ELECTRONIC SUPPLEMENTARY INFORMATION

Guidelines and Diagnostics for Charge Carrier Tuning in Thiophene-Based Wires

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Computational Methods

In this study the –SH was used instead of the $–SCH_3$ linker to simplify the *in silico* junction construction and optimization. Computations on the TDO_n wires with both types of linkers illustrate that their trends in conductance and dominant orbital peaks are consistent (Figure S1). The geometries of the isolated molecules with the thiol linkers in extended chain conformations were optimized at the PBE0-D3/cc-pVDZ level of theory using the Gaussian 09 software package.[1] The trends in their molecular orbital levels, known to be heavily method-[2] and basis set[3] dependent, were confirmed *via* computations of the vertical ionization potentials and electron affinities (with stability checks) at the ωB97X-D/maug-cc-pVTZ//PBE0-D3/cc-pVDZ level.[4] To model the binding geometry inside the junction, each molecule was attached to two Au_8 clusters *via* the thiol linkers in atop manner and its geometry was optimized (while the clusters were kept frozen). The relative position of the gold clusters and the nanogap width (Table S1) between them were chosen to afford (*i*) sufficient flexibility for the Au–S–C donor-acceptor bonds to relax[5] and (*ii*) form the tilted high-conductance junction geometries.[6] These geometry optimizations were carried out using the PBE0-D3/cc-pVDZ method including def2 effective core potential on the gold atoms. The non-equilibrium Green's function formalism[7,8] was employed to simulate the zero-bias transmission spectra, as implemented[9,10] in ADF

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2016.[11,12,13] In this approach, the junction is partitioned into an 'extended molecule' – in this work it is the studied molecule, linked to Au_8 clusters, aligned with Au_{30} slabs (111-cut surface)[14] – and the semi-infinite bulk leads. The current through the junction, *I*, is given by Landauer formula:

$$I = \frac{e}{h}\sum_{\sigma}\int \frac{d\varepsilon}{2\pi}(f_L(\varepsilon) - f_R(\varepsilon))\tau(\varepsilon), \qquad \text{Eq. 1}$$

where ε is the energy, f_L and f_R are the Fermi distributions of the left and right leads, $\tau(\varepsilon)$ is the transmission function:

$$\tau(\varepsilon) = \mathrm{Tr}_M\{\Gamma_R(\varepsilon)G_{EM}(\varepsilon)\Gamma_L(\varepsilon)G_{EM}^{\dagger}(\varepsilon)\}. \qquad \text{Eq. 2}$$

Here G_M and $G_M^{\dagger}$ are retarded and advanced Green's functions of the extended molecule and Γ_L and Γ_R are the left and right contact couplings. The Green's functions are given by

$$G_{EM}(\varepsilon) = (\varepsilon S_{EM} - H_{EM} - (\Sigma_L(\varepsilon) + \Sigma_R(\varepsilon)))^{-1}, \qquad \text{Eq. 3}$$

where S_{EM} is the overlap matrix, H_{EM} is the Hamiltonian of the extended molecule, Σ_L and Σ_R are the leads' self-energies. The couplings Γ_L and Γ_R are

$$\Gamma(\varepsilon) = i(\Sigma(\varepsilon) - \Sigma^{\dagger}(\varepsilon)), \qquad \text{Eq. 4}$$

where Σ and $\Sigma^{\dagger}$ are the retarded and advanced self-energies. In this work, we employ the so-called post-SCF NEGF+DFT approach,[9] in which the extended molecule and the semi-infinite leads are treated self-consistently separate to each other, and then combined non-self-consistently to perform the transport computations. Computations on the extended molecule are performed using the PBE functional and a DZP basis set for all atoms except gold for which a smaller DZ basis set with a large frozen core (excluding only the *d* and *s* outer shells) is used. Scalar relativistic effects are treated

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using Zero Order Regular Approximation (ZORA).[15] The classical Hirshfeld population analysis[16] of the charges on the fragments was performed on the extended molecules, as implemented in ADF.[11,12,13] The computed total charges can be non-zero due to the limited numerical integration precision (small effect) and the neglect of long-distance terms in the integral evaluations. Moreover, the 'molecule' in these results includes the two Au_8 gold clusters. To correct for these factors, we have shifted all charge distributions by constant values of –0.09 (molecule) and +0.05 (leads) that ensure neutrality for the non-substituted mid-gap-transporting $THIOQ_n$ wires (Figure S5). The self-energies of the leads are computed self-consistently for a chain of three principal layers (the aforementioned Au_{30} slabs, cut in (111) surface). The transmission is computed in the range of -0.4 to 0.0 Hartree for 1000 points. The Fermi level for each extended molecule is computed at the same level of theory using the BAND 2016 program[17] (with KSpace 7).

The NEGF+DFT formalism has become a standard for modeling molecular transport. One of the key shortcomings of the approach in its straightforward implementation is the level alignment due to several factors: (*i*) the commonly used LDA and GGA density functionals notoriously underestimate the HLG,[18] (*ii*) image charge (surface polarization) effects also contribute to the transport gap renormalization, (*iii*) positioning of the Fermi level is not always uniquely defined in the computation.[19] Several remedies to this problem exist and rely upon adjusting the self-energies to assure charge neutrality,[10] matching the gas-phase ionization potentials and electron affinities of the molecule (DFT+Σ),[8] using a more sophisticated (and computationally demanding) many-body GW approximation[20] and even empirical corrections.[21] However, none of the computational techniques offers a universal solution due to various limitations and convergence issues.[22,23] Moreover, even the most accurate treatment of charge transport in a static junction geometry cannot capture the rich

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conformational and binding mode behavior that naturally impacts the experimental outcomes.[24,25,26,27,28] Finally, such critical influences as vibrational[29] and many-body effects[30] are not automatically included in the standard NEGF+DFT approach. However, all these shortcomings do not prevent this conventional method from accurately predicting the trends (rather than absolute values) in the molecular transport characteristics.[10,19,23] Since the primary focus of this study is to elucidate the molecular-level factors dictating the performance and properties of the various oligothiophene-based SMJs, we use consistent junction models in conjunction with the standard NEGF+DFT approach in order to compare the investigated systems *ceteris paribus*.

We also note that at larger molecular lengths the transport mechanism changes from coherent off-resonant tunneling to sequential thermally activated hopping, and crossover at lengths as low as 25Å has been reported.[31,32] This process has not been included in this study and our results for wires with $n > 4$ are meaningful only to obtain the projected trends in the coherent tunneling regime.

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Table S1. Imposed *z*-axis distances between the Au_8 clusters, used to construct the junction geometries.

Wire	1	2	3	4	5	6
$THIO_n$	15.5	19.0	23.0	26.0	30.0	33.5
TDO_n	15.5	19.0	23.0	26.0	30.0	34.0
$PEDOT_n$	15.5	19.0	23.0	26.0	30.0	33.5
$TCLO_n$	15.5	19.0	23.0	26.0		
PYR_n	15.5	19.0	23.0	26.0		
TCp_n	15.5	19.0	23.0	26.0		
Cp_n	15.5	19.0	23.0	26.0		
$TDOA_n$	12.0	15.0	16.0	17.5		
$THIA_n$	12.0	15.0	16.0	17.5		
$THIOQ_n$	16.0	20.0	24.0	28.5		

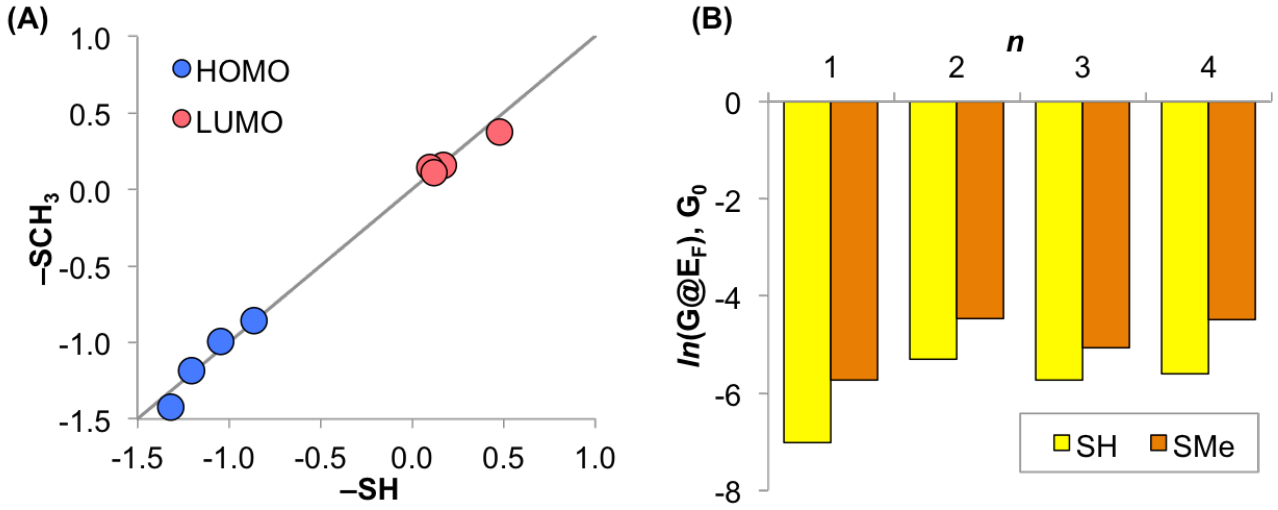

Figure S1. Role of the linker.

Computed conductance orbital peaks (A) and transmissions at Fermi level (B) in TDOn wires with $–SCH_3$ vs. –SH linkers.

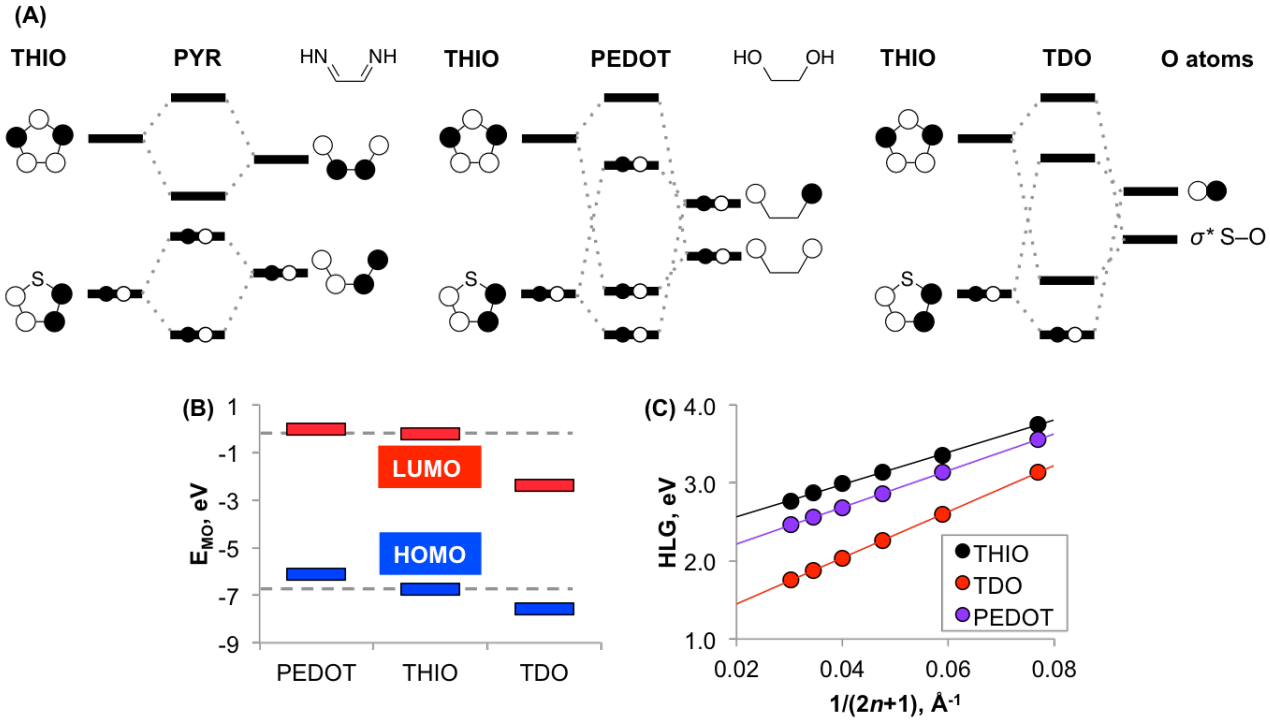

Figure S2. Orbital effects in the individual cores and their wires.

(A) Schematic MO correlation diagrams for PYR, PEDOT and TDO cores. Computed PBE0-D3/cc-pVDZ orbital energies for (B) individual cores (without (2-thio)thiophene linkers) and for (C) the studied systems with n = 1-6, plotted to illustrate the asymptotic linear dependence on the inverse chain length.

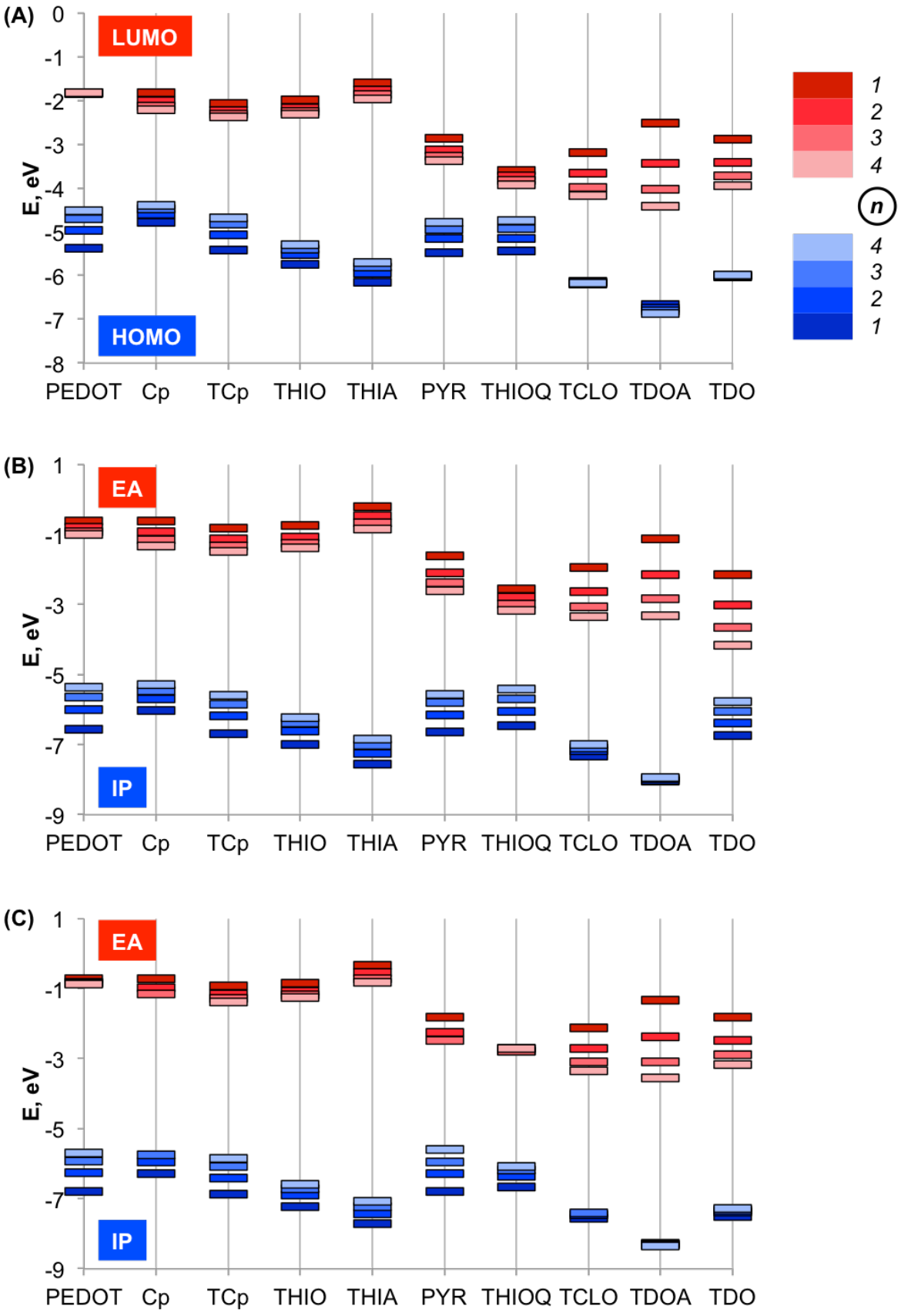

Figure S3. MO energies, IPs and EAs.

Computed PBE0/cc-pVDZ molecular orbital energies (A) and vertical ionization energies and electron affinities at the PBE0/cc-pVDZ (B) and ωB97X-D/maug-cc-pVTZ//PBE0/cc-pVDZ level of theory (C) for the investigated systems with n = 1-4.

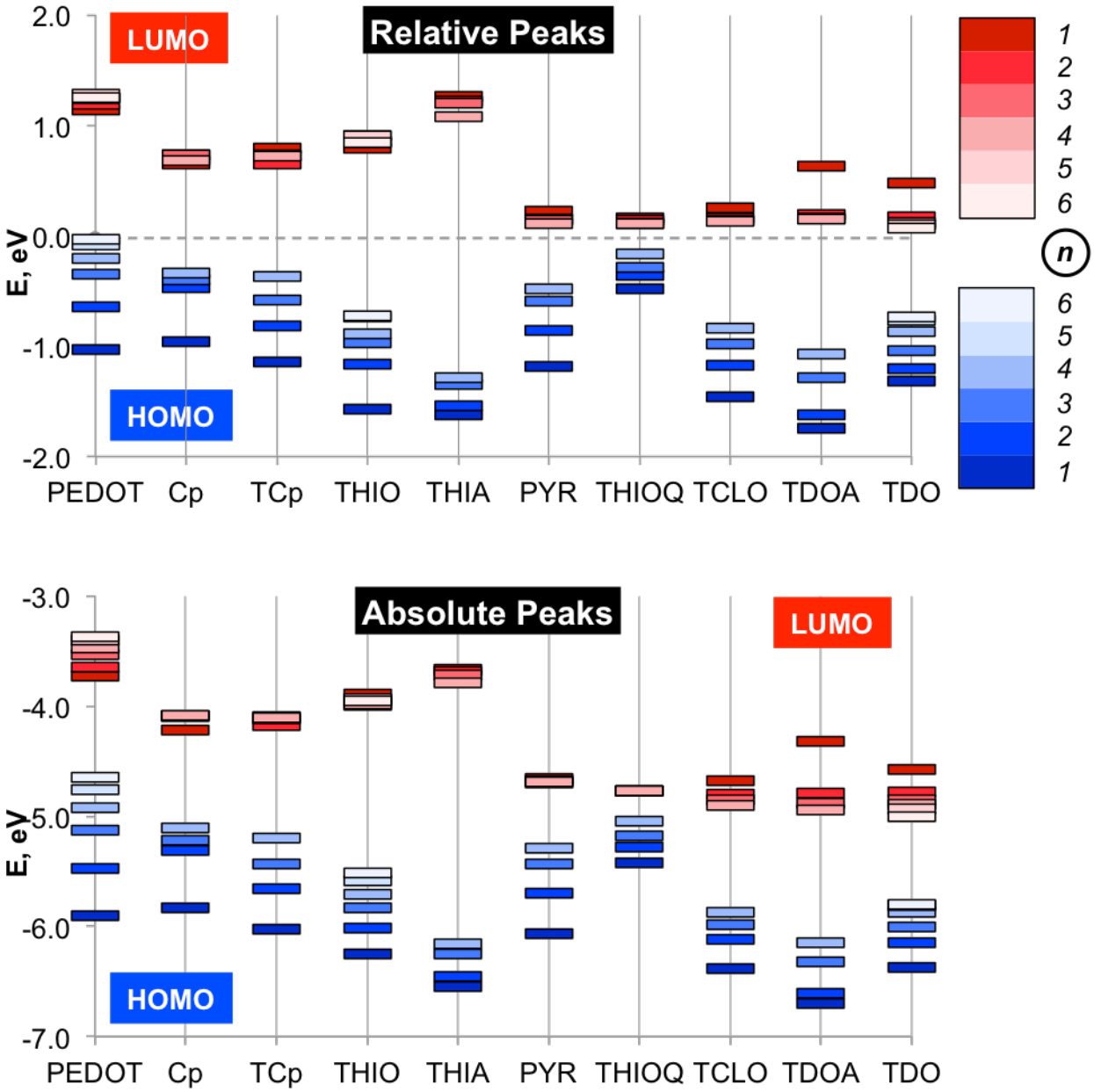

Figure S4. Transmission peaks.

Computed PBE/DZP+ZORA peaks corresponding to molecular HOMO and LUMO resonances on a relative to computed E_F (top) and an absolute (bottom) scale.

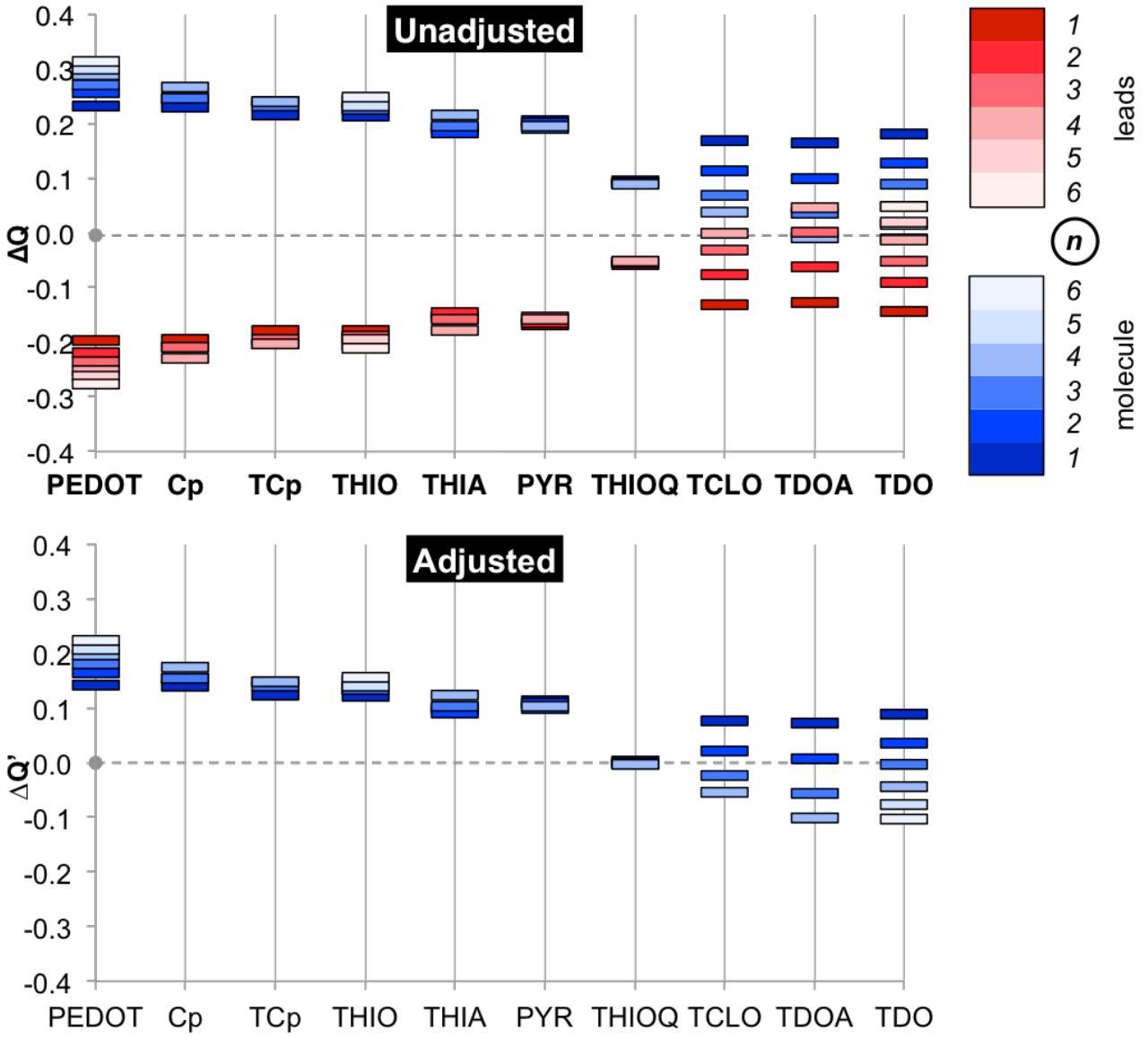

Figure S5. Charge transfer within the junction.

Computed charge transfer values (ΔQ>0 is from the molecule to the leads), based on the PBE/DZP+ZORA absolute Hirshfeld charges (top, charge on the molecule is shown in blue, sum of charges on the leads – in red) and adjusted to assure neutrality in $THIOQ_n$ junctions (bottom).

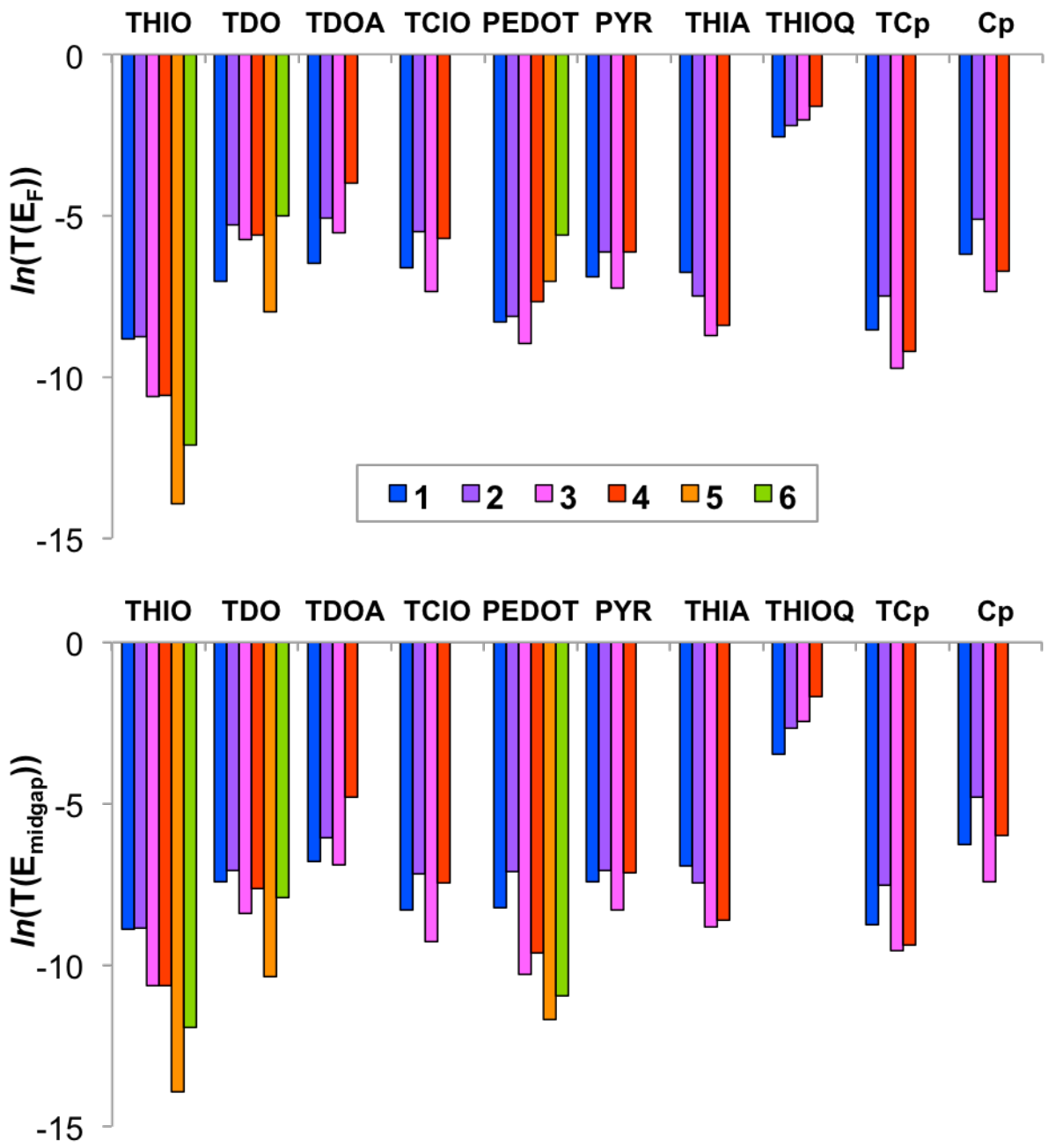

Figure S6. Comparative transmissions of the studied junctions.

Computed transmissions (PBE/DZP+ZORA) at the computed Fermi level (top) and at mid-gap energy (bottom).

We find that the computed conductance at the Fermi level does decay in the $THIO_n$ series but not in TDO_n and $PEDOT_n$ because as *n* increases the molecular resonances in these series approach the E_F closely, *i.e.* the resonant transport starts to dominate. Thus, to estimate β in the off-resonant tunneling regime we use instead the conductance values in the middle of the transport gap.

