the DZP increased the computational cost, this accuracy is necessary to know the structural changes and device performance. Overall, the mixed-basis set GENECP (LANL2DZ for gold and 6-31G\*\*) with the PBE0 exchange-correlation functional provides both accuracy and efficiency.[5]

### **3.HOMO and LUMO isosurface representation of the macrocyclic molecules**

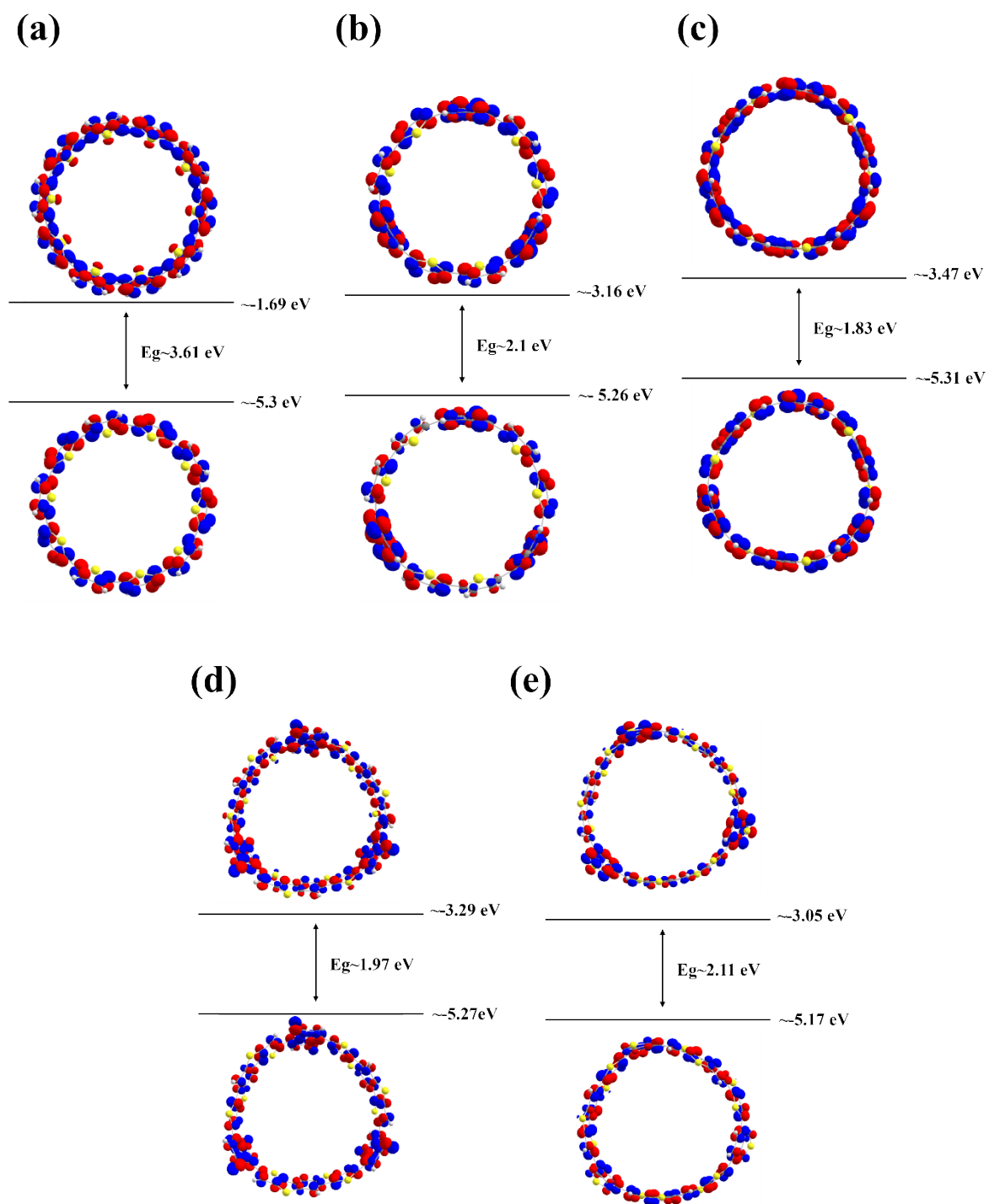


Figure S1: HOMO and LUMO isosurface representation of (a) [PT]<sub>10</sub>, (b) [TT-DPP]<sub>3</sub>, (c) [BDT-DPP]<sub>3</sub>, (d) [DTBDT-DPP]<sub>3</sub>, and (e) [DTBDT-BT]<sub>3</sub> isolated macrocyclic molecules calculated at PBE0/6-31G\*\*

Figure S1. The HOMO and LUMO isosurface representation of the five isolated macrocyclic molecules [PT]<sub>10</sub>, [TT-DPP]<sub>3</sub>, [BDT-DPP]<sub>3</sub>, [DTBDT-DPP]<sub>3</sub>, and [DTBDT-BT]<sub>3</sub> calculated

at the PBE0/6-31G\*\* level of theory (isovalue =0.025 a.u.). The HOMO is delocalized predominantly over the electron-rich donor units (thiophene, TT, BDT, and DTBDT). At the same time, the LUMO concentrates on the electron-deficient acceptor units (DPP and BT), consistent with donor-acceptor intramolecular charge transfer. In all five systems, the HOMO and LUMO densities are localized on the terminal sulphur atoms, confirming that the Au-S anchor sites are electronically accessible for coupling to the gold electrode.

#### **4.Comparative Analysis of Gold Nanocluster models and selection of the Au18 cluster as electrode model**

The electrode contacts in each molecular junction were represented by an Au18 truncated decahedral nanocluster the decahedron geometry. This cluster consists of 18 gold atoms in a truncated decahedral arrangement with approximate  $C_{2v}$  local symmetry and an Au-Au bond length of 2.88 Å, replicating the local atomic coordination environment of the Au(111) surface.<sup>[4,5]</sup> Its electronic structure was calculated at the PBE0/LANL2DZ level of theory. Table S1 compares the eight Au cluster models by their HOMO, LUMO, and HOMO-LUMO gap values. Among these, the Au18 Marks decahedron gives the HOMO energy of -5.85 eV, the closest match to the macrocyclic molecules' HOMO energies (-5.17 to -5.85 eV). This HOMO alignment reduces the energy offset at the metal-molecule interface and suppresses the charge transfer between the cluster and the molecule during geometry optimization. The Au18 Markshedron was selected over periodic slab models for two reasons. First, finite cluster models permit full geometric relaxation upon molecular adsorption, capturing the structural recognition of surface Au atoms at the binding site, a relaxation that rigid-sphere models suppress. <sup>[4,5]</sup>. The structure is substantially less computationally expensive than periodic calculations, establishing it as the standard electrode model in DFT studies of single-molecule junctions. <sup>[3,4,5]</sup> optimized Cartesian coordinates of the isolated Au18 cluster and all five molecular junctions.

**Table S1:** HOMO, LUMO, and band gap ( $E_g$ ) values for gold cluster calculated at the PBE0/LANL2DZ

Name	HOMO (eV)	LUMO (eV)	Energy (eV)
G1-Au6-Octahedron	-6.18	-4.07	2.10
G1-Au7-Pentagonal Decahedron	-5.47	-3.93	1.54
G1-Au13-cubotahedron	-5.65	-4.44	1.19
G1-Au13-Icosahedron	-5.06	-3.93	1.12
G1-Au14-Cube	-5.72	-3.43	2.28
G1-Au18-Marksüf Decahedron	-5.85	-3.82	2.03
G2-Au19-Octahedron	-5.18	-4.21	0.96

## 5.Optimized structure of the Au-S distances

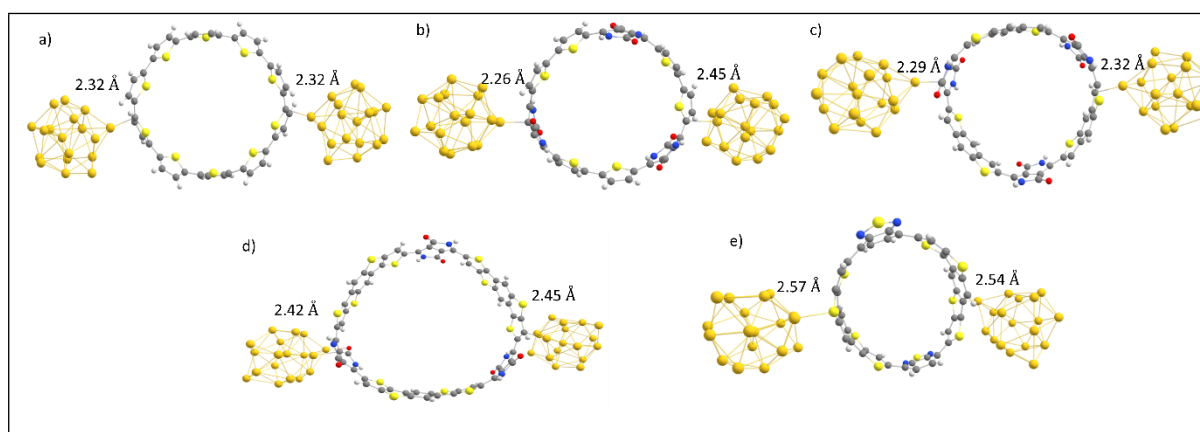


Figure S2: Geometry-optimized molecular junctions of a) [PT]<sub>10</sub>, b) [TT-DPP]<sub>3</sub>, c) [BDT-DPP]<sub>3</sub>, d) [DTBDT-DPP]<sub>3</sub>, and e) [DTBDT-BT]<sub>3</sub> anchored to Au<sub>18</sub> electrode clusters via Au-S bonds, calculated at the PBE0/GENECP level of theory.

Figure S2 shows the optimized geometry of the molecular junctions for all five macrocyclic systems anchored to Au<sub>18</sub> Marks decahedron electrode clusters, with Au-S bonds, calculated at the PBE0/GENECP level of theory. The Au-S bond distances vary systematically across the series, reflecting the differences in electronic character and metal-molecule-metal coupling strength at each interface. For [PT]<sub>10</sub>, both Au-S contacts are equivalent at 2.32 Å, consistent with the symmetric, homogeneous thiophene-based anchor environment. In [TT-DPP]<sub>3</sub>, the two Au-S distances are 2.26 Å and 2.45 Å, which indicates the asymmetric binding geometry arising from the D-A character of the macrocycle and the unequal electronic environment at the two sulphur anchor sites. Similarly, [BDT-DPP]<sub>3</sub> exhibits Au-S distances of 2.29 Å and

2.32 Å, reflecting a more symmetric contact geometry consistent with the near-equivalent HOMO density at both anchor sulphur atoms. For [DTBDT-DPP]<sub>3</sub>, the Au-S distances are 2.42 Å and 2.45 Å, the longest among the DPP-based systems, which correlates with the stronger orbital hybridization and greater Au cluster distortion observed for this junction. Finally, [DTBDT-BT]<sub>3</sub> shows the largest Au-S distances in the series, at 2.57 Å and 2.54 Å, consistent with a weaker, more elongated Au-S contact, which is consistent with the higher hole and electron injection barriers observed for this system.