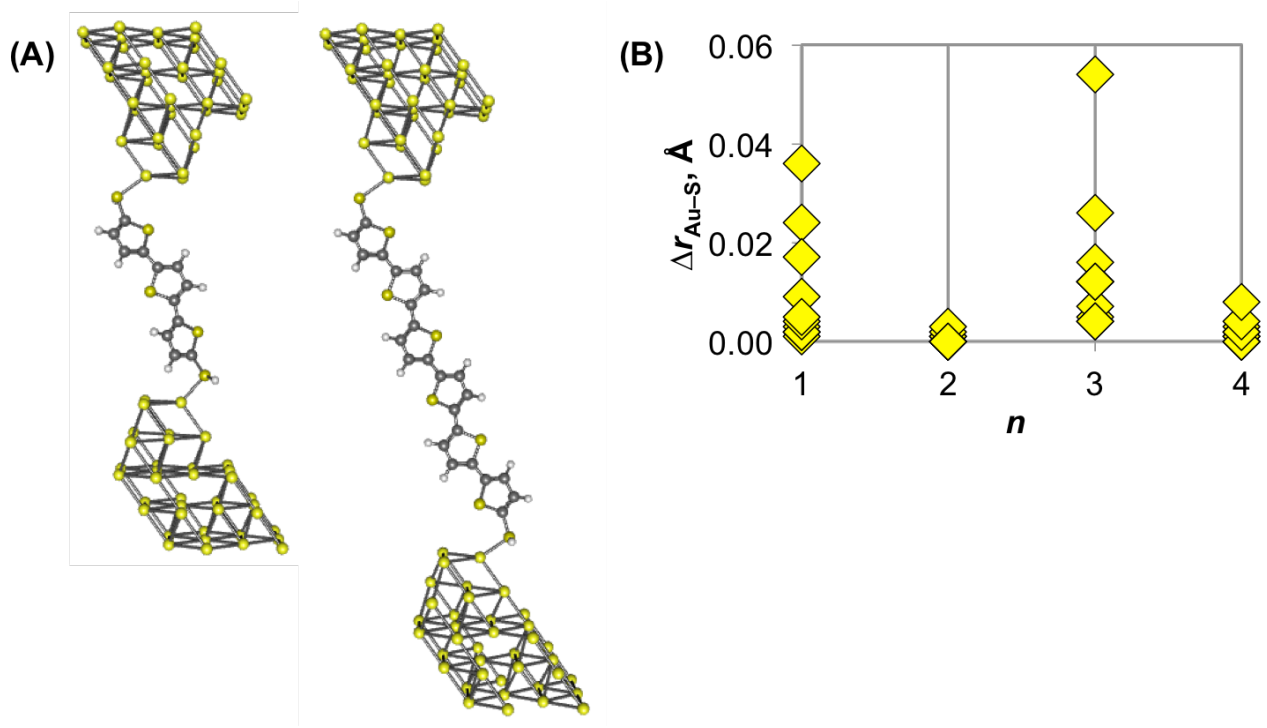

Figure S7. Role of the terminal unit binding.

(A) PBE0-D3/cc-pVDZ+ECP optimized geometries of $THIO_1$ and $THIO_4$ anchored to Au_8 cluster. Note the difference in the binding geometry to the bottom cluster. (B) Difference in the Au–S bond lengths between the molecule and the left *vs.* the right lead (in the PBE0-D3/cc-pVDZ+ECP optimized geometries of Au_8–molecule–Au_8).

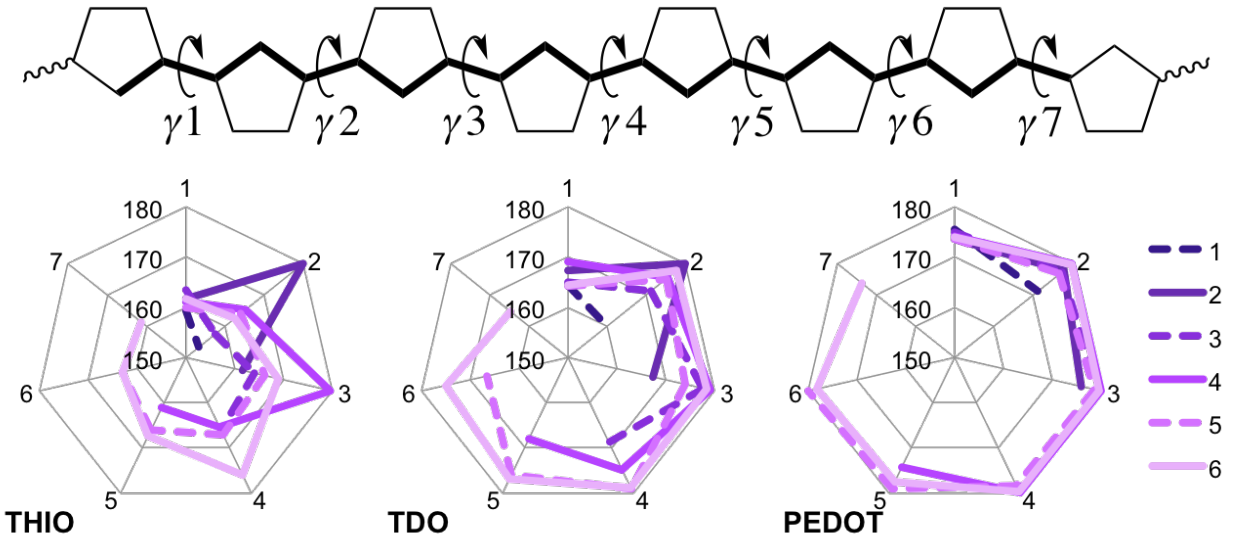

Figure S8. Planarity of the wires.

Dihedral angles along the backbones of the $THIO_n$, TDO_n and $PEDOT_n$ wires, optimized in between two Au_8 clusters at the PBE0-D3/cc-pVDZ+ECP level of theory.

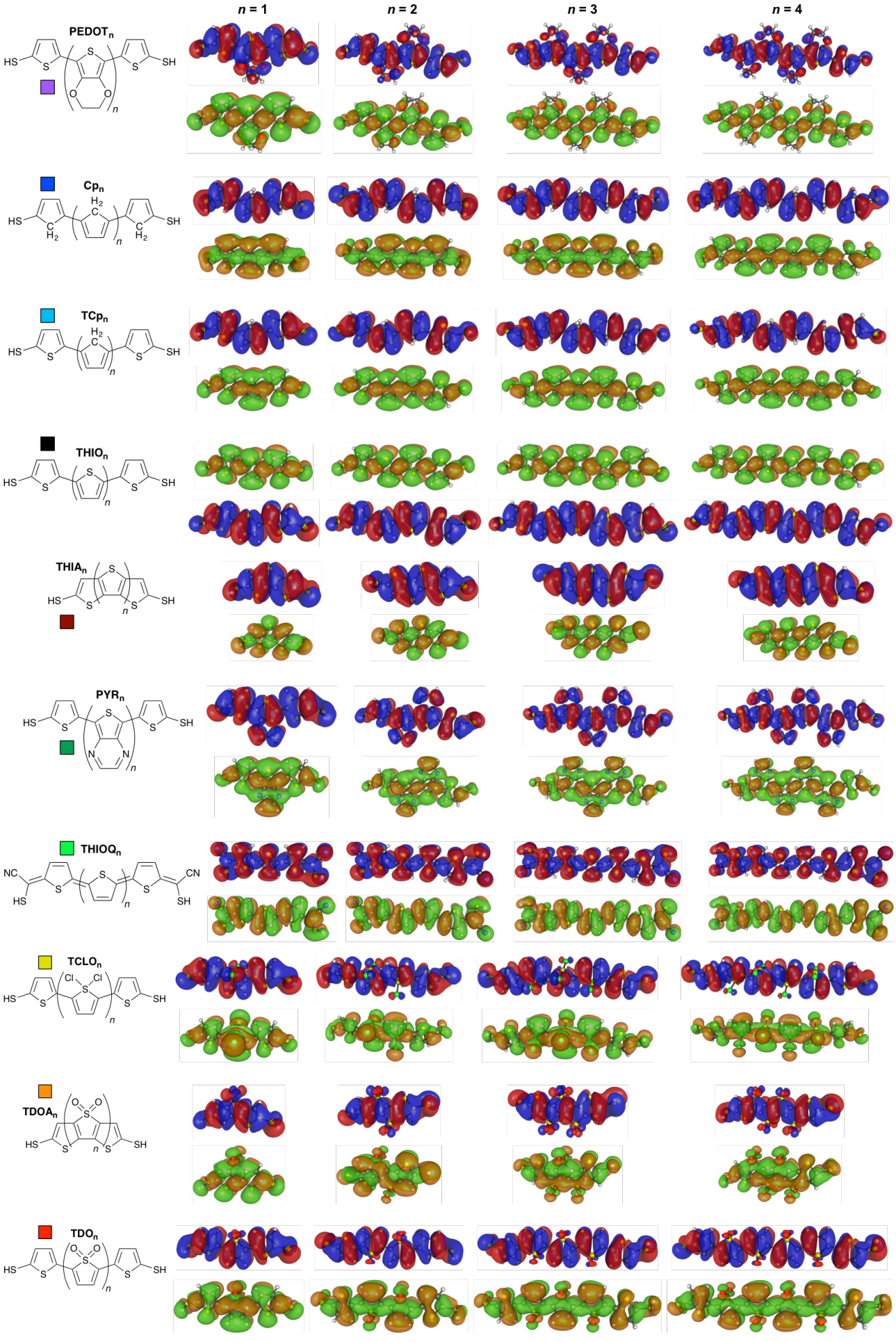
n = 1
n = 2
n = 3
n = 4
PEDOTn
Cpn
TCpn
THIOn
THIAn
PYRn
THIOQn
TCLOn
TDOAn
TDOn

Figure S9. Molecular orbital plots.

HOMO (red and blue) and LUMO (orange and green) plots (isovalue = 0.020) of the investigated wires for *n*=1-4, computed at the PBE0/cc-pVDZ level of theory.

Table S2. Molecular orbital energy levels in the isolated wires.

Orbital energies for fully optimized geometries at the PBE0/cc-pVDZ level of theory, in eV.

n	PEDOT	Cp	TCp	THIO	THIA	PYR	THIOQ	TCLO	TDOA	TDO
					HOMO					
0 [a]	-6.11			-6.76						-7.58
1	-5.38	-4.79	-5.43	-5.75	-6.15	-5.48	-5.44	-6.13	-6.67	-6.03
2	-4.97	-4.60	-5.07	-5.51	-5.96	-5.16	-5.16	-6.15	-6.75	-6.01
3	-4.71	-4.48	-4.84	-5.39	-5.81	-4.94	-4.94	-6.18	-6.81	-5.99
4	-4.52	-4.40	-4.68	-5.30	-5.71	-4.79	-4.74	-6.17	-6.87	-5.99
5	-4.39			-5.24						-5.99
6	-4.29			-5.17						-6.01
					LUMO					
0 [a]	0.00			-0.22						-2.40
1	-1.82	-1.83	-2.07	-1.99	-1.61	-2.86	-3.61	-3.20	-2.53	-2.89
2	-1.84	-2.01	-2.23	-2.17	-1.76	-3.14	-3.72	-3.67	-3.43	-3.41
3	-1.84	-2.12	-2.32	-2.25	-1.88	-3.28	-3.82	-3.98	-4.04	-3.73
4	-1.84	-2.21	-2.37	-2.31	-1.97	-3.39	-3.92	-4.18	-4.42	-3.95
5	-1.83			-2.36						-4.11
6	-1.82			-2.41						-4.25

[a] '0' refers to a single core with H atoms instead of the (2-thio)thiophene linkers.

Table S3. Vertical ionization potentials and electron affinities for the isolated wires.

ωB97X-D/maug-cc-pVTZ//PBE0-D3/cc-pVDZ level of theory, in eV.

n	PEDOT	Cp	TCp	THIO	THIA	PYR	THIOQ	TCLO	TDOA	TDO
					PBE0/cc-pVDZ					
					IP					
1	-6.57	-6.02	-6.69	-6.99	-7.56	-6.65	-6.46	-7.33	-8.05	-6.75
2	-6.01	-5.69	-6.19	-6.62	-7.26	-6.15	-6.05	-7.18	-8.01	-6.38
3	-5.63	-5.46	-5.84	-6.40	-7.02	-5.81	-5.71	-7.09	-7.97	-6.06
4	-5.37	-5.29	-5.59	-6.23	-6.84	-5.56	-5.42	-6.99	-7.93	-5.77
					EA					
1	-0.63	-0.61	-0.83	-0.76	-0.22	-1.63	-2.55	-1.95	-1.12	-2.14
2	-0.80	-0.93	-1.13	-1.07	-0.48	-2.11	-2.80	-2.63	-2.15	-3.02
3	-0.91	-1.16	-1.33	-1.25	-0.68	-2.39	-3.00	-3.07	-2.85	-3.65
4	-1.00	-1.33	-1.48	-1.40	-0.85	-2.60	-3.18	-3.36	-3.32	-4.16
					ωB97X-D/maug-cc-pVTZ//PBE0/cc-pVDZ					
					IP					

1	-6.79	-6.27	-6.88	-7.22	-7.72	-6.80	-6.66	-7.55	-8.28	-7.51
2	-6.26	-5.96	-6.40	-6.89	-7.43	-6.27	-6.36	-7.46	-8.31	-7.39
3	-5.93	-5.76	-6.08	-6.72	-7.22	-5.94	-6.17	-7.42	-8.34	-7.32
4	-5.70		-5.86	-6.60	-7.07	-5.60	-6.09		-8.35	-7.28
					EA					
1	-0.72	-0.72	-0.92	-0.84	-0.35	-1.81	-2.70	-2.12	-1.34	-1.82
2	-0.82	-0.97	-1.15	-1.07	-0.55	-2.25	-2.79	-2.70	-2.38	-2.47
3	-0.86	-1.14	-1.29	-1.17	-0.71	-2.48	-2.79	-3.09	-3.09	-2.89
4	-0.88		-1.39	-1.24	-0.83		-2.72	-3.36	-3.56	-3.18

Table S4. Hirshfeld charges.

Classical Hirshfeld charges on the 'molecule' (comprising two Au_8) cluster and sum of both Au_{30} slabs in the junction, PBE/DZP+ZORA level of theory.

n	PEDOT	Cp	TCp	THIO	THIA	PYR	THIOQ	TCLO	TDOA	TDO
					Au_8 – Molecule – Au_8					
1	0.23	0.23	0.22	0.21	0.19	0.20	0.09	0.17	0.16	0.18
2	0.26	0.25	0.24	0.23	0.18	0.20	0.09	0.11	0.10	0.13
3	0.27	0.25	0.23	0.23	0.20	0.19	0.09	0.07	0.04	0.09
4	0.29	0.27	0.24	0.24	0.22	0.19	0.09	0.04	-0.01	0.05
5	0.30			0.23						0.02
6	0.31			0.25						-0.01
					Au_{30} – – – Au_{30}					
1	-0.20	-0.19	-0.18	-0.18	-0.15	-0.17	-0.06	-0.13	-0.13	-0.14
2	-0.22	-0.21	-0.20	-0.19	-0.15	-0.16	-0.05	-0.08	-0.06	-0.09
3	-0.23	-0.21	-0.20	-0.19	-0.16	-0.15	-0.05	-0.03	0.00	-0.05
4	-0.25	-0.23	-0.20	-0.20	-0.18	-0.16	-0.05	0.00	0.05	-0.01
5	-0.26			-0.19						0.02
6	-0.28			-0.21						0.05

Table S5. Molecular lengths.

S–S distances between the thiol linkers in the PBE0-D3/cc-pVDZ optimized model junction geometries, in Å.

n	PEDOT	Cp	TCp	THIO	THIA	PYR	THIOQ	TCLO	TDOA	TDO
1	13.660	13.185	13.507	13.587	9.795	13.851	13.663	13.671	9.807	13.663
2	17.633	16.971	17.293	17.583	11.955	18.167	17.632	17.591	12.020	17.690
3	21.513	20.688	21.031	21.376	13.711	21.445	21.514	21.422	13.841	21.524
4	25.470	24.249	25.451	25.346	15.739	25.882	25.458	25.337	15.913	25.550
5	29.295			29.199						29.258

6	33.315	33.091	33.448

Table S6. Dihedral angles along molecular backbones.

PBE0-D3/cc-pVDZ optimized model junction geometries, in ° (see Figure S8 for notations).

Core	*n*	γ1	γ2	γ3	γ4	γ5	γ6	γ7
THIO	1	-159.336	153.322					
	2	-161.705	-179.969	161.683				
	3	-163.366	157.606	-164.090	-166.119			
	4	-161.086	165.300	-179.587	-165.425	161.057		
	5	159.885	164.120	-166.171	167.078	-165.975	-162.888	
	6	161.660	-162.485	168.965	176.017	-167.233	162.925	-161.402
TDO	1	-164.325	159.941					
	2	-167.388	179.998	167.383				
	3	-165.077	171.101	-177.603	-168.720			
	4	-169.039	175.524	179.096	-174.837	168.057		
	5	164.180	-175.145	174.054	-178.982	175.995	166.606	
	6	-164.437	-177.719	-178.394	-178.858	-176.865	174.986	-164.656
TDOA	1	-179.207	-176.032					
	2	178.232	179.942	-178.245				
	3	176.531	179.053	177.210	179.838			
	4	-175.255	-173.754	-172.070	-172.975	179.214		
TCLO	1	164.744	161.281					
	2	172.961	-162.565	157.823				
	3	-156.763	161.625	-161.324	168.525			
	4	-158.638	160.353	-161.969	162.963	-172.961		
PEDOT	1	-175.606	171.176					
	2	-173.664	-177.878	175.887				
	3	-174.985	177.320	-179.444	179.341			
	4	-174.184	179.977	-179.988	-179.950	174.204		
	5	173.651	-176.730	178.649	-178.362	-179.006	179.978	
	6	173.980	179.845	179.601	-179.723	-177.445	-178.215	-173.807
PYR	1	-174.138	172.246					
	2	-175.198	-179.854	175.613				
	3	-176.169	178.210	-179.568	179.182			
	4	-175.354	179.716	-179.970	-179.784	175.614		
THIA	1	-179.997	-178.397					
	2	179.424	179.965	-179.406				
	3	179.564	-179.397	179.591	-179.431			
	4	179.931	179.951	-179.990	-179.978	-179.926		

THIOQ	1	179.349	176.458			
	2	-179.011	179.729	179.624		
	3	179.843	178.723	-178.751	177.094	
	4	-179.069	-179.595	179.908	-177.717	178.228
TCp	1	-177.929	177.150			
	2	-177.383	-180.000	177.394		
	3	-178.432	-179.251	179.979	-174.097	
	4	-175.847	175.480	-177.083	177.664	-179.585
Cp	1	179.565	-173.042			
	2	-174.142	-179.993	174.128		
	3	-172.332	178.827	-178.583	-177.074	
	4	176.370	-172.781	-179.570	-176.098	-176.539

Table S7. Positions of the transmissions peaks.

PBE/DZP+ZORA spectra on an absolute scale and relative to computed E_F, in eV.

n	PEDOT	Cp	TCp	THIO	THIA	PYR	THIOQ	TCLO	TDOA	TDO
Absolute										
Peak corresponding to the HOMO resonance										
1	-5.90	-5.83	-6.03	-6.25	-6.54	-6.06	-5.42	-6.39	-6.70	-6.38
2	-5.48	-5.31	-5.66	-6.01	-6.45	-5.70	-5.28	-6.12	-6.61	-6.14
3	-5.13	-5.22	-5.43	-5.83	-6.25	-5.43	-5.18	-5.98	-6.32	-6.01
4	-4.93	-5.11	-5.20	-5.71	-6.16	-5.29	-5.05	-5.87	-6.15	-5.87
5	-4.76			-5.58						-5.81
6	-4.65			-5.52						-5.81
Peak corresponding to the LUMO resonance										
1	-3.73	-4.22	-4.09	-3.89	-3.67	-4.66	-4.77	-4.68	-4.33	-4.58
2	-3.65	-4.10	-4.18	-4.00	-3.69	-4.68	-4.77	-4.80	-4.79	-4.78
3	-3.53	-4.09	-4.12	-3.95	-3.72	-4.70	-4.77	-4.86	-4.88	-4.85
4	-3.47	-4.08	-4.11	-3.98	-3.79	-4.69	-4.77	-4.91	-4.94	-4.89
5	-3.40			-3.94						-4.94
6	-3.37			-3.96						-5.00
Relative										
Peak corresponding to the HOMO resonance										
1	-1.03	-0.96	-1.14	-1.57	-1.62	-1.18	-0.49	-1.46	-1.75	-1.32
2	-0.64	-0.47	-0.82	-1.16	-1.54	-0.86	-0.36	-1.17	-1.63	-1.20
3	-0.35	-0.40	-0.58	-0.97	-1.34	-0.60	-0.29	-0.98	-1.28	-1.04
4	-0.20	-0.34	-0.37	-0.89	-1.28	-0.49	-0.16	-0.84	-1.07	-0.86
5	-0.08			-0.74						-0.77
6	-0.03			-0.72						-0.73
Peak corresponding to the LUMO resonance										
1	1.14	0.65	0.79	0.79	1.26	0.22	0.16	0.25	0.63	0.48
2	1.19	0.74	0.65	0.86	1.22	0.15	0.14	0.16	0.19	0.17
3	1.26	0.73	0.73	0.90	1.20	0.14	0.11	0.14	0.16	0.10
4	1.25	0.68	0.72	0.85	1.08	0.11	0.11	0.13	0.15	0.12
5	1.28			0.91						0.10
6	1.25			0.85						0.07

Table S8. Fermi levels of the studied junctions.

PBE/DZP+ZORA level of theory, in eV.

n	PEDOT	Cp	TCp	THIO	THIA	PYR	THIOQ	TCLO	TDOA	TDO
1	-4.87	-4.87	-4.89	-4.68	-4.93	-4.88	-4.93	-4.93	-4.95	-5.06
2	-4.84	-4.83	-4.84	-4.85	-4.91	-4.84	-4.92	-4.95	-4.99	-4.94
3	-4.79	-4.81	-4.85	-4.86	-4.91	-4.84	-4.88	-5.00	-5.04	-4.96
4	-4.72	-4.77	-4.83	-4.82	-4.87	-4.81	-4.88	-5.04	-5.09	-5.01
5	-4.68			-4.84						-5.04
6	-4.62			-4.80						-5.07

Table S9. Values of transmission at the mid-gap between the transmission peaks.

PBE/DZP+ZORA level, in units of G_0.

Core \ *n*	1	2	3	4	5	6
THIO	1.37×10^{-04}	1.43×10^{-04}	2.40×10^{-05}	2.44×10^{-05}	8.98×10^{-07}	6.62×10^{-06}
TDO	6.02×10^{-04}	8.39×10^{-04}	2.24×10^{-04}	4.92×10^{-04}	3.13×10^{-05}	3.67×10^{-04}
TDOA	1.14×10^{-03}	2.36×10^{-03}	1.01×10^{-03}	8.16×10^{-03}		
TClO	2.49×10^{-04}	7.63×10^{-04}	9.42×10^{-05}	5.78×10^{-04}		
PEDOT	2.67×10^{-04}	8.15×10^{-04}	3.45×10^{-05}	6.58×10^{-05}	8.44×10^{-06}	1.76×10^{-05}
PYR	5.97×10^{-04}	8.51×10^{-04}	2.51×10^{-04}	7.90×10^{-04}		
THIA	9.67×10^{-04}	5.71×10^{-04}	1.48×10^{-04}	1.81×10^{-04}		
THIOQ	3.10×10^{-02}	6.94×10^{-02}	8.71×10^{-02}	1.86×10^{-01}		
TCp	1.59×10^{-04}	5.33×10^{-04}	7.17×10^{-05}	8.34×10^{-05}		
Cp	1.93×10^{-03}	8.27×10^{-03}	5.95×10^{-04}	2.48×10^{-03}		

Table S10. Values of transmission at the computed Fermi level.

PBE/DZP+ZORA level, in units of G_0.

Core \ *n*	1	2	3	4	5	6
THIO	1.49×10^{-04}	1.62×10^{-04}	2.49×10^{-05}	2.62×10^{-05}	8.81×10^{-07}	5.57×10^{-06}
TDO	8.92×10^{-04}	5.02×10^{-03}	3.23×10^{-03}	$3.71\text{E}\times10^{-03}$	3.44×10^{-04}	6.65×10^{-03}
TDOA	1.53×10^{-03}	6.25×10^{-03}	4.00×10^{-03}	1.86×10^{-02}		
TClO	1.36×10^{-03}	4.08×10^{-03}	6.39×10^{-04}	3.29×10^{-03}		
PEDOT	2.53×10^{-04}	2.93×10^{-04}	1.29×10^{-04}	4.78×10^{-04}	8.91×10^{-04}	$3.65\text{E}\times10^{-03}$
PYR	1.01×10^{-03}	2.21×10^{-03}	7.07×10^{-04}	2.20×10^{-03}		
THIA	1.15×10^{-03}	5.68×10^{-04}	1.64×10^{-04}	2.26×10^{-04}		
THIOQ	7.90×10^{-02}	1.09×10^{-01}	1.33×10^{-01}	2.01×10^{-01}		
TCp	1.94×10^{-04}	5.56×10^{-04}	6.05×10^{-05}	1.02×10^{-04}		
Cp	2.02×10^{-03}	5.97×10^{-03}	6.39×10^{-04}	1.22×10^{-03}		

Computed transmission spectra

PBE/DZP+ZORA level, post-SCF NEGF+DFT approach. Small peaks near the E_F are metal-induced peaks (in particular due to Au_8 clusters). The transmission is plotted on a logarithmic scale.