**Table S2.** Cartesian coordinates of the linear and macrocyclic molecules [PT]<sub>10</sub>, [TT-DPP]<sub>3</sub>, [BDT-DPP]<sub>3</sub>, [DTBDT-DPP]<sub>3</sub>, and [DTBDT-BT]<sub>3</sub>.

PT (Polythiophene)				PT (Polythiophene)			
Linear				Macrocycle			
	X	Y	Z		X	Y	Z
C	18.576768	0.141065	1.504887	C	4.827413	4.081759	0.146556
C	18.124468	1.382664	1.158726	C	4.67015	4.77264	1.32809
C	16.752139	1.385391	0.801803	C	3.553176	5.653571	1.328188
C	16.167148	0.141803	0.880899	C	2.844524	5.645565	0.146728
S	17.327877	-1.038136	1.414374	S	3.58086	4.540318	-0.998696
H	18.753644	2.265057	1.150428	H	5.322561	4.623309	2.18187
H	16.212853	2.267672	0.474886	H	3.256017	6.253168	2.182038
C	14.803745	-0.239063	0.593819	C	1.506208	6.139715	-0.146237
C	14.290783	-1.488718	0.326774	C	0.972874	6.606272	-1.327742
S	13.539431	0.954025	0.560718	S	0.2282	5.777906	0.999012
C	12.902351	-1.48488	0.075229	C	-0.448565	6.662398	-1.327826
H	14.9085	-2.379004	0.284664	H	1.588445	6.868916	-2.18154
C	12.335125	-0.231091	0.145796	C	-1.017158	6.239332	-0.146386
H	12.334488	-2.372332	-0.181775	H	-1.041413	6.972803	-2.181678
C	10.44231	1.411818	-0.29217	C	-3.096142	5.91634	1.327945
C	10.963547	0.156247	-0.064585	C	-2.39032	5.85239	0.146504
C	9.043562	1.4164	-0.469535	C	-4.279119	5.12626	1.327901
C	8.473827	0.164332	-0.380362	C	-4.490355	4.449828	0.14642
C	7.091412	-0.213758	-0.519924	C	-5.373861	3.329716	-0.146629
C	6.550812	-1.466485	-0.717804	C	-5.982282	2.966612	-1.328173
S	5.830479	0.982399	-0.436865	S	-5.424963	2.00257	0.998741
C	5.14514	-1.462062	-0.823977	C	-6.475013	1.632115	-1.328205
H	7.15886	-2.359424	-0.812286	H	-6.04173	3.633163	-2.182021
C	4.588755	-0.205913	-0.709032	C	-6.248542	0.960697	-0.146683
H	4.552731	-2.351339	-1.009117	H	-6.953345	1.164159	-2.182076
C	3.203634	0.180873	-0.778886	C	-6.304934	-0.464816	0.146301

C	2.661689	1.437118	-0.949241
S	1.940861	-1.007344	-0.632762
C	1.252528	1.441643	-0.984668
H	3.269823	2.326283	-1.073997
C	0.69465	0.188943	-0.841982
H	0.657183	2.334705	-1.139675
C	-0.69465	-0.188947	-0.841979
C	-1.252528	-1.441649	-0.984652
S	-1.940861	1.007342	-0.63277
C	-2.661688	-1.437124	-0.949224
H	-0.657183	-2.334712	-1.139651
C	-3.203634	-0.180877	-0.77888
H	-3.269822	-2.326291	-1.07397
C	-4.588754	0.205909	-0.709028
C	-5.145139	1.462058	-0.823981
C	-6.550811	1.466481	-0.717807
C	-7.091411	0.213756	-0.51992
H	-7.158859	2.35942	-0.812293
C	-8.473826	-0.164333	-0.380355
C	-9.043561	-1.416403	-0.469515
S	-9.692252	1.03126	-0.042603
C	-10.442309	-1.41182	-0.292151
H	-8.46729	-2.309058	-0.686633
C	-10.963547	-0.156247	-0.064581
H	-11.060608	-2.300266	-0.357986
C	-12.335125	0.231092	0.145795
C	-12.902353	1.48488	0.075213
S	-13.539431	-0.954021	0.560726
C	-14.290786	1.48872	0.326754
H	-12.334491	2.372331	-0.1818
C	-14.803747	0.239067	0.593811
H	-14.908504	2.379004	0.28463
C	-16.752152	-1.385379	0.801758
C	-16.16715	-0.141798	0.88089
C	-18.124478	-1.382652	1.158693
C	-18.576764	-0.141061	1.504899
S	-17.327867	1.038134	1.414408
S	-5.830478	-0.982401	-0.436855
H	-16.212875	-2.267653	0.474805
H	-18.753661	-2.26504	1.15037
H	-4.552731	2.351334	-1.009125
S	9.692251	-1.031259	-0.042594
H	8.467292	2.309053	-0.686666
H	11.06061	2.300262	-0.358015
H	-19.571979	0.150716	1.810888

C	-6.583836	-1.116252	1.327793
S	-5.565817	-1.568413	-0.998929
C	-6.197891	-2.485453	1.327866
H	-7.023869	-0.611997	2.181595
C	-5.619842	-2.895456	0.146414
H	-6.30988	-3.145221	2.181707
C	-4.827455	-4.081811	-0.146472
C	-4.670118	-4.772851	-1.327903
S	-3.580848	-4.540075	0.998841
C	-3.55314	-5.653778	-1.32782
H	-5.322499	-4.623659	-2.18173
C	-2.844535	-5.645593	-0.146336
H	-3.255945	-6.253505	-2.181567
C	-1.506214	-6.139676	0.146732
C	-0.972826	-6.605873	1.328354
C	0.448616	-6.66199	1.328391
C	1.017149	-6.239278	0.146795
H	1.041506	-6.972114	2.182315
C	2.390289	-5.852395	-0.146289
C	3.095968	-5.916467	-1.327809
S	3.211635	-4.808466	0.998872
C	4.278958	-5.126405	-1.327981
H	2.752319	-6.490853	-2.181545
C	4.490341	-4.449858	-0.146591
H	4.941037	-5.029173	-2.181842
C	5.373907	-3.329743	0.146251
C	5.982672	-2.966701	1.327637
S	5.424605	-2.002505	-0.999034
C	6.475392	-1.632201	1.327603
H	6.042391	-3.633307	2.181423
C	6.248573	-0.960715	0.146187
H	6.953987	-1.164298	2.181356
C	6.58363	1.116343	-1.3282
C	6.304897	0.464815	-0.146717
C	6.197683	2.485543	-1.328107
C	5.619775	2.895437	-0.146549
S	5.566064	1.568347	0.998757
S	-0.228264	-5.778273	-0.998709
H	7.023542	0.612157	-2.182106
H	6.309541	3.145379	-2.181913
H	-1.588356	-6.868241	2.182266
S	-3.211516	4.80856	-0.998856
H	-4.941293	5.02893	2.181677
H	-2.752607	6.490655	2.181776

H	19.571987	-0.150714	1.810857
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TT-DPP			
Linear			
	X	Y	Z
C	-5.570087	0.144609	0.000019
C	-4.951485	1.385131	0.000224
S	-4.383369	-1.125181	0.000054
C	-3.552032	1.321439	0.000305
H	-5.508454	2.315675	0.000272
C	-3.074197	0.019475	0.000187
H	-2.880537	2.176394	0.000423
C	-1.706394	-0.374935	0.00022
C	-0.570712	0.419567	0.000251
N	-1.271621	-1.688075	0.000205
C	-0.137653	1.80503	0.00022
C	0.570712	-0.419566	0.000257
C	0.137653	-1.80503	0.000242
H	-1.862032	-2.504976	0.000228
N	1.271621	1.688075	0.000185
C	1.706394	0.374935	0.000217
H	1.862032	2.504976	0.000198
C	3.074197	-0.019475	0.000191
C	3.552032	-1.321439	0.000328
S	4.383369	1.125181	-

TT-DPP			
Macrocycle			
	X	Y	Z
C	1.801307	-5.669981	-0.097206
C	2.552358	-5.707556	-1.259343
S	2.674177	-4.836347	1.173632
C	3.799575	-5.052753	-1.157336
H	2.185697	-6.163055	-2.172986
C	4.021226	-4.499997	0.095563
H	4.488153	-4.906525	-1.981154
C	4.988745	-3.50301	0.452555
C	-5.64601	-2.616756	-0.388487
N	5.136311	-3.021128	1.751743
C	5.584172	-2.229968	-1.795909
C	6.044806	-1.478774	0.388144
C	5.755306	-1.742435	1.795588
H	4.861849	-3.505539	2.595319
N	-5.89874	-0.844612	-1.752036
C	6.084256	-0.37606	-0.45285
H	5.986526	-0.294788	-2.595593
C	5.950644	1.006723	-0.095749
C	6.122118	1.57666	1.15732
S	-	2.11055	-1.173859

			0.000063
C	4.951485	-1.385131	0.000249
H	2.880537	-2.176394	0.000456
C	5.570087	-0.144609	0.000027
H	5.508454	-2.315675	0.000312
C	6.971665	0.160556	-
C	7.590261	1.400706	0.000652
S	8.158594	-1.109213	0.000467
C	8.990141	1.336724	-0.00064
H	7.03359	2.331468	-
C	9.467309	0.035122	-0.00007
H	9.661796	2.191502	-
C	10.836342	-0.36039	0.000075
C	11.970583	0.43288	-0.00029
N	11.269845	-1.674209	0.000649
C	12.405189	1.817354	-0.00088
C	13.113602	-0.40807	0.000057
C	12.679854	-1.792932	0.000644
H	10.678742	-2.490562	0.000981
N	13.814946	1.698115	-
C	14.24714	0.385262	0.000838
H	14.407782	2.513301	-0.00029
H	14.407782	2.513301	-
C	15.6219	-0.006228	0.001259
C	16.102909	-1.302622	-
S	16.928508	1.141463	0.000105
C	17.514291	-1.356243	0.000258
H	15.435853	-2.160868	-
C	18.096333	-0.115781	0.000318
H	18.085003	-2.277297	0.000338
C	-	0.115781	0.000464
C	18.096333	0.115781	0.000051
C	-	1.356243	0.000601
C	-	1.356243	0.000057
C	-	1.356243	0.000346