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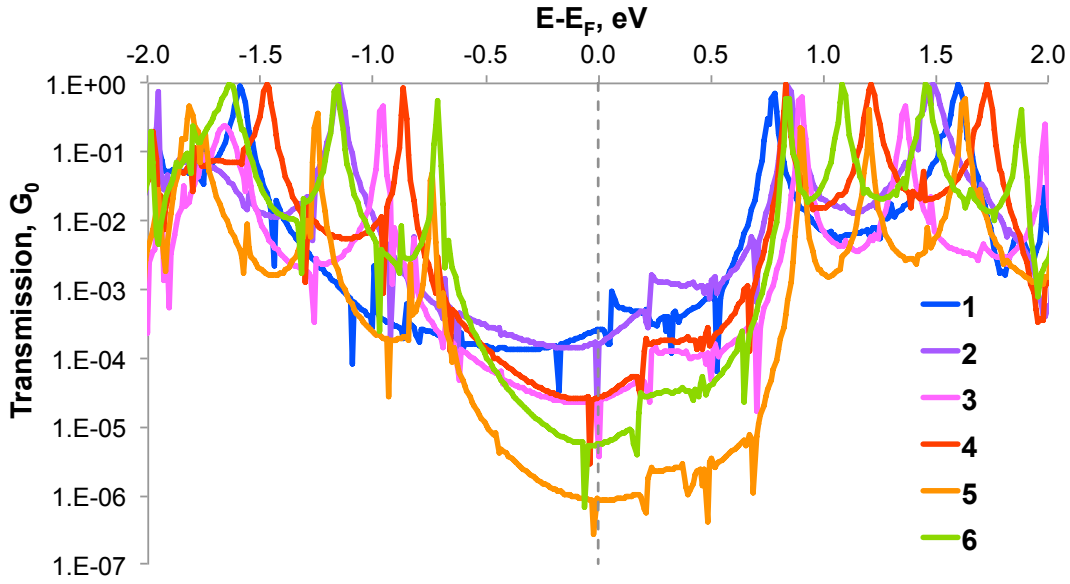
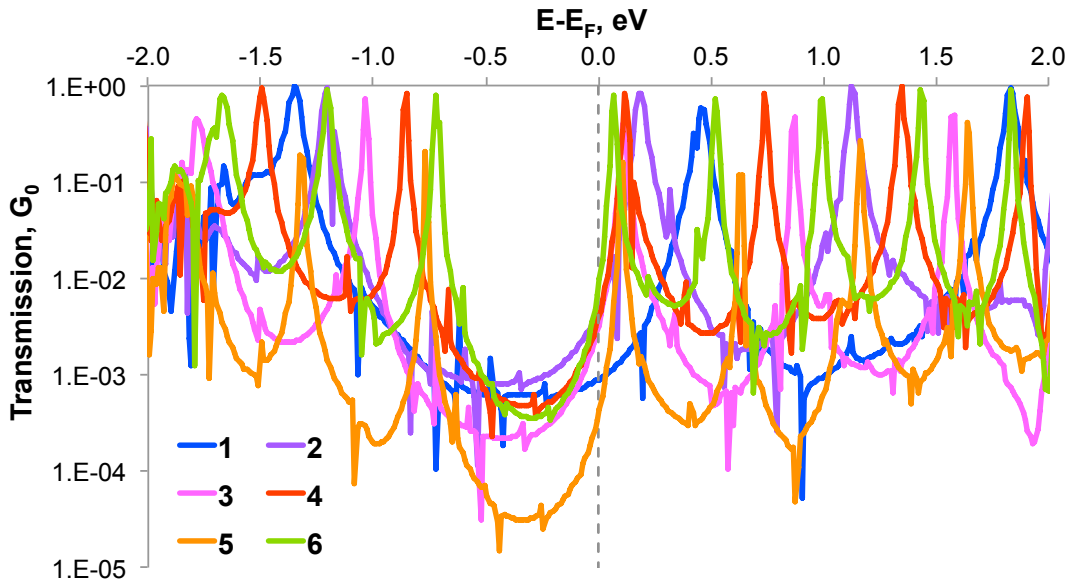
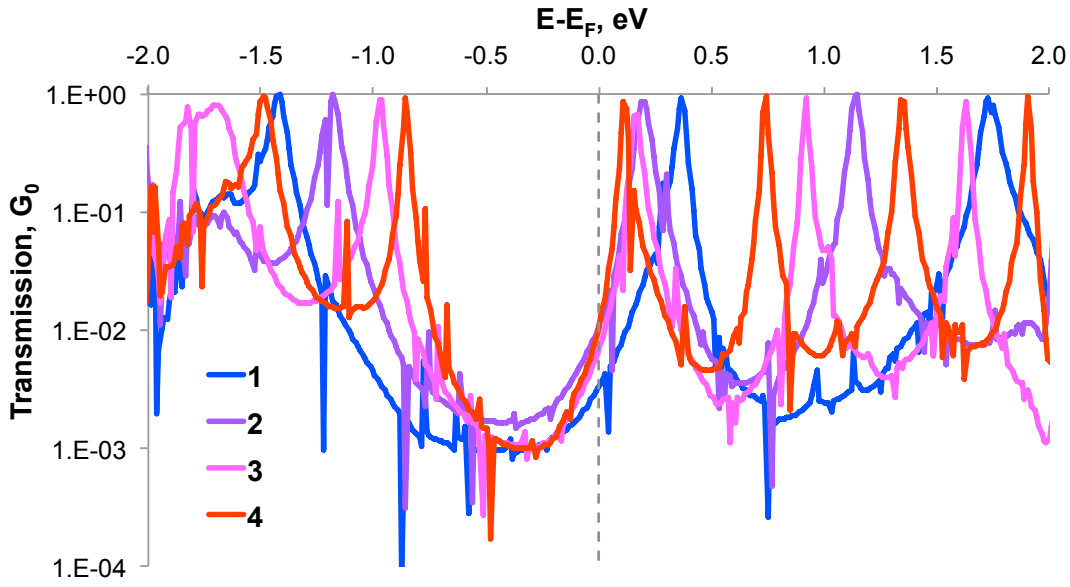


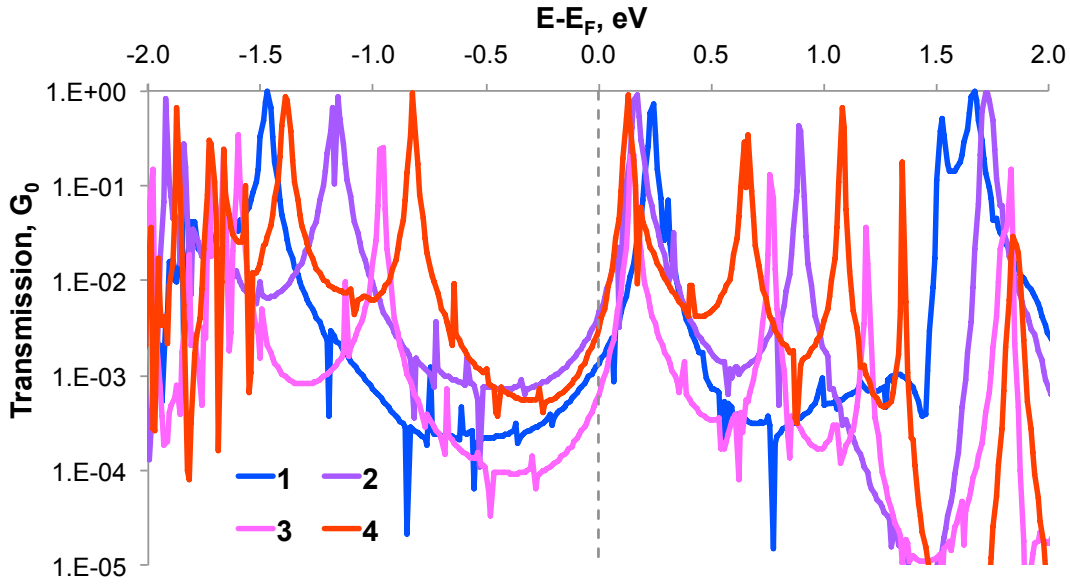
TDO_n



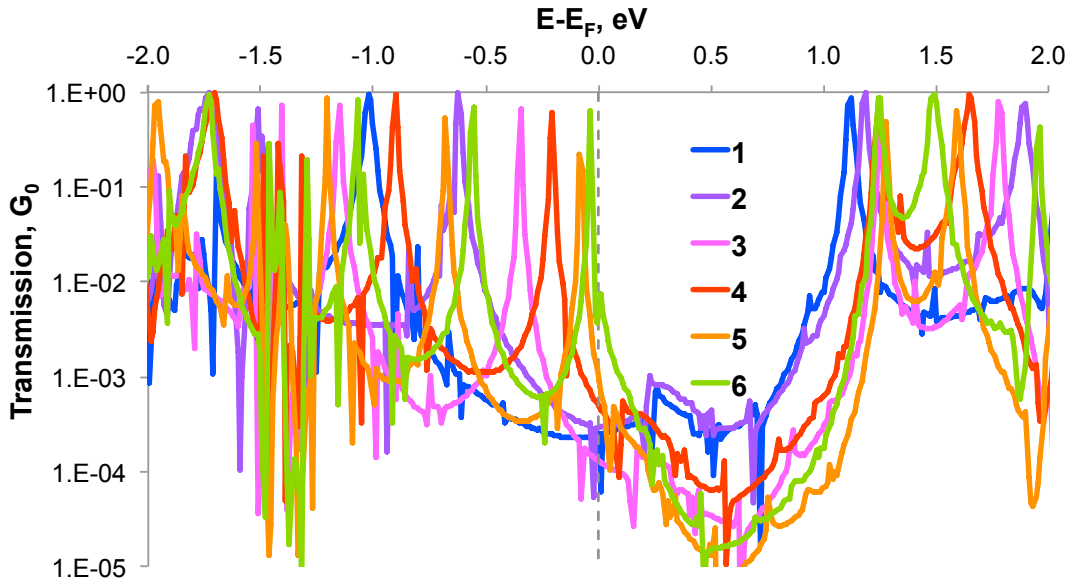
TDO_n ($-SCH_3$ linkers)



$TCLO_n$



PEDOT$_n$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-1.0
-0.5
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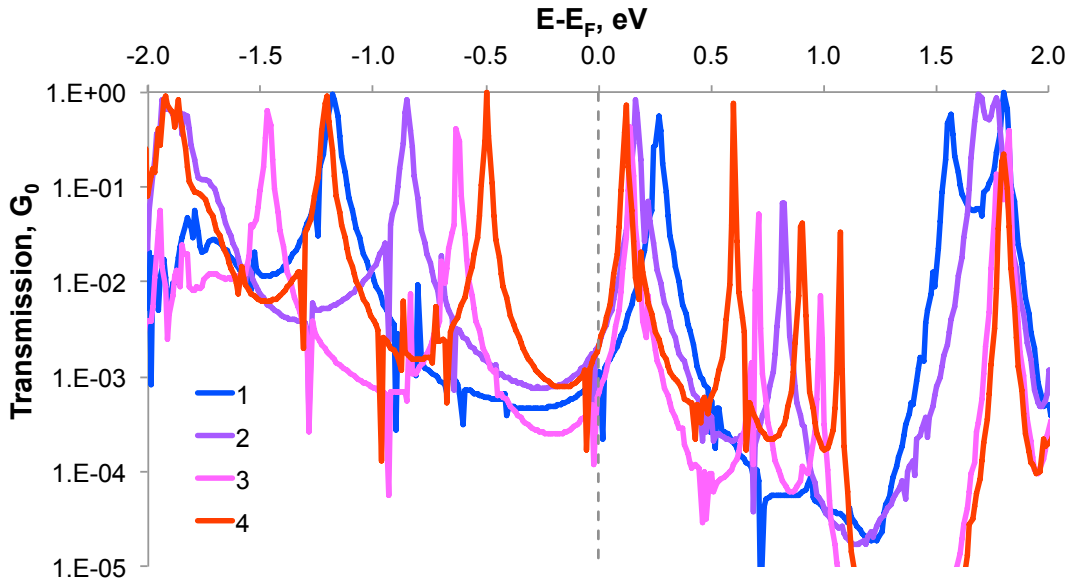
0.5
1.0
1.5
2.0
Transmission, G$_0$
1.E+00
1.E-01
1.E-02
1.E-03
1.E-04
1.E-05
1
2
3
4
5
6

PYR$_n$


E-E$_F$, eV
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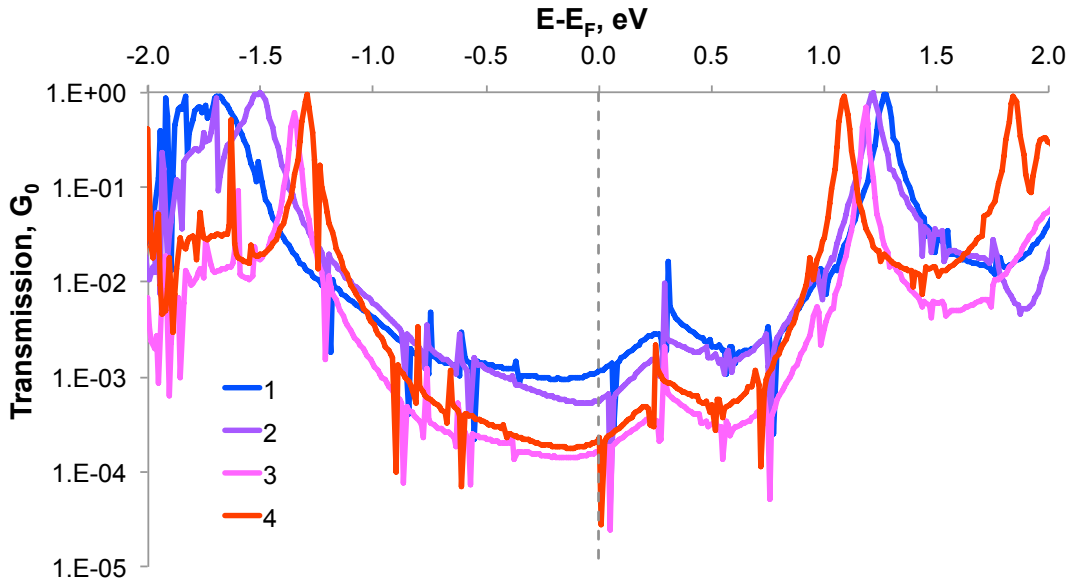
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
Transmission, G$_0$
1.E+00
1.E-01
1.E-02
1.E-03
1.E-04
1.E-05
1
2
3
4

THIA$_n$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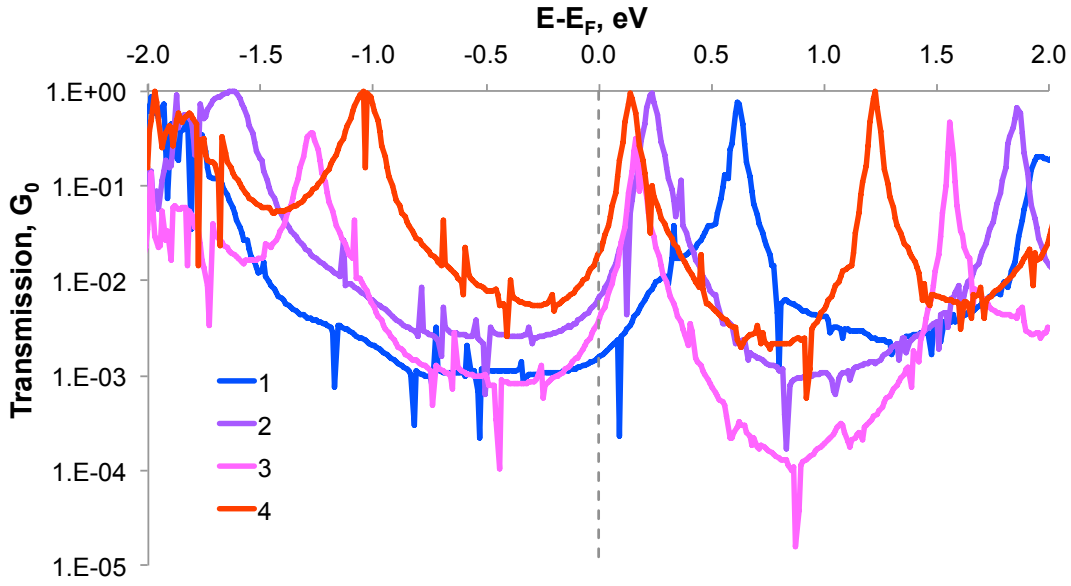
-0.5
0.0
0.5
1.0
1.5
2.0
1.E+00
1.E-01
1.E-02
1.E-03
1.E-04
1.E-05
Transmission, G$_0$
1
2
3
4

TDOA$_n$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1.0
1.5
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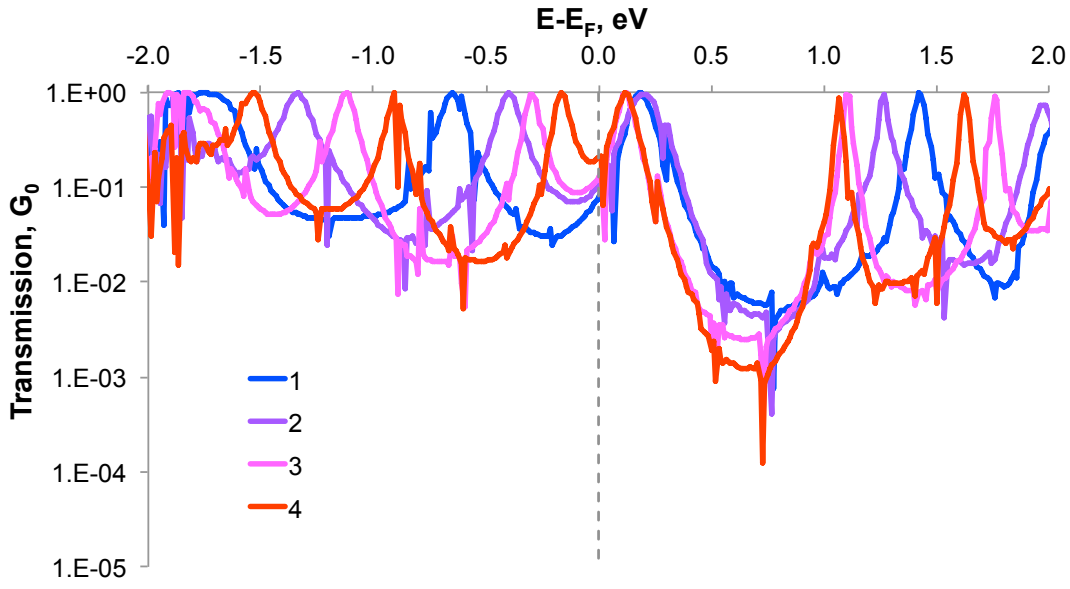
1.E+00
1.E-01
1.E-02
1.E-03
1.E-04
1.E-05
Transmission, G$_0$
1
2
3
4

THIOQ$_n$


E-E$_F$, eV
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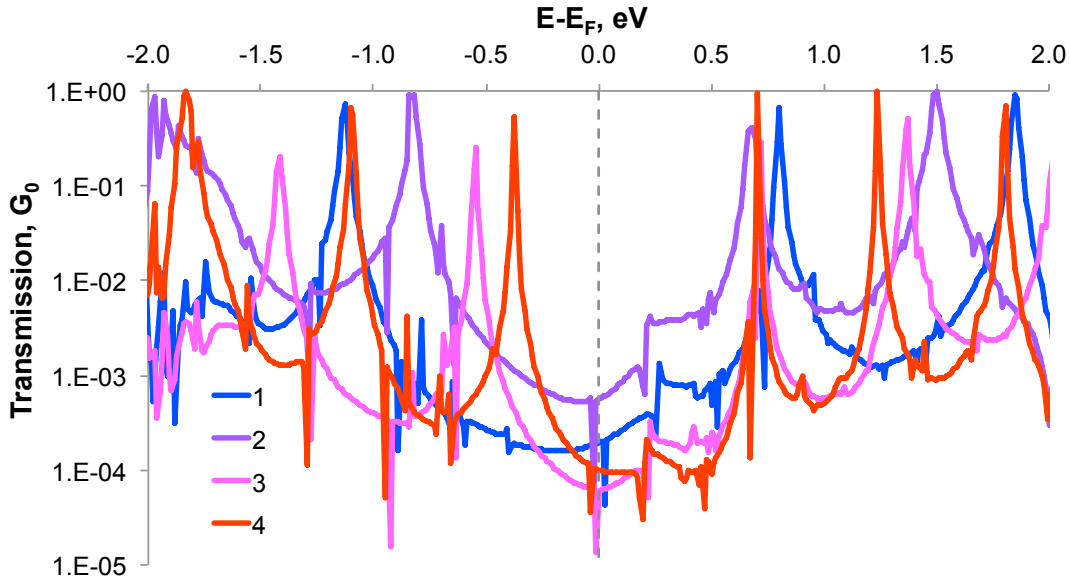
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
Transmission, G$_0$
1.E+00
1.E-01
1.E-02
1.E-03
1.E-04
1.E-05
1
2
3
4

TCp$_n$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-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
Transmission, G$_0$
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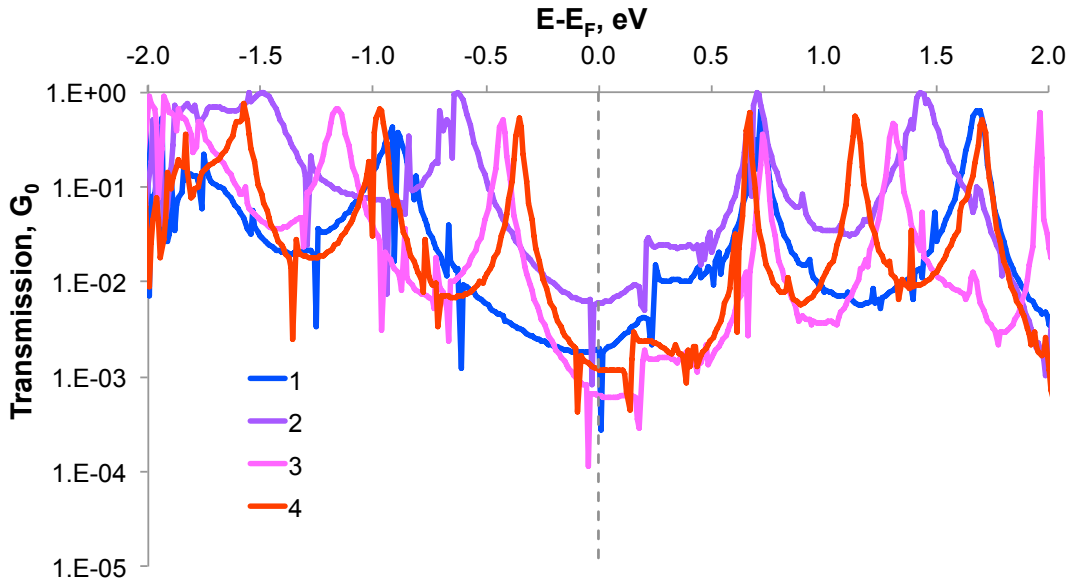
1.E-02
1.E-03
1.E-04
1.E-05
1
2
3
4

Cp_n


E-E$_F$, eV
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-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
1.E+00
1.E-01
1.E-02
1.E-03
1.E-04
1.E-05
Transmission, G$_0$
1
2
3
4

Optimized geometries

Optimized geometries of the isolated molecules and molecules bridging two 'frozen' Au_8 clusters, PBE0-D3/cc-pVDZ level of theory, in the form of Gaussian archive entries.

PEDOT1.pbe0

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2451519,0.0695571804\C,3.1363170355,0.6676232202,0.1359479376\S,5.2331
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9,-0.0935753809\S,-8.4287973197,1.32652953,-0.2387710244\H,-8.56201889
23,1.6184248631,-1.5594917904\H,-3.9376502793,-0.8493421678,-0.0349933
82\H,-6.5616767396,-1.1006705546,-0.1537773981\C,-2.4134990269,3.10455
50925,-0.0651327907\O,-3.2414599431,4.1764212486,-0.1122352775\C,-2.58
29096273,5.3767449784,0.2820420324\C,-1.2326006628,5.4907610779,-0.388
3804955\O,-0.3736456089,4.4319531768,0.0254709611\H,-2.4639256768,5.38
90396374,1.3795960369\H,-3.2403369368,6.2019853591,-0.0195167103\H,-0.
7310861201,6.4238637261,-0.1021279183\H,-1.3502187716,5.4629586466,-1.
4858150511\\Version=ES64L-G09RevD.01\HF=-2679.5318202\RMSD=4.965e-09\R
MSF=5.561e-06\Dipole=-0.0747922,0.8431781,-0.0079468\Quadrupole=-13.63
75483,18.8527368,-5.2151885,-5.1541581,9.100857,0.5890949\PG=C01 [X(C1
4H10O2S5)]\\@

PEDOT2.pbe0

1\1\GINC-LCMD08\FOpt\RPBE1PBE\Gen\C20H14O4S6\ROOT\03-Jun-2016\0\\#PBE1
PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersi
on=GD3BJ Nosymm\\DXN2.pbe0.freq\\0,1\C,-0.6962111776,-0.1731691627,-0.
1130072366\S,-1.9902864611,1.006207324,-0.0963639151\C,-3.2220771269,-
0.227774636,-0.2060320512\C,-1.2243166594,-1.4466099587,-0.1924064838\
C,-2.6398056629,-1.4771468499,-0.2485024058\O,-3.3440252532,-2.6321984
6,-0.3419719561\O,-0.4643243298,-2.5714783321,-0.2178764935\C,-4.61929
20183,0.1099415515,-0.2331266934\S,-5.8591540186,-1.1155136266,-0.2734
50695\C,-7.119119116,0.0823083812,-0.2396370837\C,-5.1858973961,1.3720
721063,-0.219346837\C,-6.5996134327,1.3541797485,-0.2229920296\S,-8.81
65326687,-0.3728397044,-0.3484409299\H,-8.9865956684,-0.7436468622,0.9
481675712\H,-7.2290278717,2.243070632,-0.211869918\H,-4.5898540451,2.2
846546034,-0.2010412536\C,7.109921289,-0.0499344911,-0.081154629\S,5.8
492600644,1.1465930478,-0.0296367652\C,4.6100796588,-0.0793306384,-0.0
728618491\C,6.5911121158,-1.3219749716,-0.1066546574\C,5.1774377838,-1
.3408267676,-0.1042685461\S,8.8077507291,0.4050326367,0.0208985329\H,8
.9665843482,0.7968388884,-1.2709594883\H,4.5819303868,-2.2536070119,-0
.1288581049\H,7.2210471608,-2.2102582173,-0.1300558548\C,3.2123696966,

0.2573543012,-0.0719872319\S,1.9791441184,-0.9776456735,-0.1466536357\
C,0.6849113383,0.1994679819,-0.071228289\C,2.6302918723,1.5052704447,0
.0023459767\C,1.2137282236,1.4726954035,0.0074543847\O,0.4534101021,2.
594613401,0.0871206332\O,3.3355732044,2.6619199028,0.0641854703\C,-2.5
513509649,-3.76968722,-0.0169781827\C,-1.2004870684,-3.6936260975,-0.6
929197327\C,1.2040057905,3.7652241442,-0.2185114814\C,2.5324934968,3.7
521244664,0.5046199662\H,-3.1135733223,-4.6463053329,-0.3632751546\H,-
2.4224737443,-3.8297340155,1.078039479\H,-0.5971700385,-4.5803787763,-
0.4603607603\H,-1.3280257199,-3.6166362395,-1.7871124996\H,0.592163639
2,4.6175107424,0.1035789028\H,1.3673026518,3.8261944157,-1.3089757265\
H,3.1042710808,4.6636596846,0.288738651\H,2.3694450134,3.6747892376,1.
5939490038\\Version=ES64L-G09RevD.01\HF=-3458.6994263\RMSD=6.593e-09\R
MSF=1.307e-05\Dipole=0.0024977,0.0063547,0.0049401\Quadrupole=-24.1307
565,28.80699,-4.6762335,4.587385,-12.3078921,0.1872702\PG=C01 [X(C20H1
4O4S6)]\\@

PEDOT3.pbe0

1\1\GINC-LCMD09\FOpt\RPBE1PBE\Gen\C26H18O6S7\ROOT\03-Jun-2016\0\\#PBE1
PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersi
on=GD3BJ Nosymm\\DXN3.pbe0.freq\\0,1\C,-2.6569088881,-0.1387450877,-0.
3576455145\S,-3.9190070123,1.0668998827,-0.2119443975\C,-5.1866879342,
-0.122064315,-0.3925520555\C,-3.2221543646,-1.3872708566,-0.5301849573
\C,-4.6386618566,-1.3777514002,-0.5506003974\O,-5.3766876783,-2.502983
617,-0.7211507443\O,-2.4941800038,-2.5262817344,-0.6679273589\C,-6.573
9913063,0.2524251894,-0.3623095841\S,-7.8482155109,-0.9344313941,-0.45
87292591\C,-9.0739800233,0.2904096669,-0.3115863248\C,-7.1056407509,1.
5247547615,-0.2462119143\C,-8.519034438,1.5437877746,-0.2179322504\S,-
10.7850687335,-0.112048868,-0.4118168184\H,-10.9414077267,-0.555416462
4,0.8637432288\H,-9.1231772351,2.4458888318,-0.1303961034\H,-6.4846228
878,2.4181853333,-0.1792435242\C,9.0683516893,0.2574992354,-0.23965654
69\S,7.8390843464,-0.959706567,-0.4169578381\C,6.5682896616,0.21550146
11,-0.2043716138\C,8.5169470526,1.494160732,-0.0063810209\C,7.10347293
1,1.472930959,0.013477995\S,10.7780152615,-0.1630109302,-0.24597838\H,
10.9378087898,-0.2517582414,-1.5931344607\H,6.484751585,2.3552263867,0
.1780075917\H,9.1236975892,2.3862229221,0.1436630288\C,1.2603690952,0.
1870552346,-0.2740069928\S,-0.0042690649,-1.0107884113,-0.4559682103\C
,-1.2662730166,0.1935842029,-0.3017396719\C,0.7051155203,1.4412664568,
-0.1045722886\C,-0.7082121282,1.4448617313,-0.1211490411\O,-1.44173338
17,2.5788647031,0.0235967797\O,1.4408255044,2.5695937273,0.0700117306\
C,5.179951833,-0.1502570083,-0.2718853566\S,3.9147145686,1.0450554627,
-0.1191592249\C,2.6500995261,-0.1519397016,-0.3087865543\C,4.629181096
2,-1.4003040391,-0.4613963508\C,3.2126618998,-1.4015140832,-0.48336623
99\O,2.482541695,-2.5329976482,-0.6644751978\O,5.3650281038,-2.5305571
865,-0.6069458667\C,-4.6078175679,-3.683401084,-0.5161199417\C,-3.2719
509477,-3.5827693738,-1.2183814348\C,-0.6666210731,3.6437221428,0.5626
607543\C,0.6670353561,3.7448482792,-0.1442485368\C,3.2589961266,-3.703
1313606,-0.4352776733\C,4.5950106995,-3.6037249433,-1.1374419729\H,-5.
2020172291,-4.5125168472,-0.9212571461\H,-4.4538096041,-3.8414183205,0
.5659183114\H,-3.4246443409,-3.4082388265,-2.2982051555\H,-2.688404014
5,-4.5018909125,-1.0795871407\H,-0.5096036544,3.4780012925,1.643150586
5\H,-1.2551999647,4.5588422865,0.4188411456\H,1.2575131252,4.580539965
1,0.2527205826\H,0.5096961797,3.8927773685,-1.2272809555\H,2.673645334
3,-4.5446223348,-0.8276006431\H,3.4118142538,-3.8410509154,0.649822586

1\H,4.4415491053,-3.4493746738,-2.2200811383\H,5.1873544088,-4.5146188
453,-0.982610522\\Version=ES64L-G09RevD.01\HF=-4237.8664954\RMSD=7.961
e-09\RMSF=3.487e-06\Dipole=-0.0002137,-0.7506219,-0.1137866\Quadrupole
=-38.4656024,41.0197206,-2.5541182,2.2856894,-16.184347,6.739614\PG=C0
1 [X(C26H18O6S7)]\\@

PEDOT4.pbe0

1\1\GINC-LCMD09\FOpt\RPBE1PBE\Gen\C32H22O8S8\ROOT\03-Jun-2016\0\\#PBE1
PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersi
on=GD3BJ Nosymm\\DXN4.pbe0.freq\\0,1\C,-0.7265148868,-0.1523587103,0.1
133196534\S,-1.9712090191,1.0688094492,0.281189795\C,-3.2547453374,-0.
1093936049,0.1001218721\C,-1.304795897,-1.3944615683,-0.0701726618\C,-
2.7177514448,-1.3703063141,-0.078572948\O,-3.4713025318,-2.4869420244,
-0.254950164\O,-0.589062221,-2.5396663099,-0.2242341747\C,-8.563023816
5,-0.0643083976,0.0628012627\S,-9.816340766,1.1288125883,0.2804187821\
C,-11.063595526,-0.0715414512,0.1118925638\C,-9.117058387,-1.314561221
8,-0.1498542891\C,-10.5305805241,-1.3160535523,-0.1221522938\S,-12.767
1290188,0.3726815615,0.1274205067\H,-12.9186884411,0.4649900336,1.4753
623362\H,-11.1504296342,-2.1999439958,-0.2670892798\H,-8.5115403391,-2
.2056938634,-0.315841067\C,11.0057485931,0.0796358945,0.1665497206\S,9
.7584869855,-1.1205736572,-0.0029041078\C,8.5051678313,0.0725114553,0.
2149094509\C,10.4727233263,1.3240806775,0.4009814871\C,9.0591986856,1.
3226485144,0.4282248751\S,12.7092776292,-0.3645950507,0.1514373014\H,1
2.861404492,-0.4557967568,-1.1965015776\H,8.4536598645,2.2137281312,0.
5944215169\H,11.0925830747,2.2078675767,0.5465104654\C,3.1969017109,0.
1177702822,0.1763153955\S,1.9133674628,-1.0604178241,-0.0048910632\C,0
.6686707536,0.1607710182,0.1627852831\C,2.6599036085,1.3787138122,0.35
48048776\C,1.246950865,1.4028805255,0.3462190857\O,0.5312306423,2.5481
268137,0.5001211147\O,3.4134679086,2.4953386405,0.5311341789\C,7.11176
67601,-0.2740062217,0.1551890791\S,5.8636836217,0.9382547981,0.3181714
088\C,4.5812488031,-0.240620448,0.1327303836\C,6.5422923227,-1.5157347
28,-0.0339094122\C,5.1258806798,-1.49735973,-0.0482419134\O,4.37925923
6,-2.6186293813,-0.2286132274\O,7.2617764668,-2.6558259688,-0.18539965
95\C,-4.6390925403,0.2489604268,0.1439538575\S,-5.9215261035,-0.929960
7106,-0.041218488\C,-7.1696138393,0.2822542644,0.12203276\C,-5.1837235
964,1.5056947357,0.3249784959\C,-6.6001368405,1.5240121293,0.310948195
4\O,-7.3196241732,2.6640833784,0.4625788666\O,-4.4370919027,2.62698869
09,0.5051184647\C,-6.5320168535,3.7261693864,0.9892625339\C,-5.1983698
302,3.8074238911,0.2800713598\C,-2.7138853429,-3.67465789,-0.054214506
8\C,-1.3826315104,-3.5871187108,-0.7678360725\C,1.324741471,3.59543442
36,1.0440822298\C,2.6560734327,3.6831107123,0.3306257516\C,5.140430367
7,-3.7990678495,-0.003240831\C,6.4742407812,-3.7179353142,-0.712143994
5\H,-6.37474805,3.5692230274,2.0710031774\H,-7.1126097066,4.6452437102
,0.8380794458\H,-4.5996221981,4.6408943224,0.6693733416\H,-5.355250196
8,3.9478746305,-0.8041989704\H,-3.3189429563,-4.4986351926,-0.45392220
99\H,-2.5521826819,-3.8332978791,1.0267420385\H,-1.5440299131,-3.41026
5419,-1.8460828735\H,-0.8074678991,-4.5125644639,-0.6354831052\H,1.486
0087995,3.4183148652,2.1223063851\H,0.7496151205,4.5209233949,0.911882
2646\H,3.2611167204,4.5069777155,0.7305828548\H,2.4944737445,3.8420094
139,-0.7503079471\H,4.5417432165,-4.6325625053,-0.3925840652\H,5.29705
85178,-3.9393981459,1.0810813769\H,6.3172092117,-3.5610961557,-1.79393
41744\H,7.0547712178,-4.6370138742,-0.5607407188\\Version=ES64L-G09Rev
D.01\HF=-5017.0334242\RMSD=7.854e-09\RMSF=2.510e-06\Dipole=-0.0001008,

0.0002741,0.000261\Quadrupole=-54.427468,54.8344721,-0.4070041,-6.0517
44,-20.2936105,9.8678254\PG=C01 [X(C32H22O8S8)]\\@

PEDOT5.pbe0

1\1\GINC-NODE02\FOpt\RPBE1PBE\Gen\C38H26O10S9\GRYNOVA\27-Feb-2017\0\\#
PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDisp
ersion=GD3BJ Nosymm\\DXN5.pbe0.freq\\0,1\C,-0.6724952312,-0.1699064745
,0.1446171858\S,-1.9249328683,1.0406511375,0.3321009796\C,-3.201524053
8,-0.1407197186,0.1220339222\C,-1.2434098371,-1.411206238,-0.066309329
1\C,-2.6563621066,-1.3945877292,-0.0799648346\O,-3.4030049953,-2.51164
20414,-0.2817545195\O,-0.5207249994,-2.549617581,-0.2400784992\C,-8.50
95577161,-0.1271908581,0.0542511731\S,-9.7723965001,1.0498189511,0.302
6770784\C,-11.0104900559,-0.152830408,0.0877679452\C,-9.0538033574,-1.
3737178934,-0.2016276332\C,-10.4673949997,-1.385512455,-0.1828156407\S
,-12.7169772161,0.2795769502,0.1067606472\H,-12.8797686372,0.319834918
2,1.455962889\H,-11.0802499849,-2.2683439231,-0.3603953477\H,-8.441074
016,-2.2547145639,-0.3932687245\C,11.0896207331,0.0139494282,0.2285279
906\S,9.8069396001,-1.160122331,0.0538540469\C,8.5591099199,0.04957952
74,0.274696467\C,10.5561817645,1.2677672178,0.4415551273\C,9.140056817
3,1.2875210437,0.4716659879\C,12.4722263506,-0.3720931626,0.1633665287
\O,8.425997836,2.4253618334,0.6801690726\O,11.3081148505,2.3850704167,
0.6057397412\C,3.2505818236,0.1183284329,0.234344792\S,1.9728641885,-1
.0624457452,0.0267606503\C,0.7205795003,0.1494704785,0.2068927908\C,2.
7053026987,1.3736199007,0.4298999675\C,1.2924151107,1.3908834871,0.413
9634906\O,0.5694663526,2.5298851886,0.582562772\O,3.4519239949,2.49234
50403,0.6281135819\C,7.1652044764,-0.2682027437,0.2252808798\S,5.91430
08419,0.9461057096,0.3980202512\C,4.6363149108,-0.2346306344,0.1928386
853\C,6.5932140319,-1.5099773375,0.0233616297\C,5.1804506805,-1.491229
9732,0.0018017827\O,4.4340248131,-2.6105318993,-0.1941694747\O,7.31606
60405,-2.6493004536,-0.1367687633\C,-4.5880749464,0.2083415496,0.16738
08218\S,-5.8621366085,-0.9736256076,-0.0531829915\C,-7.1189806148,0.22
64631296,0.132536751\C,-5.1418554879,1.4567294377,0.3765398885\C,-6.55
82598131,1.466522168,0.3557756837\O,-7.2860164615,2.5979462166,0.53157
68527\O,-4.4033621225,2.5784510134,0.5874622258\C,-6.5075144686,3.6531
865651,1.0848186085\C,-5.1711777442,3.7582449486,0.3838661973\C,-2.639
8393849,-3.6989733508,-0.1019410709\C,-1.3062947037,-3.5897007065,-0.8
082075313\C,1.3547338392,3.5738154484,1.1438219293\C,2.6891467653,3.67
72235012,0.438033463\C,5.1946202633,-3.7941456843,0.0124207809\C,6.531
931073,-3.7000731824,-0.6889584805\H,-6.3539176786,3.4737099919,2.1635
949778\H,-7.093378792,4.57165043,0.9511314577\H,-4.579945343,4.5872048
777,0.7937832126\H,-5.3241453777,3.9208634707,-0.6978986378\H,-3.23877
47951,-4.5180116362,-0.5206145058\H,-2.4814513805,-3.8784143056,0.9762
434387\H,-1.4646984669,-3.3918424926,-1.8833029808\H,-0.7267052367,-4.
5146591605,-0.6926295532\H,1.5122433377,3.3835071109,2.2204175975\H,0.
7752743762,4.4980015424,1.0211666811\H,3.2870748734,4.5000366359,0.850
9262065\H,2.5310358467,3.8488082668,-0.6416520375\H,4.5978933792,-4.62
08913009,-0.3941663196\H,5.3475467788,-3.954201089,1.0945788815\H,6.37
96244888,-3.5217041358,-1.7682067949\H,7.1108085903,-4.622691642,-0.55
30803939\C,12.9901420423,-1.6452723818,0.0011193505\C,14.4030962195,-1
.6780770623,-0.0339596506\C,14.9719720679,-0.4342968385,0.0967252134\S
,13.7594995423,0.7979831872,0.2889196414\S,16.6876303254,-0.0524555787
,0.1975930496\C,9.2171478273,3.5884708704,0.4704778276\C,10.5553751306
,3.4569017519,1.1631864499\H,12.3592318499,-2.5292971126,-0.092429805\

H,14.9972111755,-2.5831107467,-0.1540909219\H,16.8411197215,0.4272893312,-1.0652803399\H,8.6457597122,4.4300952864,0.8827552001\H,9.3669760505,3.7465445435,-0.6124476842\H,10.4055055403,3.2816607773,2.2431144356\H,11.1591878485,4.3629064652,1.0245875853\\Version=ES64L-G09RevD.01\HF=-5796.2003065\RMSD=5.083e-09\RMSF=5.331e-06\Dipole=0.0081774,0.7341737,0.1295035\Quadrupole=-70.6221903,68.7321962,1.8899941,7.7895378,-20.1845703,11.6645666\PG=C01 [X(C38H26O10S9)]\\@

PEDOT6.pbe0

1\1\GINC-NODE02\FOpt\RPBE1PBE\Gen\C44H30O12S10\GRYNOVA\27-Feb-2017\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersion=GD3BJ Nosymm\\DXN6.pbe0.freq\\0,1\C,-0.5777524412,-0.1699575934,0.1069531067\S,-1.8233693156,1.0352963381,0.3624228822\C,-3.1068039562,-0.1240661843,0.0822291298\C,-1.15581497,-1.3933317694,-0.1771285126\C,-2.5685800896,-1.3672146839,-0.1916211803\O,-3.3216542099,-2.4664853105,-0.4577780907\O,-0.4395207476,-2.5244951117,-0.4150427646\C,-8.4144137123,-0.0748074468,0.0050505929\S,-9.671366262,1.0942461267,0.3142866215\C,-10.9157398163,-0.0871125867,0.0282696535\C,-8.9650530305,-1.3015007727,-0.3228250342\C,-10.3787590713,-1.3058976293,-0.3091569251\S,-12.6199317444,0.3527850452,0.0637768718\H,-12.784701109,0.3362538661,1.4132354856\H,-10.9960334628,-2.173826636,-0.5376976099\H,-8.3567008338,-2.1739753713,-0.5616319478\C,11.1851249415,-0.0379991098,0.2167847503\S,9.9005971644,-1.2024759649,-0.0355029216\C,8.6561683785,-0.0055550003,0.2613777245\C,10.6480907533,1.2009309458,0.5111716972\C,9.235447575,1.2182174963,0.5412314632\C,12.5694063228,-0.3901376152,0.1387550156\O,8.5206302746,2.3408667889,0.8206819956\O,11.4027169544,2.3057322173,0.748426616\C,3.3471562787,0.090841138,0.2184763249\S,2.0633906271,-1.0684838155,-0.0607207833\C,0.8168516144,0.1369877205,0.1913444791\C,2.8079404566,1.3346651546,0.489738022\C,1.3952149992,1.3603479056,0.4740949344\O,0.677766621,2.4909695293,0.7095326764\O,3.5600232467,2.4362676047,0.7546145104\C,7.2612432467,-0.3139981251,0.1879440343\S,6.0152175988,0.8931473027,0.4349215552\C,4.7310351038,-0.2657024856,0.1556537077\C,6.6823229654,-1.5378336135,-0.0915389595\C,5.2697532206,-1.5103723793,-0.1126658326\O,4.5173160164,-2.6118853997,-0.3769889719\O,7.3992473516,-2.6701962193,-0.3201794263\C,-4.4913074927,0.2298205382,0.14643183\S,-5.7719035678,-0.9301066631,-0.1426352808\C,-7.0221587586,0.2652019334,0.1083328766\C,-5.0382449423,1.4675237193,0.4254379632\C,-6.4545016407,1.4871173334,0.4029660608\O,-7.1761089816,2.6112906357,0.6402149462\O,-4.2935579325,2.5716387112,0.6992801923\C,-6.3918775174,3.6322809147,1.2472590043\C,-5.0537495352,3.7647781443,0.5544969873\C,-2.5659808103,-3.6663552512,-0.3419607352\C,-1.2308861303,-3.5267650627,-1.0399189216\C,1.4684469755,3.4991974553,1.3259448423\C,2.8038233167,3.633279592,0.6272170768\C,5.2712596661,-3.8093840678,-0.2408041926\C,6.6096189208,-3.6803277639,-0.9347518126\H,-6.2410332989,3.397301166,2.3157283315\H,-6.9721239399,4.5598615164,1.1598431352\H,-4.4585632679,4.5683999399,1.006949634\H,-5.2037506142,3.9828353814,-0.5178906621\H,-3.1691577493,-4.4578622723,-0.8051623944\H,-2.4100304856,-3.9048983215,0.7250653575\H,-1.386979345,-3.2694798221,-2.1027656119\H,-0.6571174316,-4.4602919834,-0.9748767387\H,1.6245472478,3.2506771803,2.3908419534\H,0.8936063066,4.4315391853,1.2530830621\H,3.4053521308,4.4300506621,1.0836906956\H,2.6472921737,3.8628295747,-0.4419150603\H,4.6704857334,-4.6074902149,-0.6959300489\H,5.4229242651,-4.0340814286,0.8300305498\H,6.4581212909,-3.4367517274,-2.0014649104\H,7.182944975,-4.6130

575059,-0.8551533472\C,13.1147948596,-1.6240963629,-0.1590073141\C,14.
5307602999,-1.6485488757,-0.1263881661\C,15.0998645924,-0.4329411977,0
.1907215272\S,13.8513369144,0.7618079036,0.4528103058\C,16.4924262817,
-0.0979163965,0.3054675288\C,9.312087417,3.5142541185,0.6872597734\C,1
0.6491675012,3.338389103,1.3730868155\O,12.3687926571,-2.7213505707,-0
.4561232788\O,15.2508259481,-2.7707427973,-0.3772294271\H,8.7402308935
,4.3285128999,1.1508449165\H,9.4650102301,3.7406946594,-0.3830363884\H
,10.4961692871,3.0932641217,2.4390631416\H,11.2525676151,4.2520240333,
1.2952882707\C,17.044370355,1.1219862212,0.6556605713\C,18.4581367918,
1.1238622024,0.6464014128\C,18.9938557303,-0.0902618225,0.2907435492\S
,17.7481106908,-1.2643723328,-0.0185433316\S,20.6973050614,-0.53289596
52,0.2542290808\C,13.1243626262,-3.9188456233,-0.3240832282\C,14.46779
33413,-3.7799696042,-1.0052183237\H,16.4369499325,1.9915629592,0.90706
68563\H,19.0763052395,1.9867573805,0.8910354622\H,20.8658056227,-0.499
4300883,-1.0944578376\H,12.5301244036,-4.7137177548,-0.7929433335\H,13
.2659640926,-4.1535931992,0.745923443\H,14.3253100759,-3.5283508722,-2
.0710397696\H,15.0446350395,-4.710567994,-0.9278119289\\Version=ES64L-
G09RevD.01\HF=-6575.3670355\RMSD=5.121e-09\RMSF=3.099e-06\Dipole=-0.00
3173,0.0070626,-0.0082897\Quadrupole=-88.4172301,81.4972918,6.9199383,
-7.5097765,-27.0089152,19.6800766\PG=C01 [X(C44H30O12S10)]\\@

Cp1.pbe0

1\1\GINC-R01-NODE35\FOpt\RPBE1PBE\Gen\C15H14S2\GRYNOVA\07-Feb-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDis
persion=GD3BJ Nosymm\\Cp1.pbe0.freq\\0,1\C,-2.744707057,1.7549480905,-
0.0766831484\C,-1.4848264448,0.9330739251,-0.0195813719\C,-0.378569462
2,1.9509034387,0.0594626003\C,-2.3857902547,3.0756320194,-0.0338946695
\C,-0.9514727306,3.1945061934,0.0470756404\H,-0.4117669215,4.140844648
,0.0919943654\H,-3.0748880149,3.9202711731,-0.0571656115\C,1.012384094
,1.6238844275,0.1336861605\C,2.1177272078,2.6438367848,0.2233085684\C,
3.3623294716,1.8108261774,0.3368127046\C,1.5850881146,0.3826807344,0.1
576652438\C,3.0247111277,0.4967170829,0.285409371\S,4.9968171387,2.449
1167651,0.351412419\H,4.7253844239,3.5713489987,1.0632089158\H,3.71898
04578,-0.3414990629,0.3335873541\H,1.0466988645,-0.564039065,0.1091675
264\C,-6.4114202533,1.0049420642,-0.3659988448\C,-5.3213749928,2.02935
76903,-0.2306309494\C,-4.0625784137,1.2042402407,-0.1611304696\C,-5.86
13009802,-0.2361308192,-0.3428495075\C,-4.4224940121,-0.113643612,-0.2
141097962\S,-8.1289004903,1.3647148267,-0.3706754383\H,-8.0475352459,2
.5294026253,-1.0609764723\H,-3.7352942655,-0.9594500495,-0.1855736343\
H,-6.407757777,-1.1761104518,-0.4112587043\H,-1.3812166005,0.291980389
9,-0.910515501\H,-1.4784687222,0.2621037456,0.8552042851\H,1.987845616
6,3.3170650278,1.0877487997\H,2.160409139,3.2811501559,-0.6751421173\H
,-5.4677451289,2.6298770571,0.6821458884\H,-5.3056678882,2.7346787776,
-1.0789336067\\Version=ES64L-G09RevD.01\HF=-1375.473242\RMSD=3.346e-09
\RMSF=4.162e-06\Dipole=-0.04327,0.5490572,0.0054855\Quadrupole=-9.7527
074,13.1171638,-3.3644564,-3.4178572,3.7332876,0.4630941\PG=C01 [X(C15
H14S2)]\\@

Cp2.pbe0

1\1\GINC-R01-NODE71\FOpt\RPBE1PBE\Gen\C20H18S2\GRYNOVA\08-Feb-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDis
persion=GD3BJ Nosymm\\Cp2.pbe0.freq\\0,1\C,1.3272873738,-0.2291636996,
0.0228985592\C,0.1224616027,0.673795824,-0.0005118027\C,-1.0508784235,

-0.2687121973,0.0254385411\C,0.8785880141,-1.5246007371,0.0598029067\C
,-0.5605398799,-1.5479157645,0.0605851029\H,-1.1638299258,-2.455917817
8,0.0845973761\H,1.5116342327,-2.4119398672,0.0836883384\C,-2.41873456
34,0.1478508266,0.0140381288\C,-3.5921043727,-0.7968328652,0.050775765
9\C,-4.783714727,0.1169933688,0.0830980455\C,-2.9096145495,1.424207497
,-0.0095928487\C,-4.3579816384,1.4056561795,0.0359959336\S,-6.45459272
27,-0.4137477268,0.0117900793\H,-6.2962842435,-1.5427495193,0.74637896
3\H,-4.9975022442,2.2877023399,0.0344362812\H,-2.3080429825,2.33299274
73,-0.0372534103\C,8.7899664267,-0.1175173553,-0.0531976504\C,7.598352
4877,0.7962999186,-0.0208165927\C,6.4249862399,-0.1483946667,0.0159766
91\C,8.3642541659,-1.4061899075,-0.0060849853\C,6.9158908526,-1.424738
9341,0.0395711653\S,10.4608231271,0.4132994699,0.0177007101\H,10.30175
21286,1.5434478023,-0.7149323056\H,6.3143336695,-2.333533039,0.0672853
146\H,9.0037518734,-2.2882513168,-0.0045775933\C,5.0571360704,0.268171
1027,0.0046927625\C,3.8837979722,-0.6743402025,0.0306852905\C,2.678969
3152,0.2286160353,0.0073295275\C,4.5667923707,1.5473778834,-0.03037173
94\C,3.1276655528,1.5240545782,-0.0295291837\H,2.4946147007,2.41139336
31,-0.0533364412\H,5.1700766046,2.4553844533,-0.0543759544\H,0.1107242
942,1.3091104031,-0.9014728761\H,0.1111336372,1.3546389676,0.866542046
5\H,3.8950922931,-1.3551934074,-0.8363576588\H,3.8955753485,-1.3096420
994,0.9316574285\H,-3.5563671073,-1.4650528008,0.9280268268\H,-3.62536
51642,-1.4424987384,-0.8421307715\H,7.6316264195,1.4419780918,0.872082
9796\H,7.5625957709,1.4644818104,-0.8980929507\\Version=ES64L-G09RevD.
01\HF=-1568.2015917\RMSD=8.565e-09\RMSF=2.945e-06\Dipole=0.0011306,0.0
004109,0.0005055\Quadrupole=-11.0729689,14.0469433,-2.9739743,8.988840
8,-5.4348161,-2.7158573\PG=C01 [X(C20H18S2)]\\@

Cp3.pbe0

1\1\GINC-R01-NODE71\FOpt\RPBE1PBE\Gen\C25H22S2\GRYNOVA\08-Feb-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDis
persion=GD3BJ Nosymm\\Cp3.pbe0.freq\\0,1\C,1.4530817899,-0.3227354877,
0.0221371733\C,0.2639718319,0.6012860019,0.0331612071\C,-0.9255203731,
-0.3210216069,0.0211006071\C,0.9814474647,-1.6111713579,0.0075058345\C
,-0.4572,-1.6092426138,0.0058094912\H,-1.0762541966,-2.5068418536,-0.0
06559782\H,1.599162428,-2.5094903033,-0.0028365649\C,-2.2857096108,0.1
190175133,0.0261719566\C,-3.4753852484,-0.80582647,0.0242434143\C,-4.6
50923064,0.1264889687,0.0946582357\C,-2.7544307722,1.4037979802,0.0548
607311\C,-4.2027403683,1.4084403652,0.1001663591\S,-6.3308109825,-0.37
14803961,0.0013580956\H,-6.1951198119,-1.5273356137,0.6979028921\H,-4.
8269662905,2.3007008825,0.1348067131\H,-2.1372507215,2.3024345328,0.06
4135797\C,12.6532646669,0.1254401553,-0.0405284257\C,11.4774851353,-0.
8074305275,0.0172058997\C,10.2880209293,0.1176483647,0.0266945045\C,12
.205393448,1.4074686388,-0.02970928\C,10.7570628035,1.4025731182,0.014
8643582\S,14.3329852835,-0.3740613681,0.047079324\H,14.1966949414,-1.5
224254536,-0.6615907633\H,10.1400853062,2.3013948342,0.0167924834\H,12
.8298401158,2.299955309,-0.0525954299\C,5.1906111822,0.1106113313,0.02
60341084\C,4.0010577806,-0.8125234192,0.019695566\C,2.8116912454,0.110
8520535,0.0257429346\C,4.7197555652,1.4000308881,0.0344008844\C,3.2828
071553,1.4001718008,0.0347562489\H,2.6640107696,2.2978390282,0.0407307
367\H,5.3387309197,2.2975748729,0.040323783\C,8.9277314949,-0.32210728
27,0.0254725238\C,7.738445883,0.6005502538,0.0256434441\C,6.5491282387
,-0.3232718431,0.0238976974\C,8.4591208288,-1.6103108456,0.0231870768\
C,7.0204756684,-1.6118914897,0.0211350357\H,6.4025551668,-2.5101274655

,0.0192119107\H,9.0779765161,-2.5081295064,0.0235422695\H,0.2645277251
,1.2714703182,-0.8422472883\H,0.2631912378,1.2477878456,0.9261690211\H
,4.0012498098,-1.46487146,-0.8690545607\H,4.0007348913,-1.476914746,0.
8994594998\H,7.7378439402,1.2590239514,0.9098781272\H,7.7395752299,1.2
588835438,-0.8586950073\H,-3.4515521585,-1.5106073211,0.8727632815\H,-
3.5197929476,-1.4129117469,-0.894866923\H,11.4539564853,-1.5010606734,
-0.8404788711\H,11.5212026673,-1.4265217009,0.9283036691\\Version=ES64
L-G09RevD.01\HF=-1760.9300197\RMSD=9.603e-09\RMSF=6.170e-06\Dipole=0.0
018791,-0.5523957,-0.0030739\Quadrupole=-13.2906733,16.8719739,-3.5813
006,-4.1439994,-6.388395,0.1041719\PG=C01 [X(C25H22S2)]\\@

Cp4.pbe0

1\1\GINC-R02-NODE11\FOpt\RPBE1PBE\Gen\C30H26S2\GRYNOVA\08-Feb-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDis
persion=GD3BJ Nosymm\\Cp4.pbe0.freq\\0,1\C,5.3221703979,-0.2058454364,
-0.0789765931\C,4.1443872375,0.7283547814,0.009716917\C,2.9432198897,-
0.176113086,-0.0704510693\C,4.8341232839,-1.484400086,-0.195531236\C,3
.3980394052,-1.4662349332,-0.1903167134\H,2.7678506049,-2.3523997494,-
0.2696547331\H,5.4413558807,-2.3859679123,-0.2795516833\C,-2.153811002
4,-0.1174251184,-0.0610962857\C,-3.3306535893,0.8187011094,0.036362792
8\C,-4.5189942739,-0.0994111104,0.0073868374\C,-2.6402561291,-1.391432
4855,-0.1693477178\C,-4.0885222885,-1.3806861305,-0.1242706543\S,-6.19
18344693,0.4286328409,-0.0331850485\H,-6.0452738982,1.493442963,0.7941
356018\H,-4.7252130896,-2.2627113506,-0.1846331142\H,-2.0356884484,-2.
2944322775,-0.2561271851\C,16.5264125791,0.1011861893,-0.1303127861\C,
15.3379953493,-0.8168258688,-0.1594401293\C,14.1612267956,0.119374893,
-0.0617336437\C,16.0960556896,1.3824810585,0.0015370614\C,14.647789329
4,1.3933182741,0.0466683889\S,18.1991801516,-0.4270698179,-0.090176291
9\H,18.0518309466,-1.4928222231,-0.9161132755\H,14.0433123836,2.296363
5569,0.1336234998\H,16.7327826395,2.2644720343,0.0620050216\C,9.064188
4763,0.1783318334,-0.0523927358\C,7.8630032964,-0.7260988008,-0.132748
4779\C,6.6852367254,0.2081120416,-0.043911951\C,8.6093928232,1.4684590
352,0.0674833759\C,7.1733086265,1.4866526221,0.0726540557\H,6.56609527
82,2.3882303831,0.1567190408\H,9.2395955136,2.3546061061,0.1469146077\
C,12.7952116744,-0.3001460664,-0.1010709269\C,11.6180655286,0.63405700
12,-0.0150734318\C,10.4166824756,-0.270476879,-0.0968418691\C,12.30967
86189,-1.5768213251,-0.2183404865\C,10.8714012851,-1.559824175,-0.2165
440056\H,10.2421090146,-2.4464511897,-0.2969093759\H,12.9166408675,-2.
4789823228,-0.2998359258\C,1.5907083478,0.2726386501,-0.0259390375\C,0
.3893756501,-0.6319842966,-0.1074651793\C,-0.7878200247,0.3021782857,-
0.0217039576\C,1.1359214775,1.5619666367,0.0936947333\C,-0.302356515,1
.5788813408,0.095507585\H,-0.9093736145,2.4810119655,0.1769400045\H,1.
7651663782,2.4486330463,0.1740029325\H,4.1549604524,1.3028638802,0.950
5585659\H,4.1504721561,1.4646558177,-0.8107488319\H,7.8569033405,-1.46
24792687,0.6876502049\H,7.8524212075,-1.3005151275,-1.073642508\H,11.6
268660366,1.3692217171,-0.8365696373\H,11.6271163659,1.209908815,0.925
0022427\H,0.3803430099,-1.2082358938,-1.0472846871\H,0.3806318279,-1.3
668043086,0.7143530745\H,-3.2979319065,1.4284718236,0.955314983\H,-3.3
656516609,1.521119773,-0.8125483216\H,15.3729677015,-1.5194744886,0.68
92813848\H,15.3051941903,-1.4263167461,-1.0785734051\\Version=ES64L-G0
9RevD.01\HF=-1953.6585328\RMSD=5.305e-09\RMSF=5.614e-06\Dipole=0.00116
42,-0.000321,0.0003906\Quadrupole=-16.2887213,19.351569,-3.0628477,-12
.0536195,-8.8814619,4.4341364\PG=C01 [X(C30H26S2)]\\@