	5.108536		
C	-	2.86673	1.259407
H	6.568451	1.032358	1.981166
C	4.946546	3.306432	0.097178
H	5.553996	3.451234	2.173199
C	4.010272	4.395161	-0.096587
C	3.667134	5.064272	-1.258752
S	2.851713	4.734022	1.174207
C	2.476254	5.816662	-1.156838
H	4.244941	4.974554	-2.172403
C	1.886712	5.732192	0.096071
H	2.005235	6.339723	-1.980702
C	0.539424	6.071219	0.452911
C	0.556624	6.197431	-0.388274
N	-0.04814	5.957831	1.751987
C	0.860515	5.950787	-1.795777
C	1.741634	5.973597	0.388163
C	1.368729	5.854402	1.795628
H	-0.60466	5.962621	2.595713
N	2.217472	5.530223	-1.752126
C	2.716264	5.456633	-0.453054
H	2.73739	5.331563	-2.595827
C	3.847202	4.649728	-0.09622
C	4.42721	4.513694	1.156585
S	4.381542	3.368181	-1.174193
C	5.261839	3.378927	1.25855
H	4.17951	5.17264	1.980375
C	5.337104	2.630512	0.096538
H	5.76736	3.084894	2.172148
C	5.811843	1.275278	-0.097055
C	6.219736	0.643371	-1.259122

	17.514291		
S	-		
	16.928508	-1.141463	-0.00032
C	-		
	16.102909	1.302622	0.000263
H	-		
	18.085003	2.277297	0.000612
C	-		
	-15.6219	0.006228	0.000103
H	-		
	15.435853	2.160868	0.000471
C	-		
	-14.24714	-0.385262	0.000289
C	-		
	13.113602	0.40807	0.000063
N	-		
	13.814946	-1.698115	0.000837
C	-		
	12.679854	1.792932	0.000663
C	-		
	11.970583	-0.43288	0.000294
C	-		
	12.405189	-1.817354	0.000896
H	-		
	14.407782	-2.513301	-0.00125
N	-		
	11.269845	1.674209	0.000653
C	-		
	10.836342	0.36039	0.000076
H	-		
	10.678742	2.490562	0.000976
C	-		
	-9.467309	-0.035122	0.000072
C	-		
	-8.990141	-1.336724	0.000649
S	-		
	-8.158594	1.109213	0.000471
C	-		
	-7.590261	-1.400706	0.000665
H	-		
	-9.661796	-2.191502	-0.00105
C	-		
	-6.971665	-0.160556	0.000116
H	-		
	-7.03359	-2.331468	0.001112
O	-		
	11.809077	-2.882329	0.001374
O	-		
	13.275612	2.857644	0.001087
O	-		
	-0.735943	2.86863	0.000228

S	5.526008	0.102733	1.173911
C	6.275799	-0.764154	-1.156979
H	6.430947	1.188478	-2.172859
C	5.90788	-1.232234	0.095994
H	6.493082	-1.433773	-1.980748
C	5.527984	-2.568504	0.453129
C	5.08937	-3.581004	-0.38785
N	5.184181	-2.937047	1.752277
C	4.723987	-3.721096	-1.795364
C	4.302922	-4.495157	0.388701
C	4.385988	-4.112229	1.796086
H	5.46642	-2.457128	2.595853
N	3.681377	-4.686076	-1.751661
C	3.367944	-5.080822	-0.452505
H	3.249437	-5.037201	-2.595311
C	2.103446	-5.65638	-0.095711
C	1.695346	-6.090229	1.157154
S	0.726611	-5.478432	-1.173952
C	0.295236	-6.245212	1.258986
H	2.389735	-6.20517	1.981053
C	-0.39028	-5.93642	0.096761
H	-0.21237	-6.53567	2.172569
O	3.933104	-4.602631	2.820018
O	5.141587	-3.200212	-2.819247
O	-		
	5.341301	-2.851731	-2.819849

O	0.735943	-2.86863	0.00026
O	11.809077	2.882329	0.001345
O	13.275612	-2.857644	0.001068
H	19.149254	-0.131275	0.000054
H	19.149254	0.131275	0.000047

O	5.954329	-1.105313	2.819558
O	0.200536	6.051648	-2.819646
O	2.020074	5.707867	2.819505

BDT-DPP			
Linear			
	X	Y	Z
C	-5.70351	-5.96846	-0.48773
C	-6.51072	-5.23894	0.378317
N	-6.01805	-5.54537	-1.77727
C	-6.58184	-4.88922	1.791501
C	-7.20089	-4.24107	-0.37839
C	-6.8989	-4.43111	-1.7916
H	-5.61646	-5.90115	-2.63344
N	-7.31381	-3.67197	1.777179
C	-7.59853	-3.2283	0.487635
H	-7.50534	-3.17086	2.633381
C	-7.95008	0.084912	-1.05996
C	-7.8282	0.629779	0.215448
S	-7.71574	1.29249	-2.32056
C	-7.47597	2.015537	0.244656
C	-7.30111	2.503251	-1.09
C	-6.56294	4.061481	1.09017
C	-6.29651	4.505835	-0.2445
S	-5.88873	5.149256	2.320734
C	-5.44751	5.656313	-0.21529
C	-5.10308	6.095744	1.060117
O	-7.24817	-3.84626	-2.80901
O	-6.15793	-5.42242	2.808928
C	-7.15054	2.830163	1.339794
C	-6.72072	3.737991	-1.33963
H	-7.28293	2.46503	2.353877
H	-6.52217	4.071784	-2.35371
S	-4.48783	6.445312	-1.43076

BDT-DPP			
Macrocycle			
	X	Y	Z
C	-2.36707	-5.89549	-0.71412
C	-3.27088	-5.56428	0.290634
C	-3.28719	-5.3652	1.734915
C	-4.32675	-4.78997	-0.29004
C	-4.13251	-4.74647	-1.73442
H	-2.51417	-5.56893	-2.82661
C	-4.91366	-4.02679	0.714556
H	-4.5571	-4.0678	2.826881
C	-5.6158	-2.77682	0.60116
C	-5.85071	-2.10035	-0.57589
S	-5.82202	-1.72724	2.024748
C	-6.02365	-0.69561	-0.39256
H	-5.74152	-2.5764	-1.54566
C	-5.98817	-0.31391	0.986722
C	-5.77724	1.606485	-0.98653
C	-5.72896	1.9868	0.39275
S	-5.30826	2.949983	-2.0246
C	-5.25513	3.320489	0.576028
C	-4.87893	3.929737	-0.60106
H	-5.04505	3.761474	1.545763
C	-3.92219	4.997454	-0.71452
C	-3.18354	5.614896	0.29008
C	-3.00326	5.530064	1.734429
C	-1.98487	6.141664	-0.29064
C	-2.04409	5.951069	-1.73494
H	-3.56564	4.960712	-2.82695
C	-1.03065	6.268726	0.714051

C	-4.06326	7.047707	1.095006
H	-3.59453	7.447599	1.988172
C	-3.57642	7.314046	-0.17842
C	-8.02779	-1.32273	-1.09485
S	-7.83056	-0.6126	1.430892
H	-8.04022	-1.93874	-1.98802
C	-7.92508	-1.86813	0.178535
C	-4.54612	-6.75405	-0.17862
S	-3.33796	-7.10861	-1.43096
C	-4.07211	-7.04272	1.094769
C	-2.1749	-7.54546	-0.21552
C	-2.72773	-7.4671	1.059883
H	-4.65283	-6.83691	1.987954
C	-0.75405	-7.70548	-0.24468
S	-1.51525	-7.67439	2.320514
C	-0.23605	-7.71418	1.090001
C	0.123043	-7.68877	-1.33978
C	1.124096	-7.6073	1.339666
C	1.482543	-7.57396	-1.09012
H	-0.26529	-7.68357	-2.35387
C	1.992315	-7.48163	0.244564
H	1.50646	-7.53944	2.353769
S	2.73837	-7.32731	-2.32063
C	3.368505	-7.09368	0.215427
C	3.901332	-6.92667	-1.05996
S	4.445489	-6.47438	1.43093
C	5.159234	-6.29014	-1.09478
C	5.580266	-5.92872	0.178659
H	5.698965	-5.99286	-1.98791
C	6.595102	-4.96605	0.487822
C	7.273564	-4.11542	-0.37818
N	6.837049	-4.4977	1.777383
C	7.792596	-3.01881	0.378535
C	7.287215	-3.75886	-1.79139
C	7.52507	-3.25511	1.79172
H	6.499091	-4.91431	2.633592
C	8.020972	-1.95502	-0.4875
N	7.812327	-2.43914	-1.7771
O	6.95518	-4.35377	-2.80876
O	7.774577	-2.62121	2.809108
H	7.920078	-1.91359	-2.6333
C	8.12273	-0.55995	-0.17846
S	7.82586	0.663559	-1.43088
C	8.135852	-0.00504	1.094902
C	7.622702	1.889294	-0.21549

H	-1.24495	5.981746	2.82654
C	0.402932	6.251621	0.600794
C	1.106354	6.116752	-0.57618
S	1.414843	5.905527	2.024517
C	2.409396	5.564281	-0.39266
H	0.639598	6.260119	-1.54601
C	2.722056	5.342793	0.986677
C	4.280078	4.199964	-0.9863
C	4.585102	3.968063	0.393033
S	5.209461	3.122191	-2.02419
C	5.503192	2.890901	0.576497
C	5.842954	2.260461	-0.60052
H	5.779947	2.488548	1.546297
C	6.289213	0.898021	-0.71394
C	6.454454	-0.05055	0.290562
C	6.290614	-0.1645	1.734872
C	6.311439	-1.35193	-0.29038
C	6.176083	-1.20511	-1.73467
H	6.079274	0.607893	-2.82641
C	5.944324	-2.24203	0.714138
H	5.802496	-1.91327	2.826617
C	5.212869	-3.47506	0.600614
C	4.744318	-4.01649	-0.57648
S	4.407297	-4.1788	2.02418
C	3.614253	-4.86865	-0.39316
H	5.101769	-3.68361	-1.54623
C	3.266206	-5.02909	0.98616
C	1.497205	-5.80609	-0.98692
C	1.143994	-5.95477	0.392395
S	0.098934	-6.07139	-2.02472
C	-0.24788	-6.21137	0.575925
C	-0.96389	-6.18997	-0.60098
H	-0.73455	-6.25026	1.545781
O	6.007465	-2.00509	-2.64604
O	6.298943	0.653111	2.64616
O	-2.58342	-5.78162	2.646122
O	-4.74126	-4.20047	-2.64562
O	-3.71583	5.128828	2.645604
O	-1.26663	6.204647	-2.64611
C	-5.97669	0.296155	-1.39015
C	-5.8984	1.008471	1.390345
H	-5.82124	1.281642	2.438078
H	-5.96075	0.012748	-2.43789
C	3.822374	4.603951	1.390495
C	3.245009	5.027749	-1.39011