TCp1.pbe0

1\1\GINC-R01-NODE71\FOpt\RPBE1PBE\Gen\C13H10S4\GRYNOVA\08-Feb-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDis
persion=GD3BJ Nosymm\\TCp1.pbe0.freq\\0,1\C,-2.7518352718,1.8754783808
,-0.0536714642\C,-1.494008854,1.0515416254,-0.0198517776\C,-0.39038899
06,2.0722646368,0.0243496005\C,-2.3968347666,3.1932967512,-0.030595208
6\C,-0.9590589803,3.3132237175,0.0161502332\H,-0.419064994,4.260063917
6,0.0418695367\H,-3.0866301651,4.0374816684,-0.0458735007\C,1.00202446
87,1.7152636078,0.0660129018\S,2.2623879362,2.9172476583,0.0998790183\
C,3.5046956489,1.7025322287,0.1812527432\C,1.5498610835,0.4457753853,0
.0895460332\C,2.9638919081,0.4397806286,0.1549532127\S,5.2138182709,2.
1229109999,0.1575750163\H,5.3027084682,2.5666174396,1.4389215549\H,3.5
793852267,-0.4582402478,0.1886029915\H,0.9411587247,-0.4579000165,0.07
13299347\C,-6.5325528077,0.870859615,-0.2251211352\S,-5.5070230791,2.2
72577736,-0.132149653\C,-4.0662646185,1.2940694391,-0.1019448883\C,-5.
7915661016,-0.2860085229,-0.2054318851\C,-4.3978625562,-0.0479868791,-
0.13574492\S,-8.2875781053,1.0055368835,-0.2050705604\H,-8.4444841723,
1.4328336545,-1.4854121321\H,-3.6492354717,-0.8396088811,-0.121052571\
H,-6.250764817,-1.2728550442,-0.2469264056\H,-1.4104999251,0.40460132,
-0.9087597859\H,-1.467788059,0.3895722977,0.8615031109\\Version=ES64L-
G09RevD.01\HF=-2093.0928053\RMSD=9.113e-09\RMSF=1.568e-05\Dipole=0.036
5984,-0.4146639,-0.0011779\Quadrupole=-5.0316468,5.3758043,-0.3441575,
0.242018,9.6471121,0.8525706\PG=C01 [X(C13H10S4)]\\@

TCp2.pbe0

1\1\GINC-R01-NODE71\FOpt\RPBE1PBE\Gen\C18H14S4\GRYNOVA\08-Feb-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDis
persion=GD3BJ Nosymm\\TCp2.pbe0.freq\\0,1\C,1.3335880794,-0.2525046645
,-0.0179980697\C,0.1008141023,0.610244866,0.0014602385\C,-1.0371653131
,-0.372461618,-0.0484806804\C,0.9302371045,-1.5606448835,-0.0713793425
\C,-0.50864905,-1.632063544,-0.0900447383\H,-1.0819211904,-2.558885132
6,-0.1311495944\H,1.5904143786,-2.4275750701,-0.09667415\C,-2.41745937
37,0.0268234292,-0.0488474451\S,-3.7155935719,-1.134403033,-0.10275158
38\C,-4.9221186636,0.1168962219,-0.0309170327\C,-2.9269312052,1.312327
8043,-0.0042309438\C,-4.3413131286,1.3616286534,0.0054652338\S,-6.6410
959287,-0.2479479387,-0.1325791657\H,-6.7986801563,-0.7062349647,1.137
1248315\H,-4.9295799063,2.2775545082,0.0439851542\H,-2.2900122193,2.19
58133994,0.0301838753\C,8.9254803828,-0.1171555395,0.0286039829\S,7.71
89523417,1.1342375934,0.0986537766\C,6.4208223807,-0.0270470632,0.0462
237944\C,8.3446724449,-1.361926644,-0.0064415358\C,6.9302957995,-1.312
6072065,0.0030018076\S,10.6444345773,0.2479133453,0.1299574959\H,10.80
22636228,0.7038505789,-1.1405540735\H,6.2933686474,-2.1961259491,-0.03
04115486\H,8.9329512849,-2.2778957531,-0.0437435164\C,5.0405212037,0.3
722207343,0.0455186261\C,3.9025552739,-0.6105278762,-0.0042878522\C,2.
6697481872,0.2522413953,0.0146295125\C,4.5119746435,1.6318299731,0.086
5696081\C,3.0730898961,1.5604015961,0.0676756759\H,2.4129033624,2.4273
379247,0.0925237353\H,5.0852227656,2.5586735516,0.1275079138\H,0.07655
97823,1.3008409783,-0.8575935919\H,0.0567453396,1.2317045284,0.9110917
025\H,3.9469072039,-1.2324140042,-0.9136124112\H,3.9265569022,-1.30072
0197,0.8551003111\\Version=ES64L-G09RevD.01\HF=-2285.8213187\RMSD=5.71
7e-09\RMSF=5.825e-06\Dipole=-0.0001369,-0.0006347,0.0001845\Quadrupole
=-10.0383064,11.2414953,-1.2031889,-3.8449075,-12.448018,-1.2585223\PG

=C01 [X(C18H14S4)]\\@

TCp3.pbe0

1\1\GINC-R01-NODE71\FOpt\RPBE1PBE\Gen\C23H18S4\GRYNOVA\08-Feb-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDis
persion=GD3BJ Nosymm\\TCp3.pbe0.freq\\0,1\C,1.4527485059,-0.3832393989
,-0.0545861059\C,0.2642164209,0.539115815,-0.0048613179\C,-0.921724384
1,-0.3842444432,-0.0722328992\C,0.9834647831,-1.6686973475,-0.13900375
52\C,-0.4562907822,-1.6672949624,-0.1497092149\H,-1.0757300994,-2.5628
343902,-0.2108181883\H,1.5998747805,-2.5660732775,-0.1908887835\C,-2.2
803256626,0.0818640102,-0.0528276369\S,-3.6344008226,-1.0134317364,-0.
1172088336\C,-4.7779242112,0.2936935988,-0.0118424053\C,-2.7263792291,
1.3897155103,0.020842379\C,-4.1364322933,1.5076031505,0.0431533403\S,-
6.5133064937,0.0147281733,-0.105253829\H,-6.6853889221,-0.4501992251,1
.1602402952\H,-4.6788329053,2.4503041631,0.1033670297\H,-2.0471031531,
2.24053237,0.0660393345\C,12.7797539676,0.2757918323,0.0290667445\S,11
.6332328159,-1.0323151879,-0.0117214986\C,10.2815301558,0.0670734046,0
.0322561297\C,12.1408941148,1.4902118852,0.1006136642\C,10.7304518557,
1.3740670892,0.1025391611\S,14.5140378059,-0.0149245241,0.1035805872\H
,14.6904825046,-0.3627296741,-1.1982861825\H,10.0530666091,2.226621660
7,0.1431660717\H,12.6853394687,2.4326727495,0.1437008714\C,5.189063431
2,0.0478913773,-0.0030858269\C,3.9999060188,-0.8722120926,-0.070654802
8\C,2.8119758183,0.0504154177,-0.0178900088\C,4.7202089352,1.334615462
9,0.0779720051\C,3.2825130776,1.3361419571,0.0689748201\H,2.6648354977
,2.2328882703,0.1232919807\H,5.3390311414,2.2300598215,0.1400571506\C,
8.922165029,-0.395457219,-0.0072775627\C,7.7376346619,0.530738333,0.04
40959316\C,6.5476869531,-0.3887381597,-0.0229598083\C,8.4547936854,-1.
6772910232,-0.092862682\C,7.0150531099,-1.6751692988,-0.103027459\H,6.
3973148093,-2.5710038458,-0.1646947617\H,9.0729044143,-2.5742220932,-0
.1465535804\H,0.270085866,1.251796736,-0.846025181\H,0.2558725596,1.13
85632907,0.9204249649\H,4.0049102395,-1.4711674469,-0.9961995814\H,3.9
940348343,-1.5867889942,0.7688235056\H,7.7339708645,1.130194936,0.9693
921308\H,7.7457542234,1.2434033257,-0.7970761919\\Version=ES64L-G09Rev
D.01\HF=-2478.5497877\RMSD=7.693e-09\RMSF=2.451e-06\Dipole=0.007301,0.
4256018,0.0226706\Quadrupole=-16.4250521,15.937271,0.487781,3.9258609,
-14.6239698,0.9697189\PG=C01 [X(C23H18S4)]\\@

TCp4.pbe0

1\1\GINC-R02-NODE37\FOpt\RPBE1PBE\Gen\C28H22S4\GRYNOVA\08-Feb-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDis
persion=GD3BJ Nosymm\\TCp4.pbe0.freq\\0,1\C,5.3179316763,-0.1970525357
,-0.0401819514\C,4.1559914188,0.7582535878,0.0209854449\C,2.9411968052
,-0.1284698679,-0.0390136247\C,4.8103142112,-1.4700003386,-0.124652296
6\C,3.3742455092,-1.4280317268,-0.1237845174\H,2.7302029087,-2.3058483
145,-0.1820409642\H,5.4027733877,-2.3831977867,-0.1838683156\C,-2.1493
999602,-0.0115458112,-0.0409573304\S,-3.4716866185,1.1227654082,0.0120
877377\C,-4.6523751164,-0.1549813913,-0.0221034258\C,-2.6328716802,-1.
3064171214,-0.1085033068\C,-4.0458204299,-1.3855906101,-0.0978686878\S
,-6.3788196199,0.1812187789,-0.0857884655\H,-6.5400759675,0.5258526069
,1.2189329363\H,-4.6150371425,-2.313440965,-0.1381075478\H,-1.97801269
51,-2.1761699705,-0.1537675678\C,16.6584150789,0.1532070208,-0.0288538
636\S,15.4776962715,-1.1245089538,-0.0633965023\C,14.1554336226,0.0098
194315,-0.0103205499\C,16.0518779102,1.38380343,0.04724337\C,14.638927

2356,1.3046607098,0.0576806693\S,18.384837304,-0.1831483959,0.03476444
13\H,18.5462957263,-0.5264572791,-1.2702841537\H,13.9840788024,2.17441
29742,0.1031139886\H,16.6211125739,2.3116278036,0.0878332983\C,9.06483
69482,0.1269469768,-0.0131698959\C,7.8500342052,-0.7597667447,-0.07317
20419\C,6.6881035547,0.19556484,-0.0121863889\C,8.6318023537,1.4265248
117,0.0713874605\C,7.1957316431,1.4685147902,0.0721541204\H,6.60328808
68,2.3817349224,0.1311873718\H,9.2758499616,2.3043455459,0.129535076\C
,12.7842148897,-0.4164735489,-0.0408624321\C,11.6251816021,0.541119075
3,0.0165788399\C,10.4104135559,-0.3461896214,-0.0415263767\C,12.281965
7299,-1.6855322689,-0.1214932452\C,10.8429855827,-1.6450993386,-0.1227
133247\H,10.2012410195,-2.5242584958,-0.1788638267\H,12.8755727586,-2.
598781811,-0.17736007\C,1.5956095391,0.3446258354,-0.010447819\C,0.380
8684229,-0.5427355034,-0.068367077\C,-0.7781946819,0.4148095624,-0.010
688056\C,1.1629977681,1.643513778,0.0708510348\C,-0.2759857644,1.68388
70384,0.0698780121\H,-0.869621383,2.5971080718,0.1259101716\H,1.804714
1362,2.5227007285,0.1268931492\H,4.1737001956,1.3566602302,0.946720643
2\H,4.176059751,1.4728532417,-0.8182381996\H,7.8298849264,-1.474312225
9,0.7660862135\H,7.8323940733,-1.3582155174,-0.9988864052\H,11.6470246
07,1.2521204099,-0.8257494756\H,11.6435491931,1.1418256019,0.940880504
4\H,0.3623513268,-1.1433085792,-0.9927555739\H,0.3592147859,-1.2538424
885,0.7738687957\\Version=ES64L-G09RevD.01\HF=-2671.278304\RMSD=6.692e
-09\RMSF=3.320e-06\Dipole=-0.0001971,0.0003681,-0.0000864\Quadrupole=-
23.1129452,20.6393318,2.4736134,8.2928406,-16.7120576,2.6912149\PG=C01
[X(C28H22S4)]\\@

THIO1.pbe0

1\1\GINC-LCMD38\SP\RPBE1PBE\Gen\C12H8S5\ROOT\02-Jun-2016\0\\#PBE1PBE/g
en SCF=Tight IOP(2/17=4) INT(grid=finegrid)\\THIO1.pbe0.freq\\0,1\C,0,
-2.8131026928,1.7732105233,-0.0325209189\S,0,-1.4636843489,0.673338711
9,-0.0202278401\C,0,-0.3131720868,1.9796046931,0.0071385532\C,0,-2.371
1231533,3.0798186868,-0.0152147564\C,0,-0.9637616292,3.1959846153,0.00
472041\H,0,-0.4331296538,4.1481248083,0.009447328\H,0,-3.0509231526,3.
9318642585,-0.0080672723\C,0,1.1059454472,1.7092943467,0.0279095105\S,
0,2.2427177332,2.9558976121,0.4525259964\C,0,3.5911125033,1.8732374229
,0.2677793477\C,0,1.7640814532,0.5282125189,-0.2498160142\C,0,3.170278
4753,0.622639359,-0.1139474404\S,0,5.2525216237,2.43090508,0.439891315
4\H,0,5.2818799632,2.4744769176,1.7977758654\H,0,3.8646007897,-0.19778
12538,-0.2908931824\H,0,1.2430803498,-0.3805136538,-0.5521680043\C,0,-
6.6455498798,1.025369875,-0.3047770991\S,0,-5.4932629618,2.3148910684,
-0.4878160416\C,0,-4.1683999756,1.2731612435,-0.0571677291\C,0,-6.0258
31191,-0.1384729833,0.0803479128\C,0,-4.6237321935,0.0000582813,0.2204
546454\S,0,-8.3755945448,1.3021450858,-0.4818816784\H,0,-8.4086006293,
1.3355592723,-1.8399629623\H,0,-3.9608573723,-0.8096151307,0.526521019
5\H,0,-6.5763528731,-1.0615913589,0.2570890352\\Version=ES64L-G09RevD.
01\State=1-A\HF=-2452.0402366\RMSD=6.304e-09\Dipole=0.0325561,-0.38602
38,0.0037601\Quadrupole=-4.5975323,5.1785019,-0.5809696,-0.8009832,7.2
337358,0.6313856\PG=C01 [X(C12H8S5)]\\@

THIO2.pbe0

1\1\GINC-LCMD39\SP\RPBE1PBE\Gen\C16H10S6\ROOT\02-Jun-2016\0\\#PBE1PBE/
gen SCF=Tight IOP(2/17=4) INT(grid=finegrid)\\THIO2.pbe0.freq\\0,1\C,0
,1.3105635436,-0.2014401592,-0.1238005365\S,0,0.0261587004,0.945207010
7,0.1371270934\C,0,-1.1980323119,-0.2660499856,-0.1195613726\C,0,0.792

8003742,-1.4578300783,-0.3682106021\C,0,-0.6184750012,-1.4935379588,-0
.3660788385\H,0,-1.2033540485,-2.3916659935,-0.5647329078\H,0,1.420977
6183,-2.3262027734,-0.5668980498\C,0,-2.5983349492,0.0813501275,-0.055
0217494\S,0,-3.8120310727,-1.148601606,0.1450229075\C,0,-5.0913730678,
0.0296600619,0.1490505884\C,0,-3.1812733486,1.3309267312,-0.1226900792
\C,0,-4.5920807172,1.299753941,-0.007709654\S,0,-6.7848566953,-0.44797
7187,0.2179012604\H,0,-6.8374744505,-0.7135004401,1.5496322402\H,0,-5.
2343928164,2.1788715111,-0.0408417123\H,0,-2.6029145803,2.2444396515,-
0.2625036517\C,0,9.097802443,-0.0514658359,0.1044789965\S,0,7.83035330
94,1.1380856945,0.0408569909\C,0,6.5951676941,-0.0866545483,0.08877105
6\C,0,8.5787187025,-1.3207440234,0.1815040047\C,0,7.1633535331,-1.3424
184698,0.1716004275\S,0,10.7936373113,0.4138488485,0.1896702032\H,0,10
.9567128881,0.7216878543,-1.1238900977\H,0,6.5716969578,-2.2569739091,
0.2192930651\H,0,9.2098223479,-2.2065923496,0.2397571988\C,0,5.1970650
123,0.269692471,0.0374308595\S,0,3.9687313157,-0.9643536927,-0.0087724
689\C,0,2.688948664,0.2157714319,-0.0646069403\C,0,4.6206091338,1.5232
16995,0.018512615\C,0,3.2106412205,1.4936533161,-0.0404914645\H,0,2.58
68029205,2.3867424306,-0.0765733159\H,0,5.205835369,2.4425609342,0.043
8949341\\Version=ES64L-G09RevD.01\State=1-A\HF=-3003.61214\RMSD=9.644e
-09\Dipole=0.0217727,0.0189223,-0.114601\Quadrupole=-5.3316473,8.63082
68,-3.2991795,-4.3814082,-10.1243782,-1.2892797\PG=C01 [X(C16H10S6)]\\
@

THIO3.pbe0

1\1\GINC-LCMD40\SP\RPBE1PBE\Gen\C20H12S7\ROOT\02-Jun-2016\0\\#PBE1PBE/
gen SCF=Tight IOP(2/17=4) INT(grid=finegrid)\\THIO3.pbe0.freq\\0,1\C,0
,1.3530875015,-0.3114413074,-0.1771328931\S,0,0.1038753466,0.875914581
1,0.0727027592\C,0,-1.1545301182,-0.3180849817,-0.0781128478\C,0,0.800
0673575,-1.5663479929,-0.3386362483\C,0,-0.6105904352,-1.5693165266,-0
.2831954374\H,0,-1.2213654453,-2.4625284326,-0.4148390895\H,0,1.401935
48,-2.4574854473,-0.5168069815\C,0,-2.5435611419,0.0643966884,0.020420
7414\S,0,-3.7757511936,-1.1265091895,0.3200507724\C,0,-5.0277339331,0.
0808672207,0.3188653689\C,0,-3.1011676917,1.3231699534,-0.0820371683\C
,0,-4.5068901255,1.3305610169,0.0866159416\S,0,-6.7276773687,-0.352180
7301,0.4713554119\H,0,-6.7327247414,-0.5704531351,1.8126465535\H,0,-5.
1303787176,2.2224239729,0.03824596\H,0,-2.5086865116,2.2158539207,-0.2
837050003\C,0,13.0240172101,0.0946149583,0.329088568\S,0,11.7718329976
,-1.1122395269,0.3480375477\C,0,10.532695803,0.0830839126,0.1003755275
\C,0,12.4936580691,1.3526018975,0.1775547139\C,0,11.0840502014,1.34780
09574,0.045865532\S,0,14.7106805471,-0.3251212526,0.6108326091\H,0,14.
9811052698,-0.8067828211,-0.6308166119\H,0,10.48608482,2.246002422,-0.
1099995891\H,0,13.1137791246,2.247715932,0.1510254753\C,0,5.2513279811
,0.0806325472,-0.173379913\S,0,3.9972860214,-1.1244035129,-0.074916570
6\C,0,2.7407665803,0.0768434313,-0.1866827967\C,0,4.700141444,1.343534
4909,-0.262076876\C,0,3.2890368317,1.3414003103,-0.2695061929\H,0,2.68
18426096,2.2424699172,-0.3561556265\H,0,5.3054768678,2.2464424873,-0.3
423853076\C,0,9.1463086946,-0.3029686351,-0.0182525021\S,0,7.882601954
1,0.8873611816,0.1172669518\C,0,6.6399288406,-0.3034967259,-0.14945023
1\C,0,8.6084703935,-1.5552689729,-0.2330622248\C,0,7.1987023231,-1.556
1839615,-0.3072652434\H,0,6.6018432749,-2.4488970435,-0.4941473544\H,0
,9.2229648787,-2.4471246042,-0.3562297282\\Version=ES64L-G09RevD.01\St
ate=1-A\HF=-3555.1840401\RMSD=1.506e-10\Dipole=0.0706074,0.2749441,-0.
2815368\Quadrupole=-6.879271,11.6459264,-4.7666553,-1.4933324,-12.9255

043,0.472162\PG=C01 [X(C20H12S7)]\\@

THIO4.pbe0

1\1\GINC-LCMD40\SP\RPBE1PBE\Gen\C24H14S8\ROOT\03-Jun-2016\0\\#PBE1PBE/
gen SCF=Tight IOP(2/17=4) INT(grid=finegrid)\\THIO4.pbe0.freq\\0,1\C,0
,5.3120425126,-0.2055355961,0.2249868736\S,0,4.0784737441,1.0209317153
,0.1295719172\C,0,2.8021866565,-0.1642036031,0.1673728281\C,0,4.740383
3226,-1.4622432697,0.2572402942\C,0,3.3299276,-1.4389343036,0.22489922
44\H,0,2.7077051544,-2.3329819849,0.2656960721\H,0,5.3301895505,-2.376
3473389,0.3255389125\C,0,-2.4724861349,-0.0607199356,-0.2000995165\S,0
,-3.6825524108,1.1635820234,-0.4495477711\C,0,-4.9580872798,-0.0183437
426,-0.4802926694\C,0,-3.0490906992,-1.3151242379,-0.1829767591\C,0,-4
.455511721,-1.2894013105,-0.3437414631\S,0,-6.6300695953,0.440251793,-
0.7877891748\H,0,-6.9161230786,0.9046101995,0.4569087628\H,0,-5.093310
1831,-2.1724087058,-0.3478213987\H,0,-2.4717963557,-2.2275825767,-0.03
21795619\C,0,16.9679752221,0.0766310979,-0.5199123213\S,0,15.702879577
,-1.1164429639,-0.5605533441\C,0,14.4909118692,0.0675720959,-0.1648721
877\C,0,16.4667120355,1.3157058701,-0.2032376716\C,0,15.0652702638,1.3
123853781,-0.0021407407\S,0,18.6592293351,-0.3631044812,-0.7351442658\
H,0,18.6292873247,-0.5196761735,-2.0847409922\H,0,14.4878310359,2.1982
118556,0.2633620908\H,0,17.1009126611,2.1972424186,-0.1186842474\C,0,9
.2153947906,0.1232549843,0.201327685\S,0,7.9394233073,-1.044411195,-0.
0053396265\C,0,6.7055690004,0.1580005886,0.2529543618\C,0,8.6877321932
,1.3784126472,0.4310574741\C,0,7.2770987596,1.3980456925,0.4600896006\
H,0,6.6869992829,2.2943475618,0.6512779309\H,0,9.3102871152,2.25736692
94,0.5983115655\C,0,13.1001312681,-0.3055727769,-0.0576428381\S,0,11.8
543611744,0.9112167744,-0.0692262291\C,0,10.5965142977,-0.2787875246,0
.1165594616\C,0,12.544655601,-1.5633598581,0.0570710192\C,0,11.1364139
698,-1.5491340835,0.1546352131\H,0,10.5276239671,-2.4451507209,0.27547
12023\H,0,13.1460610187,-2.4718003754,0.0935185418\C,0,1.4212842164,0.
2455811137,0.1318483748\S,0,0.1629539704,-0.9120708359,-0.199981432\C,
0,-1.0817962275,0.2956061439,-0.0440344887\C,0,0.8818898228,1.50201604
58,0.3240520379\C,0,-0.5260466587,1.5295119133,0.2247955156\H,0,-1.127
210917,2.4271579941,0.3697226572\H,0,1.491009641,2.376264758,0.5538090
825\\Version=ES64L-G09RevD.01\State=1-A\HF=-4106.7559171\RMSD=8.543e-0
9\Dipole=-0.0839679,0.047111,0.3495211\Quadrupole=-8.6143718,14.183788
5,-5.5694166,6.1644758,-14.7957731,2.8936444\PG=C01 [X(C24H14S8)]\\@

THIO5.pbe0

1\1\GINC-NODE07\FOpt\RPBE1PBE\Gen\C28H16S9\GRYNOVA\27-Feb-2017\0\\#PBE
1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(GEDIIS,Maxstep=10) IOP(2/17
=4) EmpiricalDispersion=GD3BJ Nosymm\\THIO5.pbe0.freq\\0,1\C,5.3152918
326,-0.244076355,-0.3236579845\S,4.1006775304,0.9658691604,-0.01452941
96\C,2.8101068344,-0.1912733947,-0.1856353088\C,4.7279602625,-1.478497
1358,-0.5205040902\C,3.3193402182,-1.4486748048,-0.4429269853\H,2.6838
611031,-2.3209489376,-0.5951334619\H,5.3049648199,-2.3772905757,-0.737
6323806\C,-2.4462198935,-0.1011806999,0.3652563189\S,-3.6363356871,1.0
907413251,0.8007548325\C,-4.9089806672,-0.0950428996,0.8034973\C,-3.03
27938659,-1.3426495554,0.2222600365\C,-4.4266633412,-1.3374529218,0.47
07098362\S,-6.5886654472,0.3549045748,1.0762352943\H,-6.5087713401,0.5
185873378,2.4228580609\H,-5.0691144279,-2.2147421557,0.4085994434\H,-2
.4692605991,-2.2314821133,-0.0619702908\C,16.9980527749,-0.1833177417,
-0.0156106557\S,15.7048958537,-1.3485567802,-0.0619536348\C,14.4988383

326,-0.1018352362,-0.2170016325\C,16.4958258745,1.0995876404,-0.091148
282\C,15.0894500743,1.146110143,-0.204909689\H,14.5176782501,2.0691485
891,-0.2993171683\H,17.1344068543,1.9828728455,-0.0869624139\C,9.21997
98572,0.0482606887,-0.3779243461\S,7.9370690213,-1.1290253457,-0.32130
976\C,6.7109613356,0.1084762915,-0.3402650661\C,8.7008752818,1.3280589
143,-0.3851767237\C,7.2905492231,1.3618313396,-0.3639893801\H,6.705125
9952,2.2808910746,-0.3871792014\H,9.3287298449,2.2179577939,-0.4275146
023\C,13.104037661,-0.4433441687,-0.3269629377\S,11.87598886,0.7704855
768,-0.0977530098\C,10.5967660758,-0.371681436,-0.403471667\C,12.52777
31983,-1.6683907693,-0.5988900628\C,11.1179243058,-1.6282656993,-0.641
7412862\H,10.4922450193,-2.4922914248,-0.8651256719\H,13.1158081538,-2
.5668093317,-0.7858931847\C,1.436439157,0.2199190813,-0.0503608091\S,0
.1781556273,-0.9627228018,0.1739655994\C,-1.0581325166,0.2629603556,0.
2114383845\C,0.9051252655,1.4943820918,-0.0636129086\C,-0.4987802388,1
.5177328856,0.0832757327\H,-1.0954915674,2.4298076417,0.0722520233\H,1
.5163592905,2.3860847362,-0.2018259003\C,18.3704373649,-0.6163218219,0
.0950480568\C,18.894349177,-1.8795088365,-0.0951909297\C,20.2987524752
,-1.9364129891,0.074482244\C,20.8516227054,-0.7194648306,0.3911254071\
S,19.6271077935,0.5088514155,0.5196857063\H,18.2808351977,-2.736233318
2,-0.3746027118\H,20.8998626243,-2.8371200412,-0.0421166453\S,22.53738
07541,-0.3802532515,0.7676416291\H,22.8517277112,0.2497438704,-0.39459
77032\\Version=ES64L-G09RevD.01\HF=-4658.047528\RMSD=7.770e-09\RMSF=2.
256e-06\Dipole=0.1006678,-0.1526328,-0.360736\Quadrupole=-2.8383035,14
.0489095,-11.2106059,2.0872915,-24.7538783,2.681956\PG=C01 [X(C28H16S9
)]\\@

THIO6.pbe0

1\1\GINC-NODE07\FOpt\RPBE1PBE\Gen\C32H18S10\GRYNOVA\24-Feb-2017\0\\#PB
E1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDisper
sion=GD3BJ Nosymm\\THIO6.pbe0.freq\\0,1\C,5.3564064669,-0.299232449,0.
2075055328\S,4.1401065245,0.9464211378,0.1427308608\C,2.8476669722,-0.
2206464448,0.191723471\C,4.7670550821,-1.5479044807,0.2402689102\C,3.3
569041087,-1.503633021,0.2315507249\H,2.7216964718,-2.3882360789,0.275
2790069\H,5.344892709,-2.4706553435,0.2905566763\C,-2.4288384125,-0.03
92463986,-0.0681356225\S,-3.6269225309,1.2039090863,-0.2778778726\C,-4
.9186539803,0.0393046612,-0.2885871976\C,-3.0216447167,-1.2860088165,-
0.0478094064\C,-4.4309977447,-1.2398192576,-0.1746639202\S,-6.59059070
99,0.5235166522,-0.551013605\H,-6.8371297218,0.9843795369,0.7033394455
\H,-5.0813502531,-2.1134847367,-0.1709760648\H,-2.4527875452,-2.206981
882,0.080926133\C,17.0408383136,-0.2487091913,-0.32147723\S,15.7544379
323,-1.4217043409,-0.2541963429\C,14.5357572662,-0.1793036148,-0.16738
21835\C,16.5288631656,1.0326188528,-0.266888812\C,15.1214084227,1.0716
155487,-0.1791592729\H,14.5428417063,1.9940833559,-0.1315236507\H,17.1
590737934,1.921097736,-0.3035548401\C,9.2627385506,-0.032305513,0.1413
975861\S,7.9669329382,-1.1852489541,-0.0241367902\C,6.7545227619,0.042
7172829,0.2157478475\C,8.7563014002,1.2358176554,0.3497549973\C,7.3468
971061,1.277932202,0.3916962923\H,6.77204184,2.1874068188,0.5656785393
\H,9.3934034141,2.1094794447,0.4865679732\C,13.1408628378,-0.525801131
4,-0.0952831067\S,11.9213711909,0.7167396797,-0.0209986263\C,10.635000
5912,-0.4563657512,0.0524146736\C,12.5557844727,-1.77684599,-0.0738059
775\C,11.1483412533,-1.7380018679,0.0101205551\H,10.5188948874,-2.6268
55628,0.0507321115\H,13.1349375263,-2.6993997576,-0.1118410128\C,1.473
3939302,0.209395648,0.1822240741\S,0.191700258,-0.9311184615,-0.117569