C	7.831289	1.371439	1.059937
H	8.247883	-0.61083	1.98811
C	7.050692	3.199723	-0.24473
S	7.404528	2.525185	2.320496
C	6.799278	3.652783	1.089912
C	6.597611	3.95085	-1.33988
C	6.026676	4.777296	1.339519
C	5.818411	5.070801	-1.09028
H	6.787263	3.611882	-2.35396
C	5.483638	5.466229	0.244392
H	5.776776	5.07459	2.353609
S	4.976801	6.034938	-2.32082
C	4.459514	6.464022	0.215228
C	4.048352	6.84179	-1.06017
S	3.384678	7.087042	1.430733
C	2.868026	7.612701	-1.09501
C	2.34452	7.796633	0.178424
H	2.340618	7.931293	-1.98815
C	1.00337	8.194061	0.487615
C	-0.07259	8.356109	-0.37834
N	0.476866	8.16947	1.777196
C	-1.28181	8.257532	0.378454
C	-0.38828	8.189533	-1.79151
C	-0.94327	8.144252	1.791623
H	1.006667	8.084469	2.633328
C	-2.31731	7.92338	-0.48753
N	-1.79374	7.984395	-1.77711
O	0.292722	8.199892	-2.80901
O	-1.61693	8.04378	2.809104
H	-2.3028	7.814988	-2.63328

H	2.99176	5.155594	-2.43789
H	4.020257	4.400631	2.438266
C	2.731635	-5.32357	-1.39068
C	2.076173	-5.6126	1.389882
H	2.968877	-5.16778	-2.43843
H	1.801237	-5.68262	2.437655
N	-4.38015	-4.47729	1.92001
N	-2.95743	-5.52246	-1.91955
N	-3.3038	5.321684	-1.92001
N	-1.68782	6.032671	1.91952
N	6.260996	0.200527	-1.91953
N	6.068295	-1.55506	1.919727

DTBDT-DPP			
Linear			
	X	Y	Z
C	-7.45583	-0.45463	0.000196
C	-6.36583	0.398523	0.00019
N	-6.95312	-1.74305	0.000254
C	-6.00707	1.804367	0.000033
C	-5.18051	-0.37911	0.000238
C	-5.53909	-1.78477	0.000238
H	-7.49904	-2.59041	0.000234

DTBDT-DPP			
Macrocyclic			
	X	Y	Z
C	-5.70351	-5.96846	-0.48773
C	-6.51072	-5.23894	0.378317
N	-6.01805	-5.54537	-1.77727
C	-6.58184	-4.88922	1.791501
C	-7.20089	-4.24107	-0.37839
C	-6.8989	-4.43111	-1.7916
H	-5.61646	-5.90115	-2.63344

N	-4.59324	1.762728	0.000025
C	-4.09037	0.474308	0.000139
H	-4.04723	2.610029	-0.0001
C	-0.76502	-1.08926	0.000064
C	-0.22365	0.190433	0.000016
S	0.466713	-2.32407	0.00003
C	1.201554	0.232333	-1.7E-05
C	1.724	-1.09577	-1.9E-05
C	3.433021	1.082778	-5.9E-05
C	3.955645	-0.2455	-6.8E-05
S	4.69035	2.310831	-7.1E-05
C	5.380849	-0.20353	-9.4E-05
C	5.922054	1.07591	-7.5E-05
O	-4.88443	-2.8148	0.000251
O	-6.66195	2.834195	-9.4E-05
C	2.071165	1.327959	-3.8E-05
C	3.086009	-1.34102	-5.1E-05
H	1.682235	2.341581	-4.4E-05
H	3.474952	-2.35461	-6.6E-05
S	6.618838	-1.4031	-0.00011
C	7.326942	1.114583	-0.00007
H	7.956539	2.001029	-2.8E-05
C	7.858504	-0.16435	-7.2E-05
C	-2.16962	-1.12727	0.000127
S	-1.46082	1.390445	0.000058
H	-2.79947	-2.01359	0.000199
C	-2.70097	0.152064	0.000118
C	-8.84547	-0.13173	0.000133
S	-10.0857	-1.36984	0.000197
C	-9.37629	1.147619	-2E-06
C	-11.3227	-0.16956	0.000049
C	-10.7811	1.109783	-4.4E-05
H	-8.74627	2.033799	-3.1E-05
C	-12.7481	-0.21091	0.000031
S	-12.0122	2.345236	-0.0002
C	-13.2699	1.117615	-0.00011
C	-13.6179	-1.30605	0.000124
C	-14.6317	1.36331	-0.00016
C	-14.98	-1.06023	0.000081
H	-13.2294	-2.31982	0.000218
C	-15.5014	0.268083	-5.6E-05
H	-15.0204	2.37705	-0.00027
S	-16.2375	-2.28791	0.000178
C	-16.9273	0.227008	-7.4E-05
C	-17.4685	-1.05242	0.000051

N	-7.31381	-3.67197	1.777179
C	-7.59853	-3.2283	0.487635
H	-7.50534	-3.17086	2.633381
C	-7.95008	0.084912	-1.05996
C	-7.8282	0.629779	0.215448
S	-7.71574	1.29249	-2.32056
C	-7.47597	2.015537	0.244656
C	-7.30111	2.503251	-1.09
C	-6.56294	4.061481	1.09017
C	-6.29651	4.505835	-0.2445
S	-5.88873	5.149256	2.320734
C	-5.44751	5.656313	-0.21529
C	-5.10308	6.095744	1.060117
O	-7.24817	-3.84626	-2.80901
O	-6.15793	-5.42242	2.808928
C	-7.15054	2.830163	1.339794
C	-6.72072	3.737991	-1.33963
H	-7.28293	2.46503	2.353877
H	-6.52217	4.071784	-2.35371
S	-4.48783	6.445312	-1.43076
C	-4.06326	7.047707	1.095006
H	-3.59453	7.447599	1.988172
C	-3.57642	7.314046	-0.17842
C	-8.02779	-1.32273	-1.09485
S	-7.83056	-0.6126	1.430892
H	-8.04022	-1.93874	-1.98802
C	-7.92508	-1.86813	0.178535
C	-4.54612	-6.75405	-0.17862
S	-3.33796	-7.10861	-1.43096
C	-4.07211	-7.04272	1.094769
C	-2.1749	-7.54546	-0.21552
C	-2.72773	-7.4671	1.059883
H	-4.65283	-6.83691	1.987954
C	-0.75405	-7.70548	-0.24468
S	-1.51525	-7.67439	2.320514
C	-0.23605	-7.71418	1.090001
C	0.123043	-7.68877	-1.33978
C	1.124096	-7.6073	1.339666
C	1.482543	-7.57396	-1.09012
H	-0.26529	-7.68357	-2.35387
C	1.992315	-7.48163	0.244564
H	1.50646	-7.53944	2.353769
S	2.73837	-7.32731	-2.32063
C	3.368505	-7.09368	0.215427
C	3.901332	-6.92667	-1.05996

S	-18.1633	1.427348	-0.00025
C	-18.8738	-1.08947	0.000053
C	-19.4029	0.189578	-4.2E-05
H	-19.5056	-1.97492	0.000128
C	-20.7953	0.510862	0.000002
C	-21.8771	-0.34738	0.000023
N	-21.295	1.798575	-3E-06
C	-23.0756	0.429244	-2.7E-05
C	-22.2256	-1.75324	0.000002
C	-22.7161	1.845391	-5.8E-05
H	-20.7478	2.645022	0.000042
C	-24.1341	-0.43156	-0.00008
N	-23.6425	-1.71459	-7.4E-05
O	-21.5661	-2.78282	0.000003
O	-23.3606	2.87142	-0.00016
H	-24.1951	-2.55659	-0.00012
C	24.56041	-0.18517	0.000074
S	23.34329	-1.4163	-7.9E-05
C	24.04686	1.080675	0.000188
C	22.0936	-0.22455	0.000018
C	22.62828	1.050523	0.000152
H	24.65453	1.976936	0.000291
C	20.66387	-0.26775	-7E-06
S	21.3969	2.285685	0.000241
C	20.1383	1.058108	0.000109
C	19.79543	-1.3622	-0.00012
C	18.77603	1.30327	0.00011
C	18.43182	-1.11864	-0.00011
H	20.18531	-2.37543	-0.00022
C	17.90751	0.207303	-2E-06
H	18.38656	2.31677	0.000192
S	17.17632	-2.34928	-0.00024
C	16.48128	0.163239	-3.1E-05
C	15.94183	-1.11685	-0.00014
S	15.24279	1.36154	0.000059
C	14.53707	-1.15651	-0.00014
C	14.00347	0.12179	-2.3E-05
H	13.90843	-2.0437	-0.00018
C	12.61402	0.442093	0.000015
C	11.52384	-0.41172	-4.5E-05
N	12.11052	1.730391	0.000113
C	10.33818	0.365883	0.000008
C	11.16588	-1.817	-0.00018
C	10.6969	1.771755	0.000071
H	12.65668	2.577565	0.000118

S	4.445489	-6.47438	1.43093
C	5.159234	-6.29014	-1.09478
C	5.580266	-5.92872	0.178659
H	5.698965	-5.99286	-1.98791
C	6.595102	-4.96605	0.487822
C	7.273564	-4.11542	-0.37818
N	6.837049	-4.4977	1.777383
C	7.792596	-3.01881	0.378535
C	7.287215	-3.75886	-1.79139
C	7.52507	-3.25511	1.79172
H	6.499091	-4.91431	2.633592
C	8.020972	-1.95502	-0.4875
N	7.812327	-2.43914	-1.7771
O	6.95518	-4.35377	-2.80876
O	7.774577	-2.62121	2.809108
H	7.920078	-1.91359	-2.6333
C	8.12273	-0.55995	-0.17846
S	7.82586	0.663559	-1.43088
C	8.135852	-0.00504	1.094902
C	7.622702	1.889294	-0.21549
C	7.831289	1.371439	1.059937
H	8.247883	-0.61083	1.98811
C	7.050692	3.199723	-0.24473
S	7.404528	2.525185	2.320496
C	6.799278	3.652783	1.089912
C	6.597611	3.95085	-1.33988
C	6.026676	4.777296	1.339519
C	5.818411	5.070801	-1.09028
H	6.787263	3.611882	-2.35396
C	5.483638	5.466229	0.244392
H	5.776776	5.07459	2.353609
S	4.976801	6.034938	-2.32082
C	4.459514	6.464022	0.215228
C	4.048352	6.84179	-1.06017
S	3.384678	7.087042	1.430733
C	2.868026	7.612701	-1.09501
C	2.34452	7.796633	0.178424
H	2.340618	7.931293	-1.98815
C	1.00337	8.194061	0.487615
C	-0.07259	8.356109	-0.37834
N	0.476866	8.16947	1.777196
C	-1.28181	8.257532	0.378454
C	-0.38828	8.189533	-1.79151
C	-0.94327	8.144252	1.791623
H	1.006667	8.084469	2.633328

C	9.248427	-0.48711	-5.5E-05
N	9.751569	-1.77546	-9.1E-05
O	11.8203	-2.84742	-0.00042
O	10.04188	2.801647	0.000142
H	9.205937	-2.62296	-0.00016
H	25.60292	-0.4735	0.00007
H	-25.1984	-0.23862	-0.00016

C	-2.31731	7.92338	-0.48753
N	-1.79374	7.984395	-1.77711
O	0.292722	8.199892	-2.80901
O	-1.61693	8.04378	2.809104
H	-2.3028	7.814988	-2.63328

DTBDT-BT			
Linear			
C	-5.34966	-1.78932	0.000171
C	-5.22117	-0.41163	0.000016
S	-3.80309	-2.59709	0.000339
C	-3.87354	0.059397	0.000022
C	-2.97303	-1.04712	0.000197
C	-2.00138	1.542769	-7.8E-05
C	-1.10089	0.436287	0.000103
S	-1.17141	3.09282	-0.00024
C	0.246746	0.907364	0.000097
C	0.375174	2.285127	-7.2E-05
C	-3.37432	1.365578	-0.00012
C	-1.60011	-0.86992	0.000236
H	-4.05137	2.214285	-0.00026
H	-0.92306	-1.71863	0.000368
S	1.792107	0.144001	0.000296
C	1.708043	2.745126	-5.4E-05
H	2.020162	3.780228	-0.00017
C	2.611699	1.701392	0.000131
C	-6.68261	-2.24937	0.000181
S	-6.76659	0.351741	-0.00014
H	-6.99483	-3.28444	0.000265
C	-7.58618	-1.20565	0.000058
C	-13.4355	-1.27685	-0.00005
S	-14.2929	0.260173	-0.00015
C	-14.3137	-2.34189	-9E-06
C	-15.8192	-0.54036	-8.6E-05
C	-15.6576	-1.91425	-2.4E-05
H	-13.9769	-3.36923	0.000008
C	-17.1786	-0.10176	-6.4E-05

DTBDT-BT			
Macrocycle			
C	1.453266	-7.59635	-1.40999
C	0.966125	-7.65464	-0.11306
S	0.161149	-7.56939	-2.60749
C	-0.46199	-7.61421	-0.00807
C	-1.04561	-7.4776	-1.30778
C	-2.60878	-7.19358	0.967009
C	-3.16459	-6.94285	-0.32783
S	-3.7482	-6.82507	2.278516
C	-4.45376	-6.33163	-0.19862
C	-4.88507	-6.16029	1.108068
C	-1.27237	-7.52744	1.133556
C	-2.38269	-7.14656	-1.47443
H	-0.83854	-7.63485	2.123255
H	-2.79807	-6.96342	-2.46091
S	-5.45711	-5.43597	-1.3051
C	-5.99959	-5.30159	1.251746
H	-6.43459	-5.00314	2.194969
C	-6.40681	-4.76242	0.042965
C	2.840142	-7.33637	-1.50635
S	2.246944	-7.41074	1.041679
H	3.381813	-7.19643	-2.431
C	3.425726	-7.14258	-0.26655
C	7.36543	-3.079	0.461962
S	7.184949	-2.08851	1.933043
C	7.862684	-2.32063	-0.58466
C	7.670123	-0.65546	1.072203
C	8.006747	-0.95646	-0.23898
H	8.015771	-2.72981	-1.57316
C	7.510209	0.741837	1.343566

S	-17.1846	-2.7587	0.000064
C	-18.0516	-1.22903	0.000018
C	-17.7096	1.191299	-0.00012
C	-19.4293	-1.08496	0.000046
C	-19.0871	1.334004	-9.1E-05
H	-17.054	2.056723	-0.00019
C	-19.9602	0.207373	-6E-06
H	-20.085	-1.95032	0.000108
S	-19.9555	2.863333	-0.00016
C	-21.3223	0.646408	0.000009
C	-21.4821	2.019388	-5.7E-05
S	-22.8539	-0.15133	0.000114
C	-22.8368	2.442238	-1.8E-05
C	-23.6822	1.369397	0.000073
H	-23.1714	3.472165	-5.9E-05
C	18.72654	-0.88252	-0.00061
S	17.87006	0.653703	0.000054
C	17.85062	-1.94754	-0.00099
C	16.34366	-0.14714	-0.00037
C	16.50557	-1.52064	-0.00088
H	18.18944	-2.97446	-0.0013
C	14.98443	0.290894	-0.0002
S	14.9794	-2.36629	-0.00122
C	14.11154	-0.83734	-0.00065
C	14.45344	1.584274	0.000291
C	12.7345	-0.6938	-0.00061
C	13.07647	1.727822	0.000333
H	15.10948	2.449325	0.000631
C	12.20348	0.599647	-0.00012
H	12.0785	-1.55889	-0.00096
S	12.20875	3.257107	0.000915
C	10.84453	1.037632	0.000029
C	10.68237	2.411753	0.000548
S	9.318425	0.236577	-0.0003
C	9.338569	2.83891	0.000695
C	8.460796	1.773346	0.00027
H	9.001222	3.866063	0.001038
C	-11.2212	-2.50968	-0.00013
C	-9.76962	-2.49207	-8.2E-05
C	-9.03536	-1.25651	0.000062
C	-9.82076	-0.11693	0.000164
C	-11.2282	-0.13393	0.000125
C	-11.9857	-1.29236	-2.4E-05
H	-9.33973	0.857176	0.000296
H	-11.7328	0.828116	0.000249

S	8.239503	0.491422	-1.216
C	7.70919	1.500014	0.146689
C	7.04425	1.377972	2.504175
C	7.348914	2.837735	0.064178
C	6.677016	2.712765	2.418628
H	6.89246	0.809734	3.417031
C	6.770058	3.441098	1.19041
H	7.424717	3.383894	-0.87134
S	5.857742	3.637348	3.696687
C	6.0502	4.67706	1.29142
C	5.469429	4.902927	2.531902
S	5.440295	5.78644	0.098605
C	4.512856	5.939474	2.539571
C	4.320814	6.497463	1.283614
H	3.911219	6.191711	3.403722
C	-0.91414	7.853021	-0.52204
S	-2.23389	7.630319	0.654821
C	-1.34267	7.557579	-1.80546
C	-3.29156	7.028136	-0.59017
C	-2.67053	7.07052	-1.82935
H	-0.68243	7.60186	-2.66005
C	-4.49744	6.256058	-0.5508
S	-3.59435	6.221791	-3.06694
C	-4.74771	5.671768	-1.83303
C	-5.28989	5.893996	0.54866
C	-5.68735	4.665131	-2.00302
C	-6.22464	4.882634	0.380189
H	-5.10809	6.335058	1.524186
C	-6.39447	4.219206	-0.87648
H	-5.81279	4.168744	-2.96067
S	-7.16338	4.122257	1.682339
C	-7.1799	3.033716	-0.70337
C	-7.62066	2.814785	0.593017
S	-7.40661	1.61312	-1.68377
C	-8.12198	1.513851	0.832168
C	-8.02606	0.699867	-0.28404
H	-8.44956	1.141912	1.792535
C	6.640959	-5.1215	-0.85532
C	5.629852	-6.15894	-1.04177
C	4.695291	-6.48668	0.008682
C	4.99872	-5.92284	1.242021
C	5.976527	-4.91932	1.422299
C	6.734501	-4.38806	0.38546
H	4.371432	-6.14902	2.099015
H	6.024529	-4.46005	2.40527

C	20.93154	-2.13069	0.000169
C	22.37907	-2.10754	0.000111
C	23.09151	-0.8818	-0.00084
C	22.354	0.269886	-0.00172
C	20.93499	0.256393	-0.0017
C	20.1808	-0.90205	-0.00073
H	22.85638	1.232401	-0.0025
H	20.42668	1.216706	-0.00257
N	-9.23691	-3.71391	-0.00022
N	-11.724	-3.74409	-0.00022
N	22.93073	-3.32385	0.001032
N	20.4329	-3.3679	0.001114
S	-10.4679	-4.77367	-0.00035
S	21.70264	-4.38625	0.001877
C	7.010932	1.788669	0.000284
C	6.253675	0.630093	0.000333
C	6.246498	3.005919	0.000221
C	4.846283	0.612788	0.000269
H	6.758411	-0.33191	0.000448
C	4.794952	2.988065	0.000172
C	4.060747	1.75237	0.000187
H	4.365389	-0.36136	0.000281
N	6.749133	4.240409	0.000188
N	4.262087	4.209812	0.000121
S	5.492772	5.269785	0.000145
H	-24.7638	1.381868	0.000114
H	24.17525	-0.88576	-0.00086

C	1.577282	7.973382	-0.97454
C	2.915528	7.630072	-0.50742
C	3.16972	7.28759	0.867236
C	2.111697	7.563336	1.727287
C	0.815512	7.899131	1.279935
C	0.459318	7.988994	-0.06232
H	2.229023	7.387105	2.791141
H	0.040256	7.95233	2.038656
N	5.661204	-6.70921	-2.25716
N	7.397503	-4.92816	-1.93748
N	3.82939	7.625984	-1.47858
N	1.529538	8.214302	-2.28697
S	6.87555	-5.97841	-3.08921
S	3.0553	8.02838	-2.87113
C	-8.06812	-0.75429	-0.32364
C	-7.61956	-1.49015	-1.41401
C	-8.34447	-1.54423	0.853483
C	-7.21597	-2.8416	-1.33314
H	-7.43173	-0.98368	-2.35616
C	-7.9268	-2.94129	0.937297
C	-7.22799	-3.57738	-0.1543
H	-6.74693	-3.26186	-2.2177
N	-8.94736	-1.11116	1.962494
N	-8.23005	-3.50993	2.105885
S	-8.98789	-2.37137	3.017104

**Table S3.** Cartesian coordinates of the molecular junctions for the molecules [PT]<sub>10</sub>, [TT-DPP]<sub>3</sub>, [BDT-DPP]<sub>3</sub>, [DTBDT-DPP]<sub>3</sub>, and [DTBDT-BT]<sub>3</sub>.