3399\C,-1.0307452392,0.2964122098,0.0577584787\C,0.9574863103,1.474880
6807,0.3798743987\C,-0.4515897584,1.5231670164,0.3095043019\H,-1.03666
18305,2.4300744901,0.4616837845\H,1.5849892267,2.3403227539,0.59232884
56\C,18.4131292594,-0.6737878698,-0.4180638965\C,18.9162438888,-1.9312
557659,-0.6871525978\C,20.3268117425,-1.976632161,-0.7154685934\C,20.9
202197996,-0.7555976898,-0.4689750488\S,19.7108053155,0.4624152684,-0.
1757257009\H,18.2771028601,-2.7928774367,-0.8794634348\H,20.9011430012
,-2.8772093413,-0.9324134543\C,22.3230504354,-0.4188443916,-0.42932544
43\C,22.910463192,0.8306188827,-0.4398287309\C,24.3253117978,0.7863749
989,-0.4160719472\C,24.8225847396,-0.4938564622,-0.3906290554\S,23.535
8575594,-1.6636260679,-0.3582602296\S,26.5099646084,-0.9799602557,-0.2
67880815\H,22.3321273553,1.7534292928,-0.4882958691\H,24.9719030962,1.
6627299543,-0.4294498998\H,26.6665243608,-1.3910042943,-1.553559629\\V
ersion=ES64L-G09RevD.01\HF=-5209.5841377\RMSD=6.881e-09\RMSF=2.479e-06
\Dipole=-0.0314559,0.0111398,0.0915654\Quadrupole=-4.1203298,17.335388
2,-13.2150583,5.3840259,-25.2561409,4.3389543\PG=C01 [X(C32H18S10)]\\@

THIA1.pbe0

1\1\GINC-R02-NODE14\FOpt\RPBE1PBE\Gen\C8H4S5\GRYNOVA\27-Jan-2017\0\\#P
BE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispe
rsion=GD3BJ Nosymm\\THIA1.pbe0.freq\\0,1\S,0.2666557526,-2.3893303228,
-0.0546567026\C,0.7064995829,0.1969318711,-0.03378167\S,1.8286134429,1
.5105156259,-0.054393223\C,3.1803213286,0.3926706222,-0.0865314021\C,1
.3666168265,-1.0323898181,-0.0746757448\C,2.7798285659,-0.9209168562,-
0.1048289768\S,4.832279415,0.9869023077,-0.2115438332\H,4.9853241432,1
.3446693165,1.0904117669\H,3.4831159651,-1.7509495276,-0.1333639625\C,
-3.1635009527,-0.2804294982,0.0729980149\S,-2.075070989,1.0953505059,0
.0907262383\C,-0.7035001501,0.046928042,0.0238316792\C,-2.4974290334,-
1.4810888343,0.0420283023\C,-1.0922267859,-1.2937180595,0.0139391026\S
,-4.9027422927,-0.0499391392,0.2124980725\H,-5.1301487069,0.3227178697
,-1.0743825001\H,-3.0115961121,-2.4401741052,0.0343748382\\Version=ES6
4L-G09RevD.01\HF=-2297.2344811\RMSD=4.415e-09\RMSF=1.758e-05\Dipole=0.
0224017,-0.2131927,-0.0042085\Quadrupole=2.6581148,0.6657925,-3.323907
3,0.0507654,7.2428266,0.8422302\PG=C01 [X(C8H4S5)]\\@

THIA2.pbe0

1\1\GINC-R05-NODE17\FOpt\RPBE1PBE\Gen\C10H4S6\GRYNOVA\27-Jan-2017\0\\#
PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDisp
ersion=GD3BJ Nosymm\\THIA2.pbe0.freq\\0,1\C,-0.5799963318,1.3872443853
,0.050688616\S,-1.8357975595,2.5935453799,-0.0006731393\C,-3.049223574
9,1.3361372909,0.0365282511\C,-2.4939621625,0.0557434581,0.0849128064\
S,-3.7244396684,-1.1566265917,0.1197151256\C,-4.9769748617,0.072383268
8,0.0997925772\C,-4.4663794672,1.3462791306,0.043847485\S,-6.675700274
7,-0.3818239169,0.0321888448\H,-6.8269425346,-0.6810999329,1.349194037
4\H,-5.0967752352,2.232914209,0.0160179766\C,3.3208326584,1.3979278954
,0.0469789537\S,2.0683901725,2.6270719456,0.0267458456\C,2.8101758397,
0.1240561836,0.1029971634\S,5.0196027889,1.8519970218,0.1141896039\H,5
.1705657249,2.1507498928,-1.2029622016\H,3.4406028753,-0.7625563809,0.
1309563134\C,1.3930587696,0.1343510916,0.1104225677\S,0.1796108326,-1.
123137048,0.1475216175\C,-1.0761684877,0.0832317185,0.0958801021\C,0.8
378104963,1.4147009988,0.0617974536\\Version=ES64L-G09RevD.01\HF=-2771
.4374293\RMSD=7.258e-09\RMSF=1.596e-05\Dipole=-0.0000389,-0.0001203,-0
.000055\Quadrupole=3.7945977,0.0883072,-3.8829049,-1.8716664,-8.677620

2,-2.8364695\PG=C01 [X(C10H4S6)]\\@

THIA3.pbe0

1\1\GINC-R09-NODE15\FOpt\RPBE1PBE\Gen\C12H4S7\GRYNOVA\27-Jan-2017\0\\#
PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDisp
ersion=GD3BJ Nosymm\\THIA3.pbe0.freq\\0,1\S,-1.9210179736,2.1925365239
,-0.1541547603\C,-3.1646218813,0.9698052493,-0.0337658611\C,-1.2236403
404,-0.3300292666,0.0324822902\C,-2.6409219913,-0.3218544527,0.0557598
848\S,-3.9006387444,-1.4983759329,0.1738318419\C,-5.1217465805,-0.2381
581665,0.1332423573\C,-4.5801406992,1.0180896453,0.0097500813\S,-6.832
5303071,-0.6492032846,0.1278954693\H,-6.9554873185,-0.8944564184,1.458
9910708\H,-5.18809741,1.9192925353,-0.0401948686\C,5.1398299452,-0.299
3462705,-0.1242374792\S,3.9087249755,-1.5406652705,0.0311108687\C,4.60
82242128,0.9647849121,-0.2025125175\C,3.1922951617,0.9349453136,-0.155
5101929\S,6.8471353854,-0.7180662235,-0.0488624378\H,6.9709307737,-1.1
689399798,-1.3249895231\H,5.2233734205,1.8577560791,-0.2944199298\S,0.
003856441,-1.5654006299,0.103586195\C,0.7222088203,0.9492561643,-0.111
2280651\C,-0.6945778329,0.9572951461,-0.0804945445\S,1.9583609086,2.17
10567811,-0.2308224781\C,2.6583540641,-0.3505188928,-0.0411013418\C,1.
2410369704,-0.3439235612,-0.0191860596\\Version=ES64L-G09RevD.01\HF=-3
245.6402442\RMSD=4.771e-09\RMSF=1.027e-05\Dipole=0.001519,0.2259609,-0
.0176583\Quadrupole=4.481991,0.5324425,-5.0144335,-0.8242552,-10.31375
4,-0.4120036\PG=C01 [X(C12H4S7)]\\@

THIA4.pbe0

1\1\GINC-R08-NODE03\FOpt\RPBE1PBE\Gen\C14H4S8\GRYNOVA\27-Jan-2017\0\\#
PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDisp
ersion=GD3BJ Nosymm\\THIA4.pbe0.freq\\0,1\C,0.2308883717,0.6663731744,
0.0675195295\S,-1.0021259078,1.8513470177,0.4046924881\C,-3.6506174835
,0.6349664422,0.1818718026\S,-4.9057584165,1.7772682714,0.5056255912\C
,-6.1308732467,0.5426079536,0.2695122068\C,-4.1789787227,-0.6235961953
,-0.1142259998\C,-5.5939970504,-0.6766715936,-0.0651513628\S,-7.840379
1587,0.9510976794,0.3492228477\H,-7.9514378269,0.9669223127,1.70370917
26\H,-6.2048905116,-1.5565809542,-0.2570532826\C,6.067938907,-0.469948
0583,-0.4314658024\S,4.8428110999,-1.7045825081,-0.667660713\C,3.58765
55943,-0.5621559085,-0.3444379363\C,5.5310376057,0.7494353118,-0.09721
02897\C,4.1160062055,0.6964473571,-0.048480051\S,7.7774369161,-0.87855
88606,-0.5106954171\H,7.8889507322,-0.8942046227,-1.865149606\H,6.1419
339179,1.6293478025,0.0946692528\C,2.170935819,-0.5729253297,-0.305910
0041\S,0.9391588841,-1.7785131987,-0.5673635352\C,-0.2938788896,-0.593
3648142,-0.2308922005\S,2.8771700616,1.8835122229,0.2873612141\C,-1.70
96017742,-0.6058430447,-0.1872984275\S,-2.9401530365,-1.8106054948,-0.
4503070307\C,-2.2338998282,0.6457399182,0.1433214946\C,1.6466277386,0.
6787251195,0.0244360589\\Version=ES64L-G09RevD.01\HF=-3719.8430398\RMS
D=6.334e-09\RMSF=1.452e-05\Dipole=0.0000442,0.0000302,0.0000963\Quadru
pole=5.6533588,-1.1397521,-4.5136067,5.3521869,-10.8852024,3.6320626\P
G=C01 [X(C14H4S8)]\\@

PYR1.pbe0

1\1\GINC-LCMD33\FOpt\RPBE1PBE\Gen\C14H8N2S5\ROOT\03-Jun-2016\0\\#PBE1P
BE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersio
n=GD3BJ Nosymm\\THIOPYR1.pbe0.freq\\0,1\C,-2.8529812722,1.7969716696,-
0.1534299234\S,-1.4884141838,0.7382226404,-0.0140570006\C,-0.327333196

,2.017435233,0.1188555385\C,-0.9905012675,3.2453434059,0.0571928993\C,
1.0758705579,1.7560284662,0.2677437414\S,2.2429978329,3.0499291917,0.3
565207061\C,3.5551765868,1.9164322303,0.4646749209\C,1.7033785024,0.52
46384781,0.3511944727\C,3.1083603663,0.615962065,0.4618239763\S,5.2173
528867,2.4545117333,0.6875155098\H,5.4045887114,2.9550799087,-0.561566
7019\H,3.7805868777,-0.2380615496,0.5302648559\H,1.1586847096,-0.41948
66912,0.3210117734\C,-6.6587735777,1.0221830126,-0.4991089981\S,-5.564
1788028,2.366688373,-0.3867723897\C,-4.1892320571,1.2957722295,-0.3038
020157\C,-5.9919298012,-0.1803694165,-0.5025261623\C,-4.5924197274,-0.
0257707624,-0.3931940187\S,-8.3894325292,1.2617430988,-0.7204707668\H,
-8.6599318639,1.7247765214,0.5276809988\H,-3.8913108711,-0.8605305384,
-0.3688784265\H,-6.5048478754,-1.1382571501,-0.5748958888\C,-2.4121007
007,3.1213355719,-0.0970627369\N,-3.2204198034,4.2098387331,-0.1785706
367\C,-2.6058739904,5.3632825141,-0.104585876\C,-1.1864517445,5.487075
6149,0.0522237176\N,-0.3821809252,4.4573959527,0.1325444055\H,-3.22197
58801,6.2656691363,-0.1674054423\H,-0.7352969622,6.4825603279,0.109679
468\\Version=ES64L-G09RevD.01\HF=-2637.4336061\RMSD=8.313e-09\RMSF=4.2
99e-06\Dipole=-0.000789,-0.0062134,-0.0041102\Quadrupole=-5.1165851,11
.3103237,-6.1937386,-1.4425311,-9.56872,-0.8545019\PG=C01 [X(C14H8N2S5
)]\\@

PYR2.pbe0

1\1\GINC-LCMD33\FOpt\RPBE1PBE\Gen\C20H10N4S6\ROOT\03-Jun-2016\0\\#PBE1
PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersi
on=GD3BJ Nosymm\\THIOPYR2.pbe0.freq\\0,1\C,-0.6443810243,-0.1944641357
,-0.025081216\S,-1.9492865515,0.9549383017,-0.0079030748\C,-3.18455206
63,-0.2615632557,0.0595860305\C,-1.1690315007,-1.4949976146,0.01825694
1\C,-2.5995900315,-1.532552075,0.0664205606\N,-3.2804413211,-2.7049319
109,0.1148779819\N,-0.4212291968,-2.6240662093,0.016965935\C,-4.576077
7835,0.0802475342,0.1025975892\S,-5.8225033455,-1.1422713969,0.1265783
518\C,-7.0692046812,0.0672649037,0.1217639493\C,-5.1353846664,1.347912
4802,0.1221198581\C,-6.5469473689,1.3398128565,0.1316843035\S,-8.77244
68418,-0.3662779732,0.2323451308\H,-8.8941003762,-0.9030774445,-1.0098
048257\H,-7.1709868552,2.2322682149,0.1377701728\H,-4.5347380534,2.257
864838,0.1173333074\C,7.1471160381,-0.0742692222,-0.2226814396\S,5.900
4078097,1.1352649398,-0.2274150633\C,4.6539817423,-0.0872724765,-0.203
7386522\C,6.6248698566,-1.3468180907,-0.2328803313\C,5.2133054141,-1.3
549250542,-0.2234814569\S,8.8503635192,0.359296505,-0.333014825\H,8.97
17588115,0.8962809842,0.9090783627\H,4.6126701335,-2.2648871034,-0.218
9144075\H,7.2489080475,-2.2392731904,-0.2390601996\C,3.2624545046,0.25
45068149,-0.1607576516\S,2.0271846529,-0.9619980628,-0.093279553\C,0.7
222779977,0.1874094671,-0.076138924\C,2.6774843481,1.5254942077,-0.167
6107005\C,1.2469261448,1.4879412047,-0.1194807317\N,0.4991272058,2.617
0133373,-0.1182200689\N,3.3583399339,2.6978688108,-0.2160611165\C,-2.5
333404634,-3.7822543342,0.1125959399\C,-1.1047834836,-3.7433932206,0.0
631341948\C,1.1826871687,3.7363368754,-0.1643717015\C,2.6112461674,3.7
751960541,-0.2137943752\H,-3.0460011223,-4.7483182017,0.1517298248\H,-
0.5373503094,-4.6789650968,0.0636571903\H,0.615255632,4.6719100599,-0.
1649130948\H,3.1239119143,4.741257679,-0.2529022148\\Version=ES64L-G09
RevD.01\HF=-3374.5073667\RMSD=4.365e-09\RMSF=6.084e-06\Dipole=0.000122
4,0.0000523,-0.0000922\Quadrupole=-12.4012995,19.1791871,-6.7778876,-0
.7400791,12.0076034,1.8302832\PG=C01 [X(C20H10N4S6)]\\@

PYR3.pbe0

1\1\GINC-LCMD33\FOpt\RPBE1PBE\Gen\C26H12N6S7\ROOT\03-Jun-2016\0\\#PBE1
PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersi
on=GD3BJ Nosymm\\THIOPYR3.pbe0.freq\\0,1\C,-2.6467706525,-0.1626676366
,-0.222922352\S,-3.9152656275,1.0180490699,-0.0551788249\C,-5.19081723
38,-0.1517479973,-0.182369923\C,-3.2172581597,-1.4378335202,-0.3776711
522\C,-4.6483139612,-1.4306865597,-0.3542458862\N,-5.3693549653,-2.571
9402585,-0.4862982798\N,-2.5087489956,-2.5797110694,-0.534130534\C,-6.
5701054924,0.2278540239,-0.1064901847\S,-7.8567985197,-0.9407445166,-0
.2761743554\C,-9.0624544812,0.2996037598,-0.1177518333\C,-7.0879205531
,1.4981062956,0.0929988596\C,-8.4986347655,1.5380909562,0.0850123695\S
,-10.7808136598,-0.0835375672,-0.0888040879\H,-10.8990801503,-0.446135
6121,-1.3926747083\H,-9.0929352539,2.4412886147,0.215212754\H,-6.45743
85957,2.3771127171,0.2291553845\C,9.0597443879,0.3156359516,-0.3359664
247\S,7.8526999771,-0.9270716148,-0.4622016573\C,6.5684275092,0.240127
4276,-0.2664109901\C,8.4988015427,1.5539535049,-0.1243666926\C,7.08873
26074,1.5118412169,-0.0833372627\S,10.7789341482,-0.0646120701,-0.3450
837288\H,10.8675590248,-0.434333316,-1.649357062\H,6.4602417135,2.3904
128857,0.0643461802\H,9.0945127123,2.458520342,-0.0112128254\C,1.26762
88987,0.1749413364,-0.2296394193\S,-0.0018340118,-1.0118055343,-0.3638
723935\C,-1.2699013977,0.1725178457,-0.1987598198\C,0.7134282971,1.456
4283139,-0.0611973961\C,-0.7142273617,1.4550642315,-0.0437103217\N,-1.
4281638543,2.5933534207,0.1087609215\N,1.4286840483,2.5961161058,0.073
6368785\C,5.1883951386,-0.1419869662,-0.3083781283\S,3.9141624201,1.02
56004573,-0.1512524508\C,2.6441353893,-0.1576015637,-0.2870817775\C,4.
6442422793,-1.4221189594,-0.4656452588\C,3.2130704804,-1.431875068,-0.
4542958379\N,2.5030946522,-2.5752429535,-0.5921412199\N,5.3639776569,-
2.5622006322,-0.6138973601\C,-4.6587367269,-3.6640237923,-0.6361073305
\C,-3.2300210722,-3.6695134502,-0.6608130519\C,-0.7119657287,3.6881111
215,0.2383277603\C,0.7137621902,3.6894863384,0.2207522993\C,3.22309020
46,-3.6638782518,-0.7350338448\C,4.6519684456,-3.6557695056,-0.7451426
754\H,-5.2046908262,-4.6062203875,-0.7452692804\H,-2.6933800339,-4.614
2551404,-0.7897112053\H,-1.2538833024,4.630197867,0.3641836127\H,1.256
7939428,4.6326282746,0.3332055285\H,2.6852097828,-4.6097525626,-0.8496
863383\H,5.1968479331,-4.5970955728,-0.8664786731\\Version=ES64L-G09Re
vD.01\HF=-4111.5808779\RMSD=7.000e-09\RMSF=2.782e-06\Dipole=-0.0061766
,0.0841789,-0.6418647\Quadrupole=-19.6588659,25.7293641,-6.0704982,-0.
0082504,0.1539468,6.1658809\PG=C01 [X(C26H12N6S7)]\\@

PYR4.pbe0

1\1\GINC-LCMD36\FOpt\RPBE1PBE\Gen\C32H14N8S8\ROOT\03-Jun-2016\0\\#PBE1
PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersi
on=GD3BJ Nosymm\\THIOPYR4.pbe0.freq\\0,1\C,-0.7156335838,-0.1496186132
,0.0867235589\S,-1.9668607032,1.051000768,0.2855326674\C,-3.2551095178
,-0.1121618853,0.1189018847\C,-1.2947474936,-1.4204129799,-0.103781113
9\C,-2.7211305082,-1.3983629882,-0.085616502\N,-3.4557871398,-2.520878
813,-0.2517203224\N,-0.6008416899,-2.5644218558,-0.288228838\C,-8.5547
537164,-0.1002842104,0.1565392461\S,-9.8218141886,1.077720432,0.395003
4734\C,-11.0469128999,-0.1422569008,0.2272457683\C,-9.0937682597,-1.35
75544438,-0.0695353702\C,-10.5040934434,-1.3804855115,-0.0281955068\S,
-12.7601693973,0.2635389589,0.2541162446\H,-12.8468471178,0.5615486414
,1.5768219858\H,-11.1131562699,-2.2716357558,-0.1725234219\H,-8.478097
8973,-2.2392671412,-0.2490436359\C,10.9953856462,0.1337116193,0.037284

518\S,9.7682055469,-1.0828014669,-0.1397598599\C,8.5021118892,0.111895
744,0.0032527609\C,10.453644318,1.3917017756,0.1678459158\C,9.04263332
84,1.3804967133,0.1469943209\S,12.7071423505,-0.2592885711,-0.08849714
2\H,12.8095384271,-0.9569843047,1.0727054145\H,8.4278810693,2.27544114
36,0.2462287119\H,11.0638697621,2.2863996284,0.2821671384\C,3.20272846
49,0.1223031967,0.0845058178\S,1.9141785879,-1.0412378546,-0.076914331
7\C,0.663304177,0.1602206826,0.1190366406\C,2.669139757,1.4092250893,0
.2855328013\C,1.2427437973,1.4314625883,0.305402128\N,0.5491457788,2.5
761404695,0.486924336\N,3.4041330273,2.5321419522,0.4473562077\C,7.116
7750713,-0.2499629942,-0.0237966589\S,5.8612423094,0.9328304234,0.1711
570518\C,4.5723096736,-0.2285212131,0.0156787752\C,6.552698945,-1.5189
700301,-0.2020518938\C,5.1219330461,-1.5085215906,-0.1799872685\N,4.39
45958478,-2.6377412842,-0.3359571414\N,7.2546177522,-2.6653630981,-0.3
82593997\C,-4.6249396183,0.238022019,0.1862622194\S,-5.9129312613,-0.9
220803074,0.0151827919\C,-7.1695847958,0.2596660061,0.2090570687\C,-5.
17561437,1.5158496742,0.3929366891\C,-6.6065461618,1.5264367535,0.4053
865304\N,-7.3094721344,2.6716275947,0.5898065375\N,-4.4490726437,2.643
1833203,0.5653480668\C,-6.5812036935,3.7502177783,0.754345422\C,-5.152
9518022,3.737884684,0.7429097957\C,-2.7592205034,-3.622331539,-0.42975
64203\C,-1.3350468473,-3.6442295978,-0.4481158402\C,1.2836901512,3.656
4020287,0.6421497597\C,2.7078530965,3.6342681574,0.622382768\C,5.09751
64226,-3.7339193531,-0.5080620782\C,6.5256125642,-3.7457160991,-0.5315
953431\H,-7.112359299,4.6950685007,0.9056119031\H,-4.6009473501,4.6715
71734,0.8863421368\H,-3.3187642704,-4.5523105799,-0.568073088\H,-0.807
6229432,-4.590510081,-0.6005770177\H,0.7565659129,4.6032913492,0.79185
05002\H,3.2676324138,4.5646229738,0.7571697455\H,4.5447836527,-4.66915
73777,-0.6379540315\H,7.0559687337,-4.6913539592,-0.6807124796\\Versio
n=ES64L-G09RevD.01\HF=-4848.6547181\RMSD=3.539e-09\RMSF=4.581e-06\Dipo
le=0.0186378,-0.103518,0.6394975\Quadrupole=-26.8798248,34.0439641,-7.
1641393,1.3480354,0.287085,6.4079111\PG=C01 [X(C32H14N8S8)]\\@

THIOQ1.pbe0

1\1\GINC-R02-NODE22\FOpt\RPBE1PBE\Gen\C16H8N2S5\GRYNOVA\27-Jan-2017\0\
\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDi
spersion=GD3BJ Nosymm\\THIOQ1.pbe0.freq\\0,1\S,0.0120033159,1.14522621
23,-0.0360287038\C,-0.0390881336,-0.0889133433,1.2199083112\C,-0.08057
49536,-1.3860531566,0.6251049356\C,-0.0718677475,-1.3749883948,-0.7393
213415\C,-0.0222617006,-0.0683833392,-1.3123986557\C,-0.0373814289,0.2
213957653,2.5624793783\C,-0.0033023871,1.5182025429,3.1601382374\C,0.0
048143524,1.5068559585,4.5217027439\C,-0.0402611639,0.1868401282,5.084
9840203\S,-0.0780594217,-1.0239790599,3.8139719117\C,-0.0017318313,0.2
637382044,-2.6495707288\C,0.0570037004,1.5696001533,-3.2252219614\C,0.
0490740104,1.5818563861,-4.5867695211\C,-0.0003528768,0.2717675083,-5.
1723496104\S,-0.0491913681,-0.9600195601,-3.921959213\C,-0.010970925,-
0.0295270332,-6.5113770364\C,0.0749586465,1.0051473107,-7.4736404647\S
,-0.247485041,-1.6907764983,-7.0715529374\N,0.1716814041,1.8481806917,
-8.2733768232\C,-0.0533029575,-0.1371530159,6.4186856345\S,0.060561470
9,-1.8205489086,6.9506024268\C,-0.0643859292,0.8845127596,7.3985094037
\N,-0.0996974421,1.7186347015,8.2125285786\H,-0.1157930956,-2.29280361
9,1.2290425649\H,-0.099379552,-2.2719142757,-1.358157667\H,0.010058721
4,2.4272413702,2.5580186058\H,0.0333869487,2.3910536635,5.1573250562\H
,0.1080883452,2.4670827741,-2.6079832448\H,0.084198154,2.4764646823,-5
.2073161417\H,0.6846463158,-1.6516190642,-8.0561614253\H,-0.8741804304

,-1.7324265439,7.9297676674\\Version=ES64L-G09RevD.01\HF=-2713.4936898
\RMSD=7.787e-09\RMSF=3.226e-06\Dipole=-0.0429721,-1.1304043,-0.0189056
\Quadrupole=11.501856,20.3889647,-31.8908206,0.4438181,-7.2118713,0.81
16016\PG=C01 [X(C16H8N2S5)]\\@

THIOQ2.pbe0

1\1\GINC-R02-NODE57\FOpt\RPBE1PBE\Gen\C20H10N2S6\GRYNOVA\27-Jan-2017\0
\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalD
ispersion=GD3BJ Nosymm\\THIOQ2.pbe0.freq\\0,1\C,-0.6444180164,-0.19494
6391,0.0235817405\S,-1.9264583596,0.9879030934,-0.2047142824\C,-3.1750
011796,-0.2267836921,0.0469452362\C,-1.2060047333,-1.4740710617,0.2847
129304\C,-2.5746612882,-1.4930304427,0.2979321233\H,-3.1718682682,-2.3
860257558,0.481817304\H,-0.5827311422,-2.3516352231,0.457134228\C,-4.5
224138726,0.0758627325,-0.0048819638\S,-5.766599798,-1.1469889688,0.26
12789002\C,-7.0441279574,0.0354262686,0.0333579294\C,-5.1247799405,1.3
414100368,-0.2635899856\C,-6.4882036311,1.329771611,-0.2356753952\C,-8
.3772697756,-0.2888832281,0.1119615763\C,-9.3635202926,0.6973432969,-0
.1263017359\H,-7.1274550678,2.1954034643,-0.4045030072\H,-4.5278916265
,2.2307474072,-0.4685793402\C,7.0963010967,-0.0847447802,-0.0630740132
\S,5.8187928085,1.0977916382,-0.2904394255\C,4.5745900237,-0.125175204
4,-0.024850788\C,6.5403619959,-1.3792202061,0.2053449404\C,5.176938219
4,-1.3908440468,0.2332912852\C,8.429441111,0.239598418,-0.1415131597\S
,8.9477204939,1.8524623041,-0.6523228338\H,4.5800471984,-2.2802751925,
0.4378725746\H,7.179600055,-2.2449432093,0.3737484951\C,3.2271804783,0
.1774984709,-0.076584365\S,1.9786267379,-1.037334691,0.1743269897\C,0.
69659403,0.1456516086,-0.0533111494\C,2.626847575,1.4438685058,-0.3269
725144\C,1.2581894533,1.4248914287,-0.3138502205\H,0.6349269304,2.3025
641756,-0.4857594813\H,3.2240597554,2.3369801513,-0.510271987\N,-10.18
25166531,1.4977972778,-0.3472504535\S,-8.8955056561,-1.9014930703,0.62
35003746\C,9.4157009115,-0.7467464664,0.0962470245\N,10.2346952493,-1.
5472999005,0.3168472256\H,-9.8450544414,-2.0675978726,-0.3316264722\H,
9.8960975765,2.018877514,0.3039316959\\Version=ES64L-G09RevD.01\HF=-32
65.0225262\RMSD=3.562e-09\RMSF=2.445e-06\Dipole=-0.00209,-0.0000246,0.
0007996\Quadrupole=-51.4829258,33.2755869,18.2073389,28.9199358,4.2162
394,-0.7924251\PG=C01 [X(C20H10N2S6)]\\@