PT (Polythiophene)			
AU-MC			
	X	Y	Z
C	4.722123	5.810803	0.298472
C	4.476485	6.691319	1.325548
C	3.286214	7.439367	1.149227
C	2.614195	7.12725	-0.010252
S	3.473059	5.912029	-0.902302
H	5.127217	6.778691	2.188673
H	2.917575	8.170496	1.86025
C	1.253886	7.449894	-0.408204
C	0.709721	7.63136	-1.658679
S	0.00109	7.287039	0.780914
C	-0.707614	7.631824	-1.658593
H	1.315958	7.742737	-2.550997
C	-1.251745	7.450717	-0.408053
H	-1.313887	7.743593	-2.550838
C	-3.283946	7.441466	1.149585
C	-2.612206	7.128902	-0.009936
C	-4.474608	6.694081	1.326071
C	-4.720813	5.813607	0.299088
C	-5.647421	4.691613	0.241046
C	-6.423912	4.21126	-0.787496
S	-5.602285	3.556269	1.550593
C	-6.976338	2.930765	-0.524226
H	-6.578345	4.75868	-1.710488
C	-6.61862	2.43366	0.706652
H	-7.606665	2.382539	-1.217169
C	-6.705647	1.069628	1.244313
C	-6.875172	0.688438	2.592753
S	-5.744647	-0.153628	0.42369
C	-6.268106	-0.553762	2.914689
H	-7.300651	1.362923	3.329788
C	-5.610355	-1.128605	1.850646
H	-6.306311	-1.004442	3.899567
C	-4.700966	-2.260437	1.815782
C	-4.470631	-3.168698	0.80764
S	-3.452757	-2.349262	3.017639
C	-3.291794	-3.927971	1.001055
H	-5.125282	-3.270046	-0.051273

C	-2.612556	-3.595145	2.151258
H	-2.934626	-4.680951	0.30741
C	-1.253507	-3.916798	2.553171
C	-0.71008	-4.072551	3.807843
C	0.706636	-4.072937	3.807702
C	1.249897	-3.917469	2.552923
H	1.31313	-4.166946	4.701815
C	2.609052	-3.596591	2.150747
C	3.287902	-3.929885	1.000454
S	3.45013	-2.351149	3.016914
C	4.46715	-3.171304	0.806791
H	2.930183	-4.682701	0.306916
C	4.698194	-2.263136	1.814846
H	5.121587	-3.27308	-0.052232
C	5.608307	-1.131864	1.849533
C	6.266847	-0.557594	2.913381
S	5.742707	-0.156826	0.422623
C	6.874636	0.684263	2.591348
H	6.305139	-1.008406	3.898194
C	6.70482	1.065729	1.243003
H	7.300629	1.358482	3.328333
C	6.976723	2.927234	-0.52504
C	6.618337	2.429883	0.705537
C	6.424871	4.208026	-0.788127
C	5.648184	4.688349	0.240276
S	5.602108	3.552609	1.549438
S	-0.001884	-3.780535	1.360173
H	7.607111	2.378972	-1.2179
H	6.579866	4.755686	-1.710881
H	-1.316447	-4.166229	4.702077
S	-3.471805	5.914068	-0.901806
H	-5.125219	6.781888	2.189244
H	-2.914842	8.172444	1.86052
Au	-13.094527	-0.176528	-0.230083
Au	-11.716778	1.371881	-2.695353
Au	-13.602822	2.602215	-0.933906
Au	-14.413848	0.55579	-2.713607
Au	-12.308795	-1.402074	-2.770568
Au	-10.062052	-0.37671	-1.317648
Au	-10.961239	1.944597	-0.05609
Au	-12.993387	-2.021291	2.43569
Au	-14.396807	0.463299	2.298395
Au	-15.286254	-1.77467	0.812922
Au	-12.946807	-3.102563	-0.186259
Au	-10.623762	-1.907244	0.987766

Au	-11.539855	0.379453	2.287202
Au	-12.903134	2.774945	1.777589
Au	-15.743497	0.834626	-0.211895
Au	-14.902284	-2.0695	-1.923262
Au	-10.477899	-3.14478	-1.528685
Au	-8.92243	0.356427	1.186441
Au	13.094506	-0.172006	-0.227805
Au	11.717651	1.375817	-2.693255
Au	13.601316	2.606915	-0.929644
Au	10.959453	1.944794	-0.053126
Au	10.064566	-0.376184	-1.317905
Au	12.312807	-1.397429	-2.770835
Au	14.415817	0.562678	-2.709728
Au	12.991822	-2.02944	2.431328
Au	14.394884	0.456248	2.304677
Au	11.537807	0.371995	2.286563
Au	10.622185	-1.913122	0.983741
Au	12.947933	-3.099176	-0.195123
Au	15.285698	-1.774856	0.81101
Au	15.741737	0.838608	-0.204802
Au	12.902357	2.767947	1.782458
Au	8.921061	0.350825	1.185071
Au	10.479247	-3.143515	-1.53705
Au	14.907148	-2.063696	-1.926168

<b>TT-DPP</b>			
<b>AU-MC</b>			
	X	Y	Z
C	1.461461	-3.66873	4.06646
C	2.281098	-3.45572	5.157426
S	2.260604	-3.21542	2.598062
C	3.537258	-2.91403	4.820207
H	1.966875	-3.66561	6.173753
C	3.682043	-2.70549	3.459901
H	4.295281	-2.61898	5.536548
C	4.666492	-1.91015	2.786041
C	5.456264	-0.90489	3.302606
N	4.707057	-1.81227	1.40344
C	5.391448	-0.10996	4.518087
C	5.895882	-0.05893	2.200016
C	5.356541	-0.65794	0.951321
H	4.327813	-2.48733	0.755539
N	5.650783	1.205797	4.049507

C	5.829457	1.274929	2.693163
H	5.727141	1.986001	4.686663
C	5.644292	2.478899	1.951289
C	5.823792	2.687109	0.590982
S	4.746522	3.787637	2.667435
C	5.21982	3.873482	0.138969
H	6.342338	1.977669	-0.044586
C	4.575413	4.581007	1.138616
H	5.228614	4.197794	-0.895569
C	3.623046	5.666508	1.043301
C	3.302725	6.631472	1.979001
S	2.438404	5.618182	-0.22194
C	2.101936	7.310265	1.699372
H	3.910594	6.816494	2.857952
C	1.490864	6.859009	0.541543
H	1.638927	8.046865	2.347222
C	0.133592	7.073349	0.134499
C	-0.934814	7.45314	0.925804
N	-0.384074	6.578509	-1.050477
C	-1.210078	7.6571	2.342737
C	-2.13232	7.018976	0.281034
C	-1.793479	6.483401	-1.032056
H	0.150786	6.337	-1.870791
N	-2.560406	7.259769	2.455993
C	-3.08594	6.804739	1.258069
H	-3.067979	7.353921	3.322438
C	-4.236222	5.952076	1.188854
C	-4.852439	5.454505	0.05375
S	-4.757585	5.096256	2.609248
C	-5.708926	4.370587	0.330818
H	-4.616985	5.82088	-0.939617
C	-5.759515	4.03875	1.670719
H	-6.258032	3.821325	-0.427056
C	-6.255025	2.826138	2.290601
C	-6.763506	2.610257	3.551504
S	-5.942855	1.327459	1.467879
C	-6.89667	1.234882	3.884147
H	-7.016275	3.415771	4.231265
C	-6.479416	0.387067	2.84221
H	-7.0843	0.861007	4.88673
C	-6.029822	-0.98075	2.934241
C	-5.464205	-1.6089	4.020749
N	-5.757636	-1.73816	1.80908
C	-4.996481	-1.25063	5.355943
C	-4.690043	-2.70502	3.533843

C	-4.917337	-2.83805	2.098143
H	-6.250977	-1.65421	0.927049
N	-3.910105	-2.12861	5.546564
C	-3.673399	-2.93484	4.442845
H	-3.41174	-2.17233	6.422485
C	-2.420067	-3.58839	4.215308
C	-2.079553	-4.39925	3.145645
S	-1.007087	-3.10037	5.102474
C	-0.689775	-4.59494	3.033709
H	-2.818814	-4.7644	2.439999
C	0.040143	-3.94517	4.010172
H	-0.222686	-5.1729	2.243922
O	-4.532887	-3.65125	1.277584
O	-5.38285	-0.43005	6.167628
O	5.158304	-0.38187	5.677881
O	5.429379	-0.31223	-0.211643
O	-0.529431	8.061725	3.267892
O	-2.468849	6.047789	-1.946063
Au	11.576003	-0.06046	-0.77481
Au	12.509685	1.996602	1.591254
Au	11.866841	2.84899	-1.048227
Au	14.156609	1.264897	-0.605507
Au	13.526672	-0.6229	1.423367
Au	10.887898	-0.09472	2.431837
Au	9.83481	1.81635	0.685238
Au	10.073449	-2.64886	-1.83356
Au	10.245493	-0.24892	-3.353041
Au	12.569387	-1.79707	-2.869837
Au	12.371441	-2.8718	-0.222563
Au	9.809243	-2.17193	0.878733
Au	8.65868	-0.37112	-0.937384
Au	9.383017	2.080016	-2.061939
Au	12.778528	1.050053	-3.083033
Au	14.635882	-1.4317	-1.037201
Au	12.009143	-2.68119	2.561724
Au	8.144832	-0.12828	1.920126
Au	-11.283326	-0.48104	-0.861547
Au	-10.302053	2.495644	-1.507773
Au	-9.366269	0.214569	-2.937169
Au	-8.651573	0.642496	-0.180938
Au	-10.703886	2.002683	1.184584
Au	-12.927685	1.985276	-0.638006
Au	-12.059033	1.043365	-3.195371
Au	-12.249954	-2.81577	1.188984
Au	-10.65942	-3.32141	-1.133541

Au	-9.578221	-1.89556	1.093069
Au	-11.563029	-0.39726	2.381279
Au	-13.844538	-0.56685	0.659801
Au	-13.327393	-2.4468	-1.421177
Au	-11.399955	-1.73563	-3.39827
Au	-8.28214	-1.84857	-1.375513
Au	-8.928213	0.364953	2.699614
Au	-13.353839	1.765763	2.131827
Au	-14.391574	0.034238	-2.037296

<b>BDT-DPP</b>			
<b>AU-MC</b>			
	X	Y	Z
C	-3.66801	-4.23058	-1.52848
C	-4.40503	-3.76918	-0.44699
C	-4.29404	-3.64354	0.998226
C	-5.31426	-2.78213	-0.92211
C	-5.21481	-2.71598	-2.37265
H	-3.89556	-3.80808	-3.60716
C	-5.68548	-1.98585	0.148881
H	-5.26124	-2.21604	2.227142
C	-6.17596	-0.62938	0.128569
C	-6.34779	0.131197	-1.0482
S	-5.92875	0.400236	1.541778
C	-6.08039	1.528042	-0.83068
H	-6.28673	-0.34069	-2.03054
C	-5.80766	1.826981	0.534902
C	-5.26521	3.685136	-1.42027
C	-4.99354	3.987467	-0.05309
S	-4.54898	4.872171	-2.47718
C	-4.17036	5.140589	0.093333
C	-3.76493	5.658764	-1.11318
H	-3.76179	5.491383	1.038155
C	-2.58789	6.455889	-1.31754
C	-1.63374	6.842698	-0.38908
C	-1.33972	6.673807	1.026193
C	-0.41219	7.082993	-1.08331
C	-0.65593	6.954329	-2.51247
H	-2.4727	6.41789	-3.4477
C	0.630226	6.952962	-0.17852
H	0.566928	6.682307	1.93642
C	2.001266	6.611283	-0.43631
C	2.527994	6.351414	-1.679

S	3.031226	6.027105	0.864441
C	3.683153	5.521327	-1.62339
H	2.006282	6.621458	-2.59423
C	4.070883	5.219509	-0.28205
C	5.133593	3.792489	-2.38452
C	5.521085	3.490122	-1.04398
S	5.689437	2.5632	-3.49083
C	6.201564	2.245295	-0.94542
C	6.269791	1.580384	-2.15014
H	6.502882	1.781552	-0.00984
C	6.396942	0.163951	-2.30414
C	6.551749	-0.84547	-1.30937
C	6.301119	-0.89142	0.150118
C	5.977623	-2.05644	-1.87358
C	5.701058	-1.83457	-3.28052
H	5.905224	-0.02038	-4.35692
C	5.397307	-2.78337	-0.85061
H	5.431003	-2.44581	1.257489
C	4.34951	-3.76733	-0.9015
C	3.667802	-4.1521	-2.03067
S	3.512767	-4.2329	0.575021
C	2.374606	-4.67613	-1.74213
H	4.030272	-3.92696	-3.03014
C	2.121119	-4.75171	-0.3398
C	0.052227	-5.03983	-2.13231
C	-0.20013	-5.11743	-0.72922
S	-1.44127	-4.93997	-3.03076
C	-1.58845	-5.03878	-0.42381
C	-2.36688	-4.83436	-1.53833
H	-1.99708	-4.98451	0.582795
O	5.242853	-2.5345	-4.16399
O	6.504808	-0.08814	1.043798
O	-3.63109	-4.23118	1.835526
O	-5.76468	-2.01754	-3.20934
O	-2.03645	6.429324	1.99677
O	0.066917	7.04264	-3.49083
C	-5.85477	2.49562	-1.81625
C	-5.32926	3.05783	0.944435
H	-5.08966	3.261215	1.983127
H	-6.02677	2.26129	-2.86191
C	5.020032	4.260798	0.018265
C	4.27527	4.83185	-2.6927
H	3.956911	5.028404	-3.71132
H	5.280265	4.011834	1.042131
C	1.324622	-4.88129	-2.6507

C	0.868214	-5.02799	0.176189
H	1.499765	-4.7867	-3.71758
H	0.680756	-5.04611	1.244967
N	-5.16895	-2.5729	1.288311
N	-4.23921	-3.68729	-2.66653
N	-2.03074	6.644629	-2.57001
N	0.061101	6.833662	1.077131
N	6.048941	-0.47345	-3.46603
N	5.726458	-2.1508	0.338471
Au	-12.8169	0.095651	0.360832
Au	-12.467	1.591867	-2.47973
Au	-12.9198	2.981749	-0.02433
Au	-14.9439	1.352057	-1.14874
Au	-13.6607	-0.96117	-2.25749
Au	-10.8215	-0.61125	-2.10379
Au	-10.4347	1.657742	-0.5292
Au	-11.9941	-2.11512	2.549183
Au	-12.6174	0.588647	3.223596
Au	-14.6261	-1.15056	2.243221
Au	-13.4321	-2.78012	0.207261
Au	-10.602	-2.28037	0.155359
Au	-10.2108	-0.06731	1.80916
Au	-11.0574	2.588183	2.032779
Au	-14.7924	1.637495	1.681649
Au	-15.6919	-1.19346	-0.3273
Au	-11.9484	-3.18718	-2.14493
Au	-8.52418	-0.47459	-0.48197
Au	12.69385	-0.14249	0.586918
Au	11.30257	2.687234	0.993546
Au	11.76282	0.867378	3.142071
Au	9.804346	0.310829	1.100191
Au	10.63142	1.390323	-1.35483
Au	13.3248	2.296726	-0.94227
Au	13.93391	2.160002	1.863004
Au	13.1916	-2.94161	-1.04802
Au	12.97601	-2.79201	1.79546
Au	10.70535	-2.30852	0.137845
Au	11.46741	-1.14212	-2.28035
Au	14.22734	-0.46457	-1.92903
Au	15.19053	-1.64417	0.483218
Au	14.27864	-0.48247	2.904101
Au	10.64422	-1.68731	2.86422
Au	8.841926	-0.83454	-1.40158
Au	12.53152	1.201299	-3.41553
Au	15.6541	1.037183	-0.02176

<b>DTBDT-DPP</b>			
<b>AU-MC</b>			
	<b>X</b>	<b>Y</b>	<b>Z</b>
C	-5.34524	-3.36827	-2.87825
C	-6.27657	-2.93277	-1.94703
N	-5.61348	-2.69946	-4.06278
C	-6.50185	-2.92375	-0.50822
C	-7.01555	-1.86794	-2.53074
C	-6.60757	-1.71344	-3.91917
H	-5.1323	-2.83373	-4.9387
N	-7.34075	-1.80103	-0.32683
C	-7.5912	-1.1332	-1.51207
H	-7.81207	-1.62633	0.550652
C	-8.16901	2.385904	-2.40748
C	-8.01725	2.661973	-1.05764
S	-8.00291	3.809653	-3.39469
C	-7.72885	4.027169	-0.75857
C	-7.60313	4.765044	-1.97215
C	-6.90124	5.909867	0.45154
C	-6.66579	6.605324	-0.77327
S	-6.2834	6.767612	1.855239
C	-5.86876	7.762876	-0.52113
C	-5.54981	7.962092	0.816653
O	-6.97131	-0.959	-4.80665
O	-6.11221	-3.64499	0.394309
C	-7.42669	4.629558	0.467562
C	-7.07486	6.045374	-1.98877
H	-7.53397	4.07775	1.396554
H	-6.91278	6.57416	-2.92298
S	-4.94995	8.806731	-1.53953
C	-4.56243	8.937827	1.043349
H	-4.11091	9.190192	1.99936
C	-4.0947	9.457907	-0.15252
C	-8.24102	1.002687	-2.72208
S	-7.93531	1.219139	-0.11335
H	-8.1221	0.57135	-3.71577
C	-8.06015	0.222724	-1.55858
C	-4.14308	-4.10868	-2.65807
S	-2.88421	-4.15124	-3.87909
C	-3.70209	-4.58347	-1.43225

C	-1.74029	-4.71541	-2.72186
C	-2.33279	-4.89963	-1.47758
H	-4.33943	-4.58895	-0.5514
C	-0.31561	-4.79743	-2.71876
S	-1.15799	-5.25099	-0.23589
C	0.149546	-5.00837	-1.38612
C	0.597029	-4.56678	-3.75401
C	1.489266	-4.88255	-1.05989
C	1.936817	-4.44269	-3.42791
H	0.251283	-4.41847	-4.77246
C	2.387493	-4.54278	-2.07761
H	1.827316	-4.97337	-0.03214
S	3.214472	-3.97853	-4.54317
C	3.744471	-4.10768	-1.99248
C	4.311916	-3.74326	-3.20751
S	4.756922	-3.65837	-0.67395
C	5.556329	-3.0963	-3.09898
C	5.916253	-2.92977	-1.77158
H	6.1308	-2.66716	-3.91439
C	6.90817	-2.02549	-1.27395
C	7.638133	-1.06852	-1.94986
N	7.054611	-1.75794	0.083338
C	8.146219	-0.11221	-0.9905
C	7.612249	-0.45042	-3.26339
C	7.721629	-0.56749	0.337244
H	6.718576	-2.33644	0.839258
C	8.193819	1.138163	-1.65945
N	8.00403	0.883659	-2.9941
O	7.318078	-0.85792	-4.37076
O	7.892292	-0.10168	1.466973
H	8.099018	1.558167	-3.73913
C	8.153352	2.453938	-1.11536
S	7.762695	3.819267	-2.14871
C	8.096111	2.78679	0.232806
C	7.431056	4.800689	-0.77596
C	7.667641	4.110816	0.410575
H	8.265328	2.058063	1.018872
C	6.763696	6.050142	-0.61088
S	7.137856	5.007645	1.809982
C	6.464955	6.255213	0.769159
C	6.272252	6.935151	-1.57785
C	5.609119	7.263184	1.180883
C	5.411686	7.937474	-1.16716
H	6.503074	6.789094	-2.62869
C	5.031145	8.079292	0.202179