THIOQ3.pbe0

1\1\GINC-R03-NODE16\FOpt\RPBE1PBE\Gen\C24H12N2S7\GRYNOVA\27-Jan-2017\0
\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalD
ispersion=GD3BJ Nosymm\\THIOQ3.pbe0.freq\\0,1\C,-2.5982362394,-0.11441
08183,0.0692028815\S,-3.8773636013,1.0763627462,-0.1119953719\C,-5.126
6831405,-0.1379117263,0.1282672377\C,-3.1577514325,-1.3936068785,0.306
8870657\C,-4.5299407804,-1.4090404775,0.3396220624\H,-5.1271061087,-2.
3045360776,0.510617129\H,-2.5358761846,-2.2775563804,0.4493886918\C,-6
.4761991473,0.175385335,0.1027555734\S,-7.721395979,-1.0467973676,0.35
8148649\C,-8.996806619,0.1457174331,0.1767264746\C,-7.0742774837,1.447
2657638,-0.117155405\C,-8.4392235567,1.4418883828,-0.0698763283\C,-10.
3312580452,-0.176792204,0.2675122261\C,-11.317321776,0.8167534503,0.06
52095043\H,-9.0760043544,2.314538882,-0.2089423351\H,-6.4761821028,2.3
386651984,-0.3094544781\C,5.1580670381,-0.0388465143,-0.1065185039\S,3
.8758126406,1.1508083217,-0.2898220859\C,2.6295512079,-0.0644456659,-0
.0514608171\C,4.5961906381,-1.3219201846,0.1270065929\C,3.2238764675,-
1.3331061682,0.1563968906\C,6.4987472586,0.3010312426,-0.1904566251\C,

7.0615549798,1.5874504054,-0.418718957\H,2.6263070921,-2.2294148907,0.
3235534398\H,5.2176840911,-2.2060731646,0.2676728755\C,1.2747347596,0.
2542842373,-0.0777964571\S,0.0275128856,-0.959540701,0.1608729498\C,-1
.2524207218,0.2300852601,-0.0195987735\C,0.6810758027,1.5221564864,-0.
2860852115\C,-0.6933725394,1.5089903536,-0.2544549749\H,-1.3143447414,
2.3936716014,-0.3951576538\H,1.2778383305,2.4185251522,-0.4547827707\N
,-12.136572038,1.6248000885,-0.1265163986\S,-10.8466984019,-1.79865548
08,0.7519248367\S,7.7775431753,-0.9002816073,-0.0143353208\H,-11.79314
04892,-1.9540502037,-0.2083323784\C,8.426491757,1.603487086,-0.4637243
641\C,9.0197770073,0.3168207494,-0.2533786959\C,10.3628958278,0.019316
5532,-0.230293612\C,11.3209566345,1.0486504495,-0.3818572447\N,12.1171
775583,1.8956213236,-0.4795204597\S,10.924506561,-1.6556217467,-0.1310
02866\H,6.4388042124,2.4742601099,-0.54130053\H,9.0390836929,2.4881366
976,-0.6324523105\H,11.8696258643,-1.4462950516,0.8202558487\\Version=
ES64L-G09RevD.01\HF=-3816.5520388\RMSD=5.237e-09\RMSF=3.555e-06\Dipole
=0.0201848,-1.1361767,0.1942113\Quadrupole=-72.0284912,44.5485828,27.4
799084,0.690235,13.2122658,-2.9095235\PG=C01 [X(C24H12N2S7)]\\@

THIOQ4.pbe0

1\1\GINC-R04-NODE59\FOpt\RPBE1PBE\Gen\C28H14N2S8\GRYNOVA\27-Jan-2017\0
\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalD
ispersion=GD3BJ Nosymm\\THIOQ4.pbe0.freq\\0,1\C,-2.6197186794,-0.11537
49017,0.0209915405\S,-3.8889363666,1.0917050817,-0.0794458326\C,-5.146
6531073,-0.1286529088,0.0508466942\C,-3.1847376116,-1.4021080161,0.151
6459535\C,-4.5614064323,-1.4126479915,0.1686728344\H,-5.1642330149,-2.
3156591583,0.2626459948\H,-2.5693403746,-2.2984526559,0.2310566162\C,-
6.4973302046,0.1985914396,0.0335979904\S,-7.7510423439,-1.0301910507,0
.1811661444\C,-9.0179853911,0.1801279883,0.0753342016\C,-7.083420169,1
.4850654012,-0.0966147624\C,-8.4511830898,1.4856548192,-0.0665253438\C
,-10.3563817718,-0.1426740887,0.1263328268\C,-11.3359608661,0.86666275
8,-0.0155964446\H,-9.0807892337,2.3707393579,-0.1470355536\H,-6.478046
2097,2.3845695925,-0.2138058972\C,5.1426557984,-0.0843228968,-0.073388
294\S,3.8732126862,1.1223859999,-0.1712155925\C,2.6181513713,-0.095045
0703,-0.0427311167\C,4.5771934557,-1.3691921647,0.0533559513\C,3.19638
35215,-1.3741464808,0.0699837106\C,6.4963383642,0.2644413798,-0.121893
0491\C,7.0613575481,1.5511416524,-0.2528885791\H,2.592871198,-2.277248
5705,0.1612304052\H,5.1900163133,-2.2672819358,0.1297028619\C,1.258469
3185,0.2441234569,-0.0580749426\S,0.0034053423,-0.9733322607,0.0701429
648\C,-1.2660347211,0.2333963048,-0.0274420203\C,0.6802383675,1.523238
183,-0.170644618\C,-0.7005716529,1.5182839094,-0.1540149585\H,-1.31339
47454,2.4163844516,-0.2302345973\H,1.283750667,2.4263547407,-0.2617502
856\N,-12.1498331689,1.6903733879,-0.1590056955\S,-10.8828176499,-1.79
27995359,0.486564221\S,7.765558105,-0.9426060084,-0.0211055541\H,-11.8
097684593,-1.8807856564,-0.5008810514\C,8.4380235847,1.5616590424,-0.2
70082432\C,9.0232655071,0.2776785753,-0.1520706978\C,10.3739419334,-0.
0495974671,-0.1351463475\S,11.6276412923,1.1791747613,-0.2828416656\C,
10.9600322357,-1.3361127395,-0.0053343641\H,6.4459548799,2.4474613721,
-0.332530998\H,9.0408514344,2.464628279,-0.3644465214\C,12.3277864619,
-1.3367322257,-0.035851093\C,12.8945862151,-0.0311964395,-0.1775861011
\C,14.2329886659,0.291536398,-0.2289537336\C,15.2125372657,-0.71788018
57,-0.0874262324\S,14.75938445,1.9416379502,-0.5892431493\N,16.0264546
348,-1.5416033289,0.0556534788\H,10.3546614247,-2.2356229282,0.1118132
903\H,12.9573871699,-2.2218588792,0.04424612\H,15.6878460513,2.0288892

624,0.3968337242\\Version=ES64L-G09RevD.01\HF=-4368.0824121\RMSD=4.586
e-09\RMSF=6.700e-06\Dipole=0.0029578,0.000064,-0.0000284\Quadrupole=-9
8.042092,60.7356023,37.3064897,38.0191088,10.4417086,-0.1998041\PG=C01
[X(C28H14N2S8)]\\@

TCLO1.pbe0

1\1\GINC-LCMD53\FOpt\RPBE1PBE\Gen\C12H8Cl2S5\ROOT\06-Jun-2016\0\\#PBE1
PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersi
on=GD3BJ Nosymm\\TCLO1.pbe0.freq\\0,1\C,-0.0593456965,0.1880779198,1.2
801810132\S,-0.1216286274,-1.0839479797,0.0046731244\C,-0.0362965686,0
.1573988521,-1.2992752278\C,-0.0109777303,1.4123725288,0.691989884\C,0
.0017416916,1.3953490583,-0.7396872468\H,0.058891792,2.3011469794,-1.3
429464582\H,0.0350444565,2.3324392678,1.274260358\C,-0.0356060453,-0.2
997677263,-2.6544301001\S,-0.3047369373,0.801530511,-3.972769799\C,-0.
0711364118,-0.4643403078,-5.1395003104\C,0.1784903635,-1.5836995733,-3
.1172506486\C,0.1581044528,-1.6743987786,-4.5275567792\S,-0.2707488911
,-0.1771377174,-6.8639605583\H,0.8432148524,0.5806686959,-7.0348840822
\H,0.3214465005,-2.592018821,-5.0902613755\H,0.3881092506,-2.423845773
9,-2.4553996144\C,-0.1469291053,-0.3411858448,5.1334495316\S,-0.334009
1676,0.9026623839,3.9350562755\C,-0.0818094218,-0.2362529227,2.6455747
383\C,0.0567035766,-1.5708602538,4.5524882367\C,0.0939384619,-1.513961
9102,3.1407698625\S,-0.3564599708,-0.0074173399,6.8483649703\H,0.77912
80363,0.7186552335,7.0148345227\H,0.285218168,-2.3755657991,2.50132641
9\H,0.1894049927,-2.4789943241,5.1381347738\Cl,2.1867575445,-1.2373534
572,0.0273870336\Cl,-2.401579566,-0.9988329007,-0.0160885428\\Version=
ES64L-G09RevD.01\HF=-3371.970796\RMSD=4.743e-09\RMSF=5.860e-06\Dipole=
0.698725,0.7928618,-0.0046002\Quadrupole=-17.1471794,5.2111175,11.9360
619,1.0180443,-0.2287671,-0.081078\PG=C01 [X(C12H8Cl2S5)]\\@

TCLO2.pbe0

1\1\GINC-LCMD36\FOpt\RPBE1PBE\Gen\C16H10Cl4S6\ROOT\08-Jun-2016\0\\#PBE
1PBE/gen SCF=(Tight) INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispe
rsion=GD3BJ Nosymm\\TCLO2.pbe0.freq\\0,1\C,-0.6586032285,-0.1927950644
,0.00909728\S,-1.9664464119,1.0093385128,-0.2581047828\C,-3.2245463453
,-0.2711762923,-0.069875344\C,-1.1950713887,-1.4342195655,0.1713309114
\C,-2.6216660586,-1.4763494118,0.1263748797\H,-3.1930265486,-2.3934103
124,0.2662203805\H,-0.5759033405,-2.3082391813,0.3726360373\C,-4.59135
06115,0.1251650743,-0.1760737899\S,-5.8535391639,-1.05346542,-0.391123
1284\C,-7.0755759468,0.1774913191,-0.3252784082\C,-5.1133204155,1.4034
542915,-0.1093313719\C,-6.5226930117,1.4311096218,-0.1916768474\S,-8.7
777898747,-0.1863363057,-0.569113698\H,-8.9135609483,-1.0362865959,0.4
805350948\H,-7.1271477448,2.3347286969,-0.134253787\H,-4.494726842,2.2
866918849,0.049450853\C,7.1017174276,-0.1028310305,-0.1483403363\S,5.8
857697966,1.1360789068,-0.13888578\C,4.6200995362,-0.0444345319,0.0425
369555\C,6.5486720364,-1.3538189094,0.0070709902\C,5.1412821059,-1.322
4228027,0.1176739619\S,8.8176916244,0.2741343961,-0.2112205596\H,8.801
3342961,0.9049935773,-1.413182187\H,4.5200254036,-2.2061511115,0.26288
04898\H,7.1500781435,-2.2610244019,0.0295835508\C,3.2484728539,0.34790
43364,0.0908920477\S,2.0021179908,-0.9299364639,-0.1773641083\C,0.6815
610792,0.2677784847,0.0434271803\C,2.6354898729,1.549348954,0.27648397
05\C,1.2081466885,1.5069245327,0.2491654884\H,0.5792067008,2.377712764
,0.4333451153\H,3.1984912781,2.4638524128,0.4604570732\Cl,-2.050105081
,1.4402252508,2.0193762422\Cl,-1.9072766832,0.6607026318,-2.499360582\

Cl,1.9711784834,-1.3993495365,2.0930230874\Cl,2.0527143275,-0.54347871
1,-2.4142768793\\Version=ES64L-G09RevD.01\HF=-4843.5747878\RMSD=2.320e
-09\RMSF=4.093e-06\Dipole=-0.098085,-0.0563393,0.0422067\Quadrupole=27
.3918034,3.391624,-30.7834274,7.6244449,-9.5864527,-1.9368919\PG=C01 [
X(C16H10Cl4S6)]\\@

TCLO3.pbe0

1\1\GINC-LCMD09\FOpt\RPBE1PBE\Gen\C20H12Cl6S7\ROOT\08-Jun-2016\0\\#PBE
1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispers
ion=GD3BJ Nosymm\\TCLO3.pbe0.freq\\0,1\C,-2.6547078788,-0.134444466,-0
.1809650285\S,-3.9328366118,1.081160058,0.1550996372\C,-5.2208689065,-
0.1547908498,-0.1142991699\C,-3.2214194031,-1.3513470517,-0.4208472507
\C,-4.6471005191,-1.3612472378,-0.3839777104\H,-5.2404017742,-2.252738
6142,-0.5843677129\H,-2.6231227127,-2.2260635049,-0.675755365\C,-6.576
8205341,0.2655300189,0.0178113426\S,-7.8629458577,-0.8924844857,0.2084
682618\C,-9.0430909091,0.3730749395,0.3360718176\C,-7.0686942082,1.557
938121,0.0255516047\C,-8.4666247392,1.6175771951,0.2085370101\S,-10.76
31522858,0.0410313402,0.4699720009\H,-10.6912097056,-0.733293456,1.582
4980064\H,-9.0440015638,2.5391051424,0.2589953136\H,-6.4329027039,2.43
27265173,-0.1109124339\C,9.0043253266,0.4454661577,0.0330719858\S,7.83
17087186,-0.8290387435,-0.0727073257\C,6.5285943835,0.3198600397,-0.19
3716355\C,8.4123944329,1.6864694282,-0.0507207282\C,7.0092532227,1.616
46083,-0.1822872622\S,10.7311401165,0.1295128475,0.0954555597\H,10.705
3649539,-0.6910738917,1.1763177508\H,6.3613010681,2.4876669502,-0.2784
644824\H,8.9826814013,2.6126531549,-0.0052899883\C,1.2526159617,0.3021
963303,-0.2367893813\S,-0.0179629991,-0.9587843021,-0.0566012583\C,-1.
3048281529,0.2910912021,-0.1939109105\C,0.6793160637,1.536327215,-0.32
92795112\C,-0.7455880093,1.530137768,-0.3052895132\H,-1.3505548378,2.4
284358261,-0.4249442118\H,1.2723074962,2.4396245229,-0.4695322559\C,5.
1728662937,-0.1113335421,-0.2826511809\S,3.8836824439,1.1125763279,0.0
330639177\C,2.6057701694,-0.1118691719,-0.2693408021\C,4.6006692449,-1
.3212726105,-0.5405419203\C,3.17462483,-1.3229094402,-0.5328252161\H,2
.5756173289,-2.2012167216,-0.7733573574\H,5.1944804754,-2.2069158048,-
0.7640312692\Cl,-3.9973550976,1.6540052493,-2.0872476941\Cl,-3.9003747
065,0.5813302998,2.3706854689\Cl,-0.0550316815,-1.2576555712,-2.359229
734\Cl,0.0181953853,-0.7471091636,2.1918852297\Cl,3.8750821667,1.69652
55952,-2.2071997266\Cl,3.9224043146,0.6019655521,2.2461778483\\Version
=ES64L-G09RevD.01\HF=-6315.1778529\RMSD=5.827e-09\RMSF=5.796e-06\Dipol
e=0.0403714,-0.7573394,0.5355142\Quadrupole=45.9267117,-0.8396522,-45.
0870595,0.0100903,-1.6614749,2.3312266\PG=C01 [X(C20H12Cl6S7)]\\@

TCLO4.pbe0

1\1\GINC-LCMD01\FOpt\RPBE1PBE\Gen\C24H14Cl8S8\ROOT\09-Jun-2016\0\\#PBE
1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(maxstep=10) IOP(2/17=4) Emp
iricalDispersion=GD3BJ Nosymm\\TCLO4.pbe0.freq\\0,1\C,-0.6748760526,-0
.2304021675,0.1954689995\S,-1.9371783312,1.0468717858,0.1049158562\C,-
3.2314576144,-0.2005921314,0.1949135173\C,-1.2567548576,-1.4649187127,
0.2316651585\C,-2.6801981527,-1.4489220491,0.2306273748\H,-3.289957016
3,-2.3481458499,0.3119985259\H,-0.6678723189,-2.3779044228,0.316571636
4\C,-8.5020736452,-0.1152208988,0.0663286645\S,-9.7867879719,1.0610623
486,0.0303180654\C,-10.9881092406,-0.1887008984,-0.0265085609\C,-9.006
7993826,-1.4008225957,-0.0136530992\C,-10.415700087,-1.4418468343,-0.0
626423436\S,-12.7010645613,0.1610194249,-0.1815980534\H,-12.7769722297

,1.0460591534,0.8439584765\H,-11.0052655728,-2.3562957996,-0.0983033222\H,-8.3736829512,-2.2874494363,0.0202179935\C,10.9815218178,0.1805418564,-0.2893420384\S,9.7907649387,-1.0804017183,-0.2649822135\C,8.5057902635,0.0767375027,-0.0461912492\C,10.4111018149,1.4215204624,-0.1045218431\C,9.0094284588,1.3624187838,0.0374872263\S,12.701727967,-0.1495407549,-0.393809484\H,12.6354429029,-1.0108482064,-1.4399823569\H,8.3773597736,2.2366069054,0.1930802924\H,10.9942412654,2.3406390222,-0.090067031\C,3.2380862601,0.1382294919,0.1911391798\S,1.9388014631,-1.0547375444,-0.1668193801\C,0.681440589,0.1673207999,0.23245691\C,2.6911300095,1.3450125841,0.5197402423\C,1.2678134291,1.3604418312,0.5434709415\H,0.6834001388,2.2302984081,0.8424797294\H,3.3046940929,2.2019451201,0.7959106993\C,7.1461016462,-0.3384258224,0.0136023607\S,5.8758702571,0.9450658262,-0.009465251\C,4.5814699046,-0.2931653403,0.0998973208\C,6.5541450465,-1.5669061618,0.0658171999\C,5.1312993947,-1.5424134302,0.1122499505\H,4.5198136871,-2.4400207621,0.204512408\H,7.1330541524,-2.4893778903,0.0924864105\C,-4.5762987629,0.2350688752,0.2244203156\S,-5.8714343804,-0.9495736263,-0.1515489828\C,-7.1419268534,0.2862072847,0.1931920687\C,-5.1271078065,1.445545486,0.5311206857\C,-6.5509490095,1.4739671571,0.5115476632\H,-7.1311700865,2.3621524744,0.7588833622\H,-4.5154615484,2.3006094471,0.8190817148\Cl,-5.8600485652,-0.3484898741,-2.3405546818\Cl,-5.922825337,-1.6195104571,2.0637651518\Cl,-1.9444541238,0.9520360923,-2.1518468709\Cl,-1.9407906212,1.2158351982,2.4193517188\Cl,1.9184688409,-0.4395845516,-2.3399585137\Cl,1.9720484504,-1.7549946558,2.0454076875\Cl,5.8296374328,0.8714747603,-2.2816816261\Cl,5.9636420827,1.08158451,2.2947843934\\Version=ES64L-G09RevD.01\HF=-7786.7807108\RMSD=3.066e-09\RMSF=7.302e-06\Dipole=-0.0083546,0.0157615,-0.0677506\Quadrupole=73.957329,-8.0254256,-65.9319035,-14.4994863,-16.3634215,9.0241462\PG=C01 [X(C24H14Cl8S8)]\\@

TDOA1.pbe0

1\1\GINC-NODE05\FOpt\RPBE1PBE\Gen\C8H4O2S5\GRYNOVA\02-Mar-2017\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersion=GD3BJ Nosymm\\TDOA1.pbe0.freq\\0,1\S,0.2810243314,-2.5715751232,-0.074010558\C,0.7723162473,0.0098147704,-0.003963316\S,1.8740370483,1.3239992988,0.0597501776\C,3.2386587432,0.2259014648,0.0935249561\C,1.438852175,-1.1976200154,-0.0178893683\C,2.8427816491,-1.092860714,0.0353077667\S,4.8858912563,0.8445130477,0.0783503869\H,4.9801380253,1.1010852414,1.409297381\H,3.5425261984,-1.9261875689,0.0357660114\C,-3.1344170747,-0.3501727632,-0.130634769\S,-1.9905878042,0.9739244258,-0.0438921172\C,-0.6692224358,-0.1210089211,-0.0332834129\C,-2.5064406337,-1.576882015,-0.1286171862\C,-1.1065081134,-1.4285035194,-0.0749767654\S,-4.8663218703,-0.0410136807,-0.0959566589\H,-5.0112400948,0.2452308699,-1.416269737\H,-3.0442083995,-2.5219823037,-0.1680440388\O,0.3253661901,-3.3317392303,1.1855213147\O,0.3701345619,-3.2717032639,-1.365550067\\Version=ES64L-G09RevD.01\HF=-2447.4359409\RMSD=7.647e-09\RMSF=9.745e-06\Dipole=-0.1424379,1.5632737,0.0339456\Quadrupole=11.7168049,-9.4284991,-2.2883058,1.9245743,8.1045972,0.5371488\PG=C01 [X(C8H4O2S5)]\\@

TDOA2.pbe0

1\1\GINC-NODE07\FOpt\RPBE1PBE\Gen\C10H4O4S6\GRYNOVA\02-Mar-2017\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersion=GD3BJ Nosymm\\TDOA2.pbe0.freq\\0,1\C,-0.5296767424,1.3427967732,-0.0087677368\S,-1.7622481551,2.6629517882,-0.1219861118\C,-3.084005913

3,1.4609141133,0.065661868\C,-2.566100864,0.1858263143,0.1948579285\S,
-3.812936696,-0.9757512765,0.3790543539\C,-5.0324445191,0.2758310294,0
.314610621\C,-4.4870707507,1.5310475693,0.1309320313\S,-6.7436372313,-
0.1313640707,0.3593172857\H,-6.8237409279,-0.3506516671,1.6975847613\H
,-5.0857804984,2.4365696424,0.0580387256\C,3.3752389921,1.2079412103,-
0.1686316727\S,2.1557013902,2.4594543888,-0.2339018399\C,2.8298860003,
-0.0471833375,0.0157269698\S,5.0863996297,1.6153053372,-0.2133460145\H
,5.1668765927,1.8326638638,-1.5519083662\H,3.4286117413,-0.9526472369,
0.0892157769\C,1.4268362174,0.0230075492,0.0812393938\S,0.105059935,-1
.1791194884,0.268280428\C,-1.1275781758,0.1408645194,0.1537329431\C,0.
9088990871,1.2980035446,-0.048761673\O,-1.6653177089,3.5314219475,1.05
98900222\O,-1.7512816757,3.2322949268,-1.476954312\O,0.0926699492,-1.7
479687767,1.6234467876\O,0.0095803235,-2.048028664,-0.9133921699\\Vers
ion=ES64L-G09RevD.01\HF=-3071.8301958\RMSD=8.868e-09\RMSF=8.220e-06\Di
pole=-0.000118,-0.0005967,-0.0003465\Quadrupole=21.2699298,-14.3017644
,-6.9681654,4.7743292,-10.7835895,-1.9127466\PG=C01 [X(C10H4O4S6)]\\@

TDOA3.pbe0

1\1\GINC-NODE07\FOpt\RPBE1PBE\Gen\C12H4O6S7\GRYNOVA\02-Mar-2017\0\\#PB
E1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDisper
sion=GD3BJ Nosymm\\TDOA3.pbe0.freq\\0,1\S,-1.9970464656,2.3457741248,-
0.268820016\C,-3.2772420476,1.1002796333,-0.0560050825\C,-1.2855533613
,-0.1328994418,0.1934848643\C,-2.7209825803,-0.1472412193,0.1591368339
\S,-3.9329741471,-1.3309436331,0.4356728634\C,-5.1866134513,-0.1195899
021,0.3053156759\C,-4.6790491785,1.1374594202,0.0377751959\S,-6.887298
6784,-0.5634104784,0.3610987912\H,-6.9294253697,-0.8666931914,1.684306
6035\H,-5.3036272091,2.0203500421,-0.0815175858\C,5.1524725512,-0.2662
521212,-0.2473757168\S,3.8814189541,-1.4530528626,-0.0688735015\C,4.66
39711546,1.0252178286,-0.3023605835\C,3.262252824,1.0333849659,-0.2002
267483\S,6.8468032967,-0.7323739423,-0.1904260866\H,6.868326184,-1.398
1744438,-1.3738108628\H,5.3012679524,1.9005373801,-0.4096338593\S,-0.0
258304968,-1.4288106978,0.1905808154\C,0.7023369351,1.0434162695,-0.22
90737197\C,-0.7175234612,1.0796609814,-0.0249396004\S,2.0007727947,2.3
113054502,-0.3072295332\C,2.687228175,-0.2197778983,-0.0969733202\C,1.
2522988764,-0.1934374639,-0.136631928\O,0.1896600425,-1.9816416848,1.5
335389296\O,-0.2510173686,-2.3007211326,-0.9690383164\O,1.9400031615,3
.1071437695,0.9246185982\O,2.040730637,2.9451439375,-1.6293214322\O,-1
.926062304,2.8077972652,-1.6602198733\O,-2.0256274195,3.2903490453,0.8
528685951\\Version=ES64L-G09RevD.01\HF=-3696.2192849\RMSD=5.251e-09\RM
SF=2.977e-06\Dipole=-0.0006652,-1.6761453,0.2133007\Quadrupole=33.6168
306,-21.9916617,-11.6251689,-2.0762402,-12.0992774,1.4672238\PG=C01 [X
(C12H4O6S7)]\\@

TDOA4.pbe0

1\1\GINC-NODE08\FOpt\RPBE1PBE\Gen\C14H4O8S8\GRYNOVA\02-Mar-2017\0\\#PB
E1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDisper
sion=GD3BJ Nosymm\\TDOA4.pbe0.freq\\0,1\C,0.2258161987,0.6419273767,0.
0708952919\S,-1.0911514286,1.718045316,0.6964753977\C,-3.7355211963,0.
4006867063,0.323755026\S,-4.9843691406,1.4493382425,0.8667430083\C,-6.
1984556574,0.2671070747,0.4413668727\C,-4.2556466365,-0.7713045613,-0.
1961190956\C,-5.6538961095,-0.8745869705,-0.1186810018\S,-7.9137495202
,0.6193523462,0.5728318217\H,-7.9196619574,0.8773930558,1.905502227\H,
-6.2501379731,-1.7242002122,-0.4450652889\C,6.1398338341,-0.241524782,

-0.5473025228\S,4.9422169344,-1.50200197,-0.7076100717\C,3.6852218201,
-0.3911570229,-0.342123314\C,5.5863805726,0.9728352715,-0.1845718799\C
,4.1893915817,0.8715087971,-0.0841735341\S,7.8539266448,-0.5892757362,
-0.7314102515\H,7.826364008,-0.8189945304,-2.0696319041\H,6.1745384527
,1.8756043052,-0.0336174004\C,2.2643267068,-0.4840098818,-0.17519315\S
,1.0437317883,-1.742788664,-0.6232423186\C,-0.291764763,-0.5566546055,
-0.3140476597\S,2.8687705679,2.0119567261,0.3541673019\C,-1.6993310252
,-0.7022391311,-0.1034769758\S,-2.9384222102,-1.8988818785,-0.67717048
01\C,-2.3045264181,0.4091947872,0.3921882509\C,1.6521025825,0.67472563
15,0.1825608115\O,-2.9682701257,-3.0906849938,0.1768351158\O,-2.824098
7501,-2.0029167961,-2.1369587638\O,0.9614775917,-2.7997966859,0.389516
8304\O,1.2061752618,-2.0411956485,-2.0492603442\O,-0.8690728962,1.9264
525514,2.1307057999\O,-1.3888582319,2.8269373682,-0.2149617893\O,3.008
632707,2.4301422177,1.75261255\O,2.624816787,2.9854762967,-0.717428559
4\\Version=ES64L-G09RevD.01\HF=-4320.6091758\RMSD=4.188e-09\RMSF=5.754
e-06\Dipole=-0.1184309,-0.0219658,0.0987585\Quadrupole=47.3429398,-30.
1986245,-17.1443153,-8.819745,-18.2756899,-0.3530632\PG=C01 [X(C14H4O8
S8)]\\@