H	5.33077	7.371336	2.224646
S	4.534092	9.022611	-2.23608
C	3.942759	8.996401	0.30501
C	3.535255	9.54615	-0.90456
S	2.813271	9.347465	1.558204
C	2.312406	10.23963	-0.84878
C	1.765994	10.17941	0.422926
H	1.774419	10.67038	-1.68912
C	0.400749	10.44451	0.761174
C	-0.66331	10.69273	-0.09061
N	-0.13666	10.1707	2.007145
C	-1.86985	10.40475	0.608843
C	-0.95066	10.75236	-1.51508
C	-1.5442	10.07178	1.986409
H	0.386007	9.982285	2.848451
C	-2.86667	10.17209	-0.32545
N	-2.3332	10.47354	-1.56676
O	-0.25739	10.96844	-2.49526
O	-2.22368	9.76335	2.951591
H	-2.8232	10.43094	-2.44684
Au	-13.5657	-0.81907	0.706946
Au	-13.0261	2.208172	1.536619
Au	-12.3168	0.008424	3.19661
Au	-15.0467	0.614737	2.737497
Au	-15.2985	1.520892	0.038962
Au	-12.6917	1.688439	-1.16069
Au	-10.9489	0.493492	0.700572
Au	-13.8782	-3.203	-1.48787
Au	-12.8851	-3.62306	1.156619
Au	-15.5849	-2.89291	0.771594
Au	-15.6883	-1.06481	-1.40291
Au	-13.0645	-0.75141	-2.51395
Au	-11.3692	-2.12029	-0.74689
Au	-10.7633	-1.98042	1.974677
Au	-14.2423	-2.09671	3.153302
Au	-16.9669	-0.50526	1.04521
Au	-14.9948	1.293204	-2.74604
Au	-10.4915	0.192534	-2.16256
Au	13.24427	-0.18183	-0.00895
Au	15.01301	0.950267	2.597478
Au	12.90489	-0.83801	2.944431
Au	12.35361	1.767147	1.938285
Au	14.50441	2.458608	0.254327
Au	16.19082	0.17726	0.130861
Au	15.44476	-1.73565	2.041174

Au	12.25324	-2.47835	-1.82659
Au	11.60833	-2.43169	0.889984
Au	10.54657	-0.39164	-0.80843
Au	12.61876	0.156128	-2.77583
Au	14.88456	-1.52696	-2.09913
Au	14.17677	-3.34292	-0.02939
Au	13.45422	-3.59852	2.673866
Au	10.36747	-0.20422	2.116666
Au	11.91608	2.159047	-0.87261
Au	15.12069	1.266083	-2.20229
Au	16.83325	-2.49469	-0.28792

<b>DTBDT-BT</b>			
<b>AU-MC</b>			
C	5.165744	2.935708	-0.54498
C	5.030313	2.257501	0.649814
S	5.30161	1.831424	-1.91072
C	4.919422	0.828273	0.524102
C	4.86901	0.468422	-0.8525
C	4.073091	-1.34011	1.064593
C	3.840299	-1.61096	-0.31462
S	3.3273	-2.5294	2.121618
C	2.88661	-2.66989	-0.44619
C	2.474413	-3.21256	0.758579
C	4.605627	-0.12994	1.491914
C	4.335593	-0.72853	-1.28664
H	4.657925	0.114596	2.548151
H	4.204845	-0.93701	-2.34382
S	1.770403	-3.06407	-1.70896
C	1.25305	-3.91901	0.692654
H	0.726567	-4.33365	1.541898
C	0.685827	-3.85174	-0.5652
C	4.824266	4.303123	-0.49777
S	4.508378	3.334066	1.893469
H	4.783931	4.970139	-1.34851
C	4.354493	4.665402	0.751039
C	-0.68375	6.853448	0.726803
S	-1.77329	6.078653	1.874925
C	-1.24842	6.911345	-0.53245
C	-2.89005	5.679485	0.613699
C	-2.47304	6.210255	-0.59434
H	-0.71864	7.315642	-1.38459
C	-3.84466	4.620199	0.488417

S	-3.32295	5.516703	-1.95426
C	-4.07173	4.335823	-0.88912
C	-4.33942	3.744033	1.465775
C	-4.59512	3.118911	-1.30716
C	-4.86849	2.541036	1.040438
H	-4.20263	3.956877	2.521447
C	-4.90571	2.168201	-0.33263
H	-4.6349	2.861783	-2.36105
S	-5.25424	1.175956	2.11271
C	-4.99195	0.737396	-0.44592
C	-5.09466	0.065925	0.754546
S	-4.53647	-0.35335	-1.70249
C	-4.77798	-1.3073	0.704003
C	-4.35008	-1.67999	-0.55758
H	-4.71828	-1.96927	1.557353
C	1.694183	7.248379	-0.01447
C	3.024104	6.666807	-0.00991
C	3.421929	5.74988	1.023944
C	2.593949	5.752501	2.135387
C	1.299777	6.316419	2.130164
C	0.742458	6.917104	1.012063
H	2.84809	5.131651	2.989889
H	0.66436	6.079137	2.978506
N	3.750515	7.022643	-1.06614
N	1.468331	8.018856	-1.07512
S	2.828912	8.015743	-1.96713
C	-3.42326	-2.76425	-0.84777
C	-2.59703	-2.7526	-1.96102
C	-3.02243	-3.6926	0.17459
C	-1.30136	-3.31273	-1.96292
H	-2.85191	-2.11969	-2.80629
C	-1.69038	-4.26873	0.172469
C	-0.7403	-3.92069	-0.85035
H	-0.66781	-3.06495	-2.80964
N	-3.74604	-4.06053	1.228202
N	-1.46261	-5.05281	1.222596
S	-2.8236	-5.06667	2.113941
Au	11.15067	-0.45947	0.232551
Au	9.601553	1.054352	2.6481
Au	8.173235	-0.13672	0.546477
Au	9.611785	2.246747	0.13988
Au	12.0541	1.960562	1.624952
Au	11.97508	-0.53423	3.013146
Au	9.505045	-1.7536	2.488727
Au	11.74665	-1.2055	-2.98897

Au	9.12464	-1.15406	-1.96294
Au	10.5497	1.234259	-2.33279
Au	13.22757	0.68992	-1.52443
Au	13.3895	-2.02889	-0.74398
Au	10.90281	-3.22216	-1.20363
Au	8.489058	-2.88556	0.145585
Au	7.825062	1.369488	-1.90344
Au	12.04788	3.15562	-0.92241
Au	13.96579	-0.01836	1.098502
Au	11.82771	-2.94574	1.450504
Au	-12.5916	-1.38244	-2.02753
Au	-12.5404	1.111507	2.744719
Au	-13.4161	-0.19501	0.36243
Au	-12.8657	2.633274	0.485947
Au	-10.2668	2.183308	1.388674
Au	-10.0832	-0.33962	2.654918
Au	-12.5563	-1.62754	2.700722
Au	-8.16445	-1.10852	-2.12553
Au	-10.4732	-2.09699	-3.67739
Au	-10.4677	0.471534	-2.64251
Au	-8.58725	1.201053	-0.65017
Au	-8.353	-1.30645	0.648396
Au	-10.2347	-2.66522	-0.97993
Au	-12.737	-2.94324	0.239028
Au	-13.053	1.334475	-1.98799
Au	-10.7105	2.882681	-1.30437
Au	-7.81001	1.142356	2.111777
Au	-10.2782	-2.99259	1.764488

**Table S4. Optimized Cartesian coordinates of the gold clusters**

<b>G1-Au6-Octahedron</b>			
Au	0	1.38045	0
Au	0	0	2.364032
Au	2.364032	0	0
Au	0	-	0
Au	0	1.38045	0
Au	0	0	-2.36403
Au	-2.36403	0	0

<b>G1-Au7-Pentagonal Decahedron</b>			
Au	0	1.523052	0
Au	0	-1.52305	0
Au	0	0	2.389077
Au	-2.27215	0	0.738265
Au	-1.40426	0	-1.9328
Au	1.404264	0	-1.9328
Au	2.272147	0	0.738265

<b>G1-Au13-cubotahedron</b>			
Au	0	2.116195	0
Au	0	0	2.116195
Au	2.116195	0	0
Au	0	-2.1162	0
Au	0	0	-2.1162
Au	-2.1162	0	0
Au	1.951774	1.951774	1.951774
Au	-1.95177	1.951774	1.951774
Au	1.951774	-1.95177	1.951774
Au	1.951774	1.951774	-1.95177
Au	-1.95177	-1.95177	-1.95177
Au	1.951774	-1.95177	-1.95177
Au	-1.95177	1.951774	-1.95177
Au	-1.95177	-1.95177	1.951774

<b>G1-Au14-Cube</b>			
Au	0	2.116195	0
Au	0	0	2.116195
Au	2.116195	0	0
Au	0	-2.1162	0
Au	0	0	-2.1162
Au	-2.1162	0	0
Au	1.951774	1.951774	1.951774
Au	-1.95177	1.951774	1.951774

Au	1.951774	-1.95177	1.951774
Au	1.951774	1.951774	-1.95177
Au	-1.95177	-1.95177	-1.95177
Au	1.951774	-1.95177	-1.95177
Au	-1.95177	1.951774	-1.95177
Au	-1.95177	-1.95177	1.951774

<b>G1-Au18-Marksüf Decahedron</b>			
Au	0	0	0
Au	0	2.995704	0
Au	-4.9E-05	1.595283	2.439883
Au	-2.32048	1.595283	0.753918
Au	-1.43409	1.595283	-1.97394
Au	1.434167	1.595283	-1.97388
Au	2.320451	1.595283	0.754012
Au	0	-2.9957	0
Au	-4.9E-05	-1.59528	2.439883
Au	-2.32048	-1.59528	0.753918
Au	-1.43409	-1.59528	-1.97394
Au	1.434167	-1.59528	-1.97388
Au	2.320451	-1.59528	0.754012
Au	2.22627	0	3.064095
Au	-2.22617	0	3.064166
Au	-3.60212	0	-1.17034
Au	-6.1E-05	0	-3.78747
Au	3.602083	0	-1.17045

<b>G2-Au19-Octahedron</b>			
Au	0	0	0
Au	2.072105	2.072535	0
Au	0	2.072535	2.072105
Au	-2.07211	2.072535	0
Au	0	2.072535	-2.07211
Au	2.071086	0	2.071086
Au	-2.07109	0	2.071086
Au	-2.07109	0	-2.07109
Au	2.071086	0	-2.07109
Au	-2.07211	-2.07254	0
Au	0	-2.07254	-2.07211
Au	2.072105	-2.07254	0
Au	0	-2.07254	2.072105
Au	0	3.913992	0
Au	0	0	3.914799
Au	3.914799	0	0
Au	0	-3.91399	0

Au	0	0	-3.9148
Au	-3.9148	0	0

<b>G1-Au13-Icosahedron</b>			
Au	0	0	0.382639
Au	0	2.875212	0.468753
Au	0	3.754497	-2.06038
Au	1.447011	1.344393	-1.6456
Au	1.441362	1.408821	2.345757
Au	-1.44136	1.408821	2.345757
Au	-1.44701	1.344393	-1.6456
Au	0	-2.87521	0.468753
Au	0	-3.7545	-2.06038
Au	1.447011	-1.34439	-1.6456
Au	1.441362	-1.40882	2.345757
Au	-1.44136	-1.40882	2.345757
Au	-1.44701	-1.34439	-1.6456

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