TDO1.pbe0

1\1\GINC-LCMD22\FOpt\RPBE1PBE\CC-pVDZ\C12H8O2S5\ROOT\01-Mar-2016\0\\#P
BE1PBE/cc-pVDZ SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalD
ispersion=GD3BJ Nosymm\\TDO1\\0,1\C,-2.8923588947,1.8346784315,-0.0651
273555\S,-1.4856304427,0.7022684269,0.0431890782\C,-0.2821286732,2.051
2420867,-0.00982711\C,-2.4101722658,3.0993857453,-0.1028521033\C,-0.96
36566129,3.2194810564,-0.0719304701\O,-1.4578397154,0.0485224263,1.364
5451187\O,-1.3928507777,-0.1271710347,-1.1752837609\H,-0.4725499685,4.
1927623546,-0.1063034837\H,-3.0525375357,3.9788716013,-0.1630072585\C,
1.1106282748,1.7319901286,0.0451908017\S,2.3279178631,2.9636380173,0.2
394006116\C,3.5962933808,1.7759736635,0.2519388469\C,1.6871734511,0.47
71799929,-0.0332380055\C,3.0952091917,0.5059993262,0.085967881\S,5.294
6290249,2.230858168,0.328213318\H,5.2798762243,2.7207653576,1.59481816
76\H,3.7343680695,-0.3753234289,0.0611310603\H,1.1004566173,-0.4302666
711,-0.1709407801\C,-6.6802204447,0.9308639781,-0.1887258501\S,-5.6266
640121,2.310044117,-0.1058966006\C,-4.2138734692,1.2902964969,-0.08674
59929\C,-5.9683080021,-0.2456815686,-0.1675206019\C,-4.5704062648,-0.0
459714351,-0.1089351615\S,-8.4318065494,1.0982040536,-0.1490562002\H,-
8.5708161007,1.6886128188,-1.3644156708\H,-3.835583282,-0.850111487,-0
.1077271363\H,-6.450689086,-1.2212326222,-0.2052813421\\Version=ES64L-
G09RevD.01\HF=-2602.0829126\RMSD=6.328e-09\RMSF=5.629e-05\Dipole=-0.11
80755,1.1256836,-0.1316829\Quadrupole=5.6662146,5.6477732,-11.3139878,
-3.6229664,10.2541078,0.5257438\PG=C01 [X(C12H8O2S5)]\\@

TDO2.pbe0

1\1\GINC-LCMD49\FOpt\RPBE1PBE\CC-pVDZ\C16H10O4S6\ROOT\02-Mar-2016\0\\#
PBE1PBE/cc-pVDZ SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) Empirical
Dispersion=GD3BJ Nosymm\\TDO1\\0,1\C,1.3327887077,-0.2267435401,-0.029
0410612\S,-0.0186120005,0.9652165993,0.0405549504\C,-1.2742037705,-0.3
342749078,-0.0805230416\C,0.8055775467,-1.4765900644,-0.1059094024\C,-
0.6401072655,-1.5330992035,-0.1334837899\O,-0.0686069289,1.6000443493,
1.3704389389\O,-0.0220570363,1.8154238525,-1.165960933\H,-1.1707505596
,-2.4835001768,-0.2000956552\H,1.4216884041,-2.3747490663,-0.150003146
3\C,-2.6506749488,0.0403805017,-0.079291404\S,-3.9268776614,-1.1444758

174,0.0151396609\C,-5.1416650784,0.0960166461,0.0193929225\C,-3.171830
4478,1.3214454085,-0.1399718727\C,-4.5823400541,1.3497905509,-0.080774
0104\S,-6.8602033334,-0.2759393866,0.0050454465\H,-6.8871369418,-0.973
1606255,1.1696912542\H,-5.1820852729,2.2584638182,-0.0970272579\H,-2.5
428671329,2.2073654993,-0.2197104377\C,9.1447890501,-0.0934060299,-0.0
380449469\S,7.9299274064,1.1470375304,-0.0327770647\C,6.65371519,-0.03
79874423,0.0582990022\C,8.5853906516,-1.3473538681,0.0592985584\C,7.17
48250756,-1.3191727384,0.1172217698\S,10.8632617987,0.279056346,-0.021
5463402\H,10.892221205,0.9729450154,-1.188143463\H,6.5458553693,-2.205
2937925,0.1945473007\H,9.1852035749,-2.2559989411,0.0746184921\C,5.277
2014016,0.3365819807,0.0589751946\S,4.0216753108,-0.9631273227,-0.0604
598697\C,2.6702283626,0.228886691,0.0072672401\C,4.643045826,1.5354126
653,0.1108708996\C,3.1973712724,1.4788240599,0.0831131978\O,4.07184189
41,-1.6000481146,-1.3893773425\O,4.0250466308,-1.8114210577,1.14734233
93\H,2.5811988436,2.3770026972,0.1258879858\H,5.1736369105,2.485907884
1,0.1765568852\\Version=ES64L-G09RevD.01\HF=-3303.8131331\RMSD=5.296e-
09\RMSF=5.068e-06\Dipole=-0.0022802,-0.0008805,-0.0033315\Quadrupole=2
1.589627,-2.8541597,-18.7354673,10.8855589,-9.561441,-2.4201142\PG=C01
[X(C16H10O4S6)]\\@

TDO3.pbe0

1\1\GINC-LCMD49\FOpt\RPBE1PBE\CC-pVDZ\C20H12O6S7\ROOT\01-Mar-2016\0\\#
PBE1PBE/cc-pVDZ SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) Empirical
Dispersion=GD3BJ Nosymm\\TDO1\\0,1\C,1.3461846572,-0.3341983292,-0.063
1716045\S,0.0387337696,0.9009299852,0.0645393404\C,-1.2624217918,-0.35
21233383,-0.083631349\C,0.7738310772,-1.5637206314,-0.1669123238\C,-0.
670913144,-1.5717985689,-0.1748262668\O,0.0184056983,1.4876267079,1.41
59389197\O,0.0533226122,1.7919291294,-1.1123593084\H,-1.2343958849,-2.
5013684706,-0.261341637\H,1.3599417256,-2.4782161471,-0.2604473055\C,-
2.6228124011,0.0691257288,-0.0551848496\S,-3.9402783133,-1.0739265646,
0.0075469454\C,-5.1089768467,0.2072842254,0.0729057416\C,-3.100180671,
1.3692087246,-0.0631620857\C,-4.5071200601,1.4448271986,0.0137711613\S
,-6.8396452615,-0.0947266847,0.0632306731\H,-6.8601668538,-0.957399741
9,1.1106994329\H,-5.0734711167,2.3743604629,0.0415094846\H,-2.44149485
61,2.2354351987,-0.1148935718\C,13.1116644617,0.2041526044,0.015478544
4\S,11.9390260798,-1.0736594023,0.0757066501\C,10.6221543085,0.0699003
426,0.0143749175\C,12.5096023144,1.4427283159,-0.009225342\C,11.100405
2976,1.3695980609,-0.0068092537\S,14.8382611648,-0.0975378079,0.136407
865\H,14.9180843599,-0.9941303948,-0.8792509653\H,10.4418907487,2.2359
440083,-0.0584780669\H,13.0782442004,2.3704825516,-0.047701949\C,5.299
85585,0.0678586188,-0.0370213908\S,3.9998304143,-1.1844644938,0.001063
5578\C,2.6996534699,0.0672802368,-0.0482738171\C,4.7213567692,1.299864
0753,-0.0511217403\C,3.2777370169,1.2995322232,-0.057488134\O,4.005456
5963,-1.9814476131,-1.2419533541\O,3.9943666175,-1.8781214338,1.301185
6864\H,2.6966945965,2.2211854257,-0.0891381697\H,5.3021297959,2.221862
2007,-0.0770676842\C,9.2621646341,-0.3514873784,-0.0289528314\S,7.9593
544829,0.901900352,0.1022018446\C,6.6535261855,-0.3331732159,-0.041325
4466\C,8.6717113696,-1.5709967812,-0.1291686579\C,7.2270558868,-1.5625
608888,-0.1400270602\O,7.9597752231,1.4929569117,1.4517062818\O,7.9628
659003,1.7888990953,-1.0778831055\H,6.6419440734,-2.4769341865,-0.2407
645773\H,9.236155843,-2.5004713119,-0.2100411987\\Version=ES64L-G09Rev
D.01\HF=-4005.5424751\RMSD=7.054e-09\RMSF=4.521e-06\Dipole=0.0268498,-
1.2464288,-0.4191714\Quadrupole=41.801166,-10.2434739,-31.5576922,-9.6

73004,-15.2420977,0.4425263\PG=C01 [X(C20H12O6S7)]\\@

TDO4.pbe0

1\1\GINC-LCMD56\FOpt\RPBE1PBE\CC-pVDZ\C24H14O8S8\ROOT\02-Mar-2016\0\\#
PBE1PBE/cc-pVDZ SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) Empirical
Dispersion=GD3BJ Nosymm\\TDO1\\0,1\C,5.3204428819,-0.1884561176,-0.039
6372279\S,4.0432156964,1.075196714,0.1352062294\C,2.7207966566,-0.1434
192144,-0.0364403317\C,4.7186262245,-1.4020972989,-0.1876626553\C,3.27
71065659,-1.3780033843,-0.1853566822\O,4.0511992149,1.6306303463,1.500
0898336\O,4.0574816126,1.9934366086,-1.0196863823\H,2.6816583885,-2.28
26586766,-0.3073171082\H,5.2826500794,-2.3262561504,-0.314379375\C,-2.
5978422759,-0.0354213915,-0.0050175091\S,-3.8933236537,1.1292932783,0.
1152481988\C,-5.0877811772,-0.1283062646,0.0833938027\C,-3.1026078376,
-1.3218250457,-0.105121008\C,-4.5109570419,-1.372673276,-0.0503984923\
S,-6.8112984321,0.2056878615,0.0728703031\H,-6.8124667659,1.0808963925
,1.1095844116\H,-5.0957366499,-2.2903406428,-0.0884384847\H,-2.4620323
358,-2.1984713759,-0.1931634424\C,17.0901404843,0.1365183022,-0.016085
6279\S,15.8967415022,-1.1214111361,0.0305482233\C,14.5987716032,0.0464
040163,0.0001061393\C,16.5101537373,1.3866630444,-0.0144304687\C,15.10
07008203,1.3377612831,-0.0012123822\S,18.8119658236,-0.1903520502,0.08
37993081\H,18.8437967457,-1.1742269223,-0.8496476353\H,14.457417178,2.
2164607813,-0.0328516694\H,17.0938391024,2.3053778838,-0.0431105332\C,
9.2802047248,0.1385549675,-0.0041988363\S,7.9590810584,-1.0925227792,-
0.0519919479\C,6.6807829711,0.1812200765,-0.0061221647\C,8.722707608,1
.3798785808,0.0607579415\C,7.2813100992,1.4027258104,0.0597949331\O,7.
9492744312,-1.7927556393,-1.3507479112\O,7.948007588,-1.8794302829,1.1
937688638\H,6.7161224239,2.3342124407,0.0937617173\H,9.3177569192,2.29
2248955,0.0973510975\C,13.232873081,-0.3502586701,-0.041237141\S,11.95
38494461,0.9244383427,0.1197431836\C,10.6253309433,-0.2845018372,-0.03
24240075\C,12.6195175622,-1.5577929087,-0.1609828507\C,11.1767957452,-
1.5226371238,-0.1601569402\O,11.9740119775,1.4952905886,1.4778897958\O
,11.9669000784,1.8278368824,-1.0471473136\H,10.5751517832,-2.425424166
6,-0.2682138151\H,13.1661761884,-2.4957001205,-0.2630043217\C,1.376645
6615,0.2813959016,0.0085352293\S,0.04366848,-0.929958677,-0.061856334\
C,-1.2305009047,0.3572182208,0.0176303844\C,0.8298086448,1.5251784044,
0.0956962137\C,-0.6126010453,1.5654624229,0.1016573649\O,0.0267935495,
-1.6002051698,-1.3757123207\O,0.0205643451,-1.7438475317,1.1668272197\
H,-1.155477314,2.5089422915,0.1655652593\H,1.4351338063,2.4305634566,0
.1460482668\\Version=ES64L-G09RevD.01\HF=-4707.2715919\RMSD=3.634e-09\
RMSF=2.247e-06\Dipole=0.0315447,-0.0022844,-0.2736482\Quadrupole=64.95
31532,-19.5422882,-45.4108651,-23.1366571,-18.7281752,4.2038366\PG=C01
[X(C24H14O8S8)]\\@

TDO5.pbe0

1\1\GINC-NODE08\FOpt\RPBE1PBE\Gen\C28H16O10S9\GRYNOVA\27-Feb-2017\0\\#
PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDisp
ersion=GD3BJ Nosymm\\TDO5.pbe0.freq\\0,1\C,5.3976562953,-0.1231796215,
-0.0955406953\S,4.0928087439,1.1116776042,0.0626847935\C,2.8010221239,
-0.1444122414,-0.0509848429\C,4.8254110429,-1.3553170821,-0.2142817428
\C,3.3850563666,-1.3682047612,-0.1886648067\O,4.1075500457,1.710204643
1,1.4098068747\O,4.0641665032,1.9915447978,-1.1199207961\H,2.810131706
6,-2.2901223314,-0.2723814349\H,5.411942353,-2.2676644149,-0.322833764
9\C,-2.5104252348,-0.1656909814,0.0780435855\S,-3.834852665,0.97252856

21,0.1047402532\C,-4.9965408389,-0.3138056784,0.1594970687\C,-2.982505
0028,-1.4686823809,0.0691560975\C,-4.3889398773,-1.5508254102,0.119721
299\S,-6.7267269634,-0.0284164306,0.1158036481\H,-6.7436355177,0.98749
72821,1.0142075525\H,-4.9505469062,-2.4830660207,0.1480666256\H,-2.318
3071453,-2.3321143244,0.066265228\C,17.2455993333,0.3956305984,-0.0996
140022\S,15.9601428819,-0.8723382692,-0.2554583613\C,14.6403784766,0.3
456080015,-0.1195251603\C,16.6401226221,1.6082334579,0.0171608358\C,15
.198396795,1.5815936537,0.0088756612\C,18.6066086017,-0.0116750746,-0.
1335996814\H,14.6006728151,2.4885221376,0.1020364452\H,17.1929148915,2
.5424902634,0.1179842308\C,9.342948691,0.2997169118,-0.1046565487\S,8.
0529667855,-0.9594103273,-0.194813018\C,6.7464923293,0.2804113632,-0.0
775814986\C,8.7566056788,1.525762463,0.0072249602\C,7.3168203713,1.515
0803112,0.0222967786\O,8.0439529992,-1.5951477469,-1.5247779991\O,8.07
18471799,-1.8029637092,1.0132349837\H,6.7299349698,2.4298206302,0.1038
338676\H,9.3316216913,2.4490390241,0.0760543872\C,13.2940316259,-0.066
4376154,-0.1616382359\S,11.9864704189,1.169560993,-0.01268186\C,10.696
9991412,-0.0836334688,-0.1513969888\C,12.72529218,-1.2982306191,-0.292
3530195\C,11.2846922781,-1.3065912614,-0.2876372015\O,11.9916515261,1.
7587748605,1.3384879441\O,11.9765109132,2.0576531635,-1.1895736767\H,1
0.7093346714,-2.2268096858,-0.3892607259\H,13.3116526291,-2.2111175288
,-0.3938732315\C,1.4498958978,0.2479591818,0.0178467959\S,0.1451167491
,-0.9876872201,-0.1022729116\C,-1.1548578722,0.2606613604,0.0885717566
\C,0.8770851072,1.4750976384,0.1641523053\C,-0.5644625897,1.4811576919
,0.2002737333\O,0.106381381,-1.5605010979,-1.4593146779\O,0.1756473748
,-1.8883319995,1.0654190292\H,-1.1283418336,2.4068171115,0.3176256202\
H,1.4637934468,2.3896100331,0.2530210043\C,19.0967977134,-1.3078650699
,-0.1517884637\C,20.5049310847,-1.3702141336,-0.1257657112\C,21.095665
0815,-0.1247903403,-0.0955047191\S,19.9151908562,1.1450766728,-0.12876
38914\S,22.8206150068,0.1850210465,-0.1689245981\H,18.4450257295,-2.18
06776834,-0.1446239871\H,21.0799981064,-2.29447841,-0.1080698091\H,22.
8388012619,1.2004561096,0.7300087567\O,15.9798817423,-1.4563810399,-1.
6082360203\O,15.966288229,-1.7629835881,0.9200819602\\Version=ES64L-G0
9RevD.01\HF=-5409.0462291\RMSD=9.510e-09\RMSF=3.319e-06\Dipole=-0.0024
174,1.3143783,0.6869749\Quadrupole=91.739239,-30.5806622,-61.1585768,2
0.9395973,8.6404685,4.2794504\PG=C01 [X(C28H16O10S9)]\\@

TDO6.pbe0

1\1\GINC-NODE01\FOpt\RPBE1PBE\Gen\C32H18O12S10\GRYNOVA\28-Feb-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDis
persion=GD3BJ Nosymm\\TDO6.pbe0.freq\\0,1\C,5.4582384445,-0.1367417354
,0.0212203995\S,4.1755207143,1.1206431045,0.1813031042\C,2.8616234336,
-0.1084614898,0.0260412595\C,4.8639299047,-1.3561453049,-0.1227527615\
C,3.4240494416,-1.3417600246,-0.120531455\O,4.1839435741,1.6946788942,
1.5386060053\O,4.1787233413,2.0210216671,-0.9863528219\H,2.8329840288,
-2.2499715388,-0.235666953\H,5.4347930142,-2.2780827637,-0.2339894631\
C,-2.4491206208,-0.0292770304,0.0672247319\S,-3.7526078222,1.117483623
8,0.2601642953\C,-4.9386902896,-0.127099083,0.0367584836\C,-2.94547237
41,-1.3103439736,-0.1171279524\C,-4.3536543917,-1.3636158316,-0.138736
5647\S,-6.6613294702,0.1707941018,0.1738202849\H,-6.6758689381,1.34001
39775,-0.513247004\H,-4.9329408747,-2.2714826993,-0.2983377441\H,-2.29
78575226,-2.1732033944,-0.2675124261\C,17.304670059,0.0901870063,0.019
9970529\S,15.9894758685,-1.139526037,-0.1178046438\C,14.7080864972,0.12
02262443,0.0335406449\C,16.7434707105,1.3246800028,0.1616167238\C,15.3

036498799,1.3399056377,0.1698646747\C,18.6481639144,-0.3279371295,-0.0
348993612\H,14.7337292448,2.2629562737,0.2766035817\H,17.3352666895,2.
2343146345,0.2604861779\C,9.4106387865,0.1981720923,0.0562619916\S,8.0
939703971,-1.0263277442,-0.0966716596\C,6.8145569134,0.2370663605,0.06
42912519\C,8.8504536753,1.432943567,0.2073592252\C,7.4112970185,1.4547
969228,0.2115912444\O,8.080517281,-1.6007235215,-1.4537699723\O,8.0837
589306,-1.9237820971,1.0722855283\H,6.8444673719,2.3786598571,0.325193
5931\H,9.4451834758,2.3396004447,0.3182056661\C,13.3515158431,-0.25320
45621,-0.0043012211\S,12.0726270554,1.0118561639,0.1477028852\C,10.755
486831,-0.2134719668,0.0056968408\C,12.7542877784,-1.471563098,-0.1442
981695\C,11.3151854487,-1.4492898036,-0.1385673384\O,12.0865783441,1.5
98257652,1.4996842438\O,12.0829629828,1.8988040074,-1.0291802371\H,10.
7200585728,-2.3566368011,-0.2413320025\H,13.320765502,-2.3962382927,-0
.2529125432\C,1.5175593057,0.3093426582,0.0711159202\S,0.1924179901,-0
.9084732767,0.0092994161\C,-1.0870870004,0.3730493673,0.0867456711\C,0
.9652737994,1.5516424724,0.1626129925\C,-0.475637366,1.5856452534,0.17
38322252\O,0.1724319912,-1.5837509,-1.3020381547\O,0.1785149121,-1.715
9341539,1.2414678706\H,-1.0238128031,2.5257019066,0.2397435283\H,1.567
8494892,2.4588257132,0.2128889877\C,19.1992421465,-1.5658807946,-0.178
3547752\C,20.6400934288,-1.6002284191,-0.1954794859\C,21.2527213534,-0
.3914965868,-0.0709401848\S,19.9748335266,0.8819579636,0.1036200227\C,
22.6152893189,0.0086344742,-0.0408124992\H,18.5961591567,-2.4687345099
,-0.2768106595\H,21.1872802439,-2.5364214327,-0.3079772332\S,23.918566
4422,-1.1541637949,-0.0709380122\O,15.9784161765,-1.7288974972,-1.4689
589331\O,15.9873960406,-2.0264448048,1.0595330267\O,19.9786452619,1.78
2350707,-1.0644010244\O,20.0062897314,1.4541677401,1.461131972\C,23.11
21213612,1.3022820672,-0.0072172137\C,24.5199541124,1.3585161847,-0.04
12327463\C,25.1044726425,0.1104783401,-0.092915074\S,26.8282407344,-0.
2064474757,-0.0368539787\H,22.4646343998,2.1782503837,0.0029976906\H,2
5.0990875317,2.2803699238,-0.0494826161\H,26.8297274071,-1.2354778223,
-0.9202078051\\Version=ES64L-G09RevD.01\HF=-6110.7820234\RMSD=8.336e-0
9\RMSF=1.874e-06\Dipole=-0.0082483,0.0529543,-0.607822\Quadrupole=120.
3405985,-42.332849,-78.0077495,-35.2067433,-15.2096346,3.7813607\PG=C0
1 [X(C32H18O12S10)]\\@

PEDOT1g.pbe0

1\1\GINC-R05-NODE05\FOpt\RPBE1PBE\Gen\C14H10Au16O2S5\GRYNOVA\10-Aug-20
16\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\DXN1g.pbe0.freq\\0,1\C,0
.5629614831,0.2881799586,6.2668381155\S,0.1135196359,0.7455233477,7.88
85634206\C,1.6959106052,0.3655777454,8.5181380086\C,2.5119961959,-0.09
65335053,7.5076898501\C,1.9781847905,0.5165034811,9.919192441\S,3.4597
753303,-0.0583454166,10.631329613\C,2.9314271194,0.4375668889,12.21121
75042\C,1.1487541002,1.0656525877,10.881275187\C,1.6847443634,1.012325
6107,12.1838364225\S,3.9337017155,0.0872307394,13.6219374725\H,4.46384
52202,1.3252516624,13.8195138739\H,1.1703541145,1.3503470069,13.084763
1951\H,0.1698538168,1.48536652,10.6496924194\C,-1.5716024746,0.1956615
108,3.0228997012\S,0.0217611547,-0.191264109,3.5861003208\C,-0.3800798
473,0.3685805382,5.1868702004\C,-2.3537881828,0.7564548215,4.003572886
4\C,-1.676151039,0.8523305369,5.2374982561\S,-2.0534938881,-0.01915024
64,1.3440605227\H,-2.2246108432,-1.3700801144,1.3389589373\H,-2.120927
1683,1.2617472759,6.1443082412\H,-3.3792757423,1.0819996379,3.83344079
9\C,1.873658645,-0.1387660463,6.2386507792\O,2.4984643268,-0.565951781

3,5.118342564\C,3.916958585,-0.6007344308,5.27758814\C,4.2907221354,-1
.2437951762,6.5938743969\O,3.7966635923,-0.4773923287,7.6931757223\H,4
.3146302624,0.4272880204,5.2264206884\H,4.3060931808,-1.1814726931,4.4
320889027\H,5.3806242726,-1.2829621587,6.7126839858\H,3.8816439979,-2.
2673390176,6.6485910282\Au,0.,0.,0.\Au,2.49762,1.44199,0.\Au,2.49762,-
1.44201,0.\Au,-1.66508,0.,-2.35478\Au,0.83254,1.442,-2.35478\Au,0.8325
4,-1.442,-2.35478\Au,3.33017,2.88401,-2.35478\Au,3.33016,-2.88402,-2.3
5478\Au,2.35161,0.,15.5\Au,-0.14596,-1.44199,15.5\Au,-0.14596,1.44201,
15.5\Au,4.01674,0.,17.85478\Au,1.51914,-1.442,17.85478\Au,1.51914,1.44
2,17.85478\Au,-0.97851,-2.88401,17.85478\Au,-0.9785,2.88402,17.85478\\
Version=ES64L-G09RevD.01\HF=-4851.8732564\RMSD=7.301e-09\RMSF=9.680e-0
6\Dipole=0.5470451,-0.0800832,-0.3362296\Quadrupole=59.2859829,15.7478
163,-75.0337992,-2.0310083,45.2264375,7.5338682\PG=C01 [X(C14H10Au16O2
S5)]\\@

PEDOT2g.pbe0

1\1\GINC-R05-NODE20\FOpt\RPBE1PBE\Gen\C20H14Au16O4S6\GRYNOVA\09-Aug-20
16\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\DXN2g.pbe0.freq\\0,1\C,1
.068039782,-0.0289145288,8.7975639874\S,-0.5221981328,0.0768456183,8.0
737243353\C,0.1217418126,-0.0715340228,6.4564273221\C,2.0258194105,-0.
1785207123,7.811820955\C,1.494374439,-0.2013547631,6.4985104596\O,2.26
6006285,-0.3343304482,5.3951755351\O,3.3528951633,-0.292016588,8.06563
56121\C,-0.7372336095,-0.0672220066,5.3053063005\S,-0.1222841305,-0.37
72967405,3.7004431493\C,-1.718223842,-0.2467555731,3.0315460287\C,-2.1
04971325,0.1484835817,5.2793109671\C,-2.6614051965,0.0491665073,3.9867
107841\S,-2.0499758573,-0.383281697,1.3079409575\H,-2.0102127194,-1.73
88521935,1.183576906\H,-3.7169135745,0.1879274,3.7555444909\H,-2.68422
83128,0.3733472752,6.1745469305\C,4.0632509887,0.3436811151,15.9746712
269\S,2.466265284,0.4601194342,15.3056810665\C,3.0871984331,0.18276103
92,13.6973862827\C,5.0119610485,0.0780724885,15.0159412151\C,4.4587395
204,-0.0083279573,13.7211477126\S,4.3920053574,0.4575831944,17.7002679
908\H,4.3147647474,1.8089202003,17.8506038315\H,5.0426485087,-0.208261
0563,12.8230462866\H,6.06940816,-0.0469272424,15.2460936171\C,2.226122
5422,0.1718444799,12.547939678\S,2.8672145592,-0.0005421823,10.9319959
917\C,1.2721807661,0.0508114214,10.2126220962\C,0.850596748,0.26799120
08,12.5087412826\C,0.3143736508,0.1955477413,11.1990365466\O,-1.016442
2081,0.2602437229,10.9483952682\O,0.0795952553,0.4169864999,13.6105612
201\C,3.5808595923,-0.7906854284,5.7099780756\C,4.1365173634,-0.042107
0366,6.9004915128\C,-1.7413379351,0.7790377448,12.0618008607\C,-1.2918
966181,0.1228373823,13.3478517094\H,4.1895570226,-0.6124036884,4.81469
9859\H,3.5509646366,-1.8734503686,5.9213790584\H,5.1530938166,-0.38253
87937,7.1339156832\H,4.1539256631,1.0422467679,6.6943141334\H,-2.79988
75656,0.5669922946,11.8658588867\H,-1.5936327125,1.8714742723,12.12018
51752\H,-1.8581311252,0.5081764291,14.2049007933\H,-1.4253124326,-0.97
08006209,13.2851706738\Au,0.0000137859,0.0000005725,0.0000378331\Au,2.
4976177503,1.4419938964,-0.000008487\Au,2.497617919,-1.442013604,-0.00
00112474\Au,-1.6650787133,-0.0000002143,-2.3547809098\Au,0.8325398691,
1.4419977896,-2.3547813998\Au,0.8325397702,-1.4419978569,-2.3547813936
\Au,3.3301686019,2.8840124216,-2.3547790114\Au,3.3301581457,-2.8840232
116,-2.3547786889\Au,2.3514681806,0.0000098838,18.9999509509\Au,-0.146
1137968,-1.4420007434,19.000025185\Au,-0.1461176357,1.4420140942,19.00
00253605\Au,4.016597194,-0.0000027821,21.3547819842\Au,1.5189798691,-1

.4420037749,21.354774107\Au,1.5189847958,1.4419980758,21.3547758035\Au
,-0.9786644422,-2.8840196264,21.35477607\Au,-0.9786512936,2.8840350797
,21.3547738436\\Version=ES64L-G09RevD.01\HF=-5631.0427289\RMSD=4.809e-
09\RMSF=1.320e-05\Dipole=-0.0098933,0.0548998,0.017057\Quadrupole=74.8
270137,20.6096775,-95.4366912,0.6741936,39.177648,16.3686803\PG=C01 [X
(C20H14Au16O4S6)]\\@

PEDOT3g.pbe0

1\1\GINC-R06-NODE23\FOpt\RPBE1PBE\Gen\C26H18Au16O6S7\GRYNOVA\09-Aug-20
16\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\DXN3g.pbe0.freq\\0,1\C,1
.5725975624,0.1594470353,8.6486110368\S,-0.0333359906,0.390997604,7.99
01906684\C,0.5073785737,0.0825808903,6.3590700152\C,2.4592516872,-0.14
05818487,7.6310374428\C,1.8614749679,-0.1820726234,6.3466620408\O,2.55
95812099,-0.452228089,5.2188189415\O,3.7800352424,-0.3799817813,7.8319
969654\C,-0.4164067964,0.099593615,5.2614580614\S,0.0716231656,-0.3308
652501,3.6418540483\C,-1.553417407,-0.1229363928,3.0662577315\C,-1.765
3913008,0.4128658792,5.307265242\C,-2.4102687954,0.2873737615,4.059386
6318\S,-2.0028990709,-0.3186308842,1.3773005616\H,-1.9997959661,-1.678
6415388,1.3008206384\H,-3.4671064012,0.4873500341,3.8861529534\H,-2.26
89835364,0.7206777967,6.2232423768\C,5.550727003,0.2546392691,19.66683
34829\S,6.243991237,-0.0701920986,18.1039882903\C,4.7217114405,0.25914
09088,17.3196124902\C,4.2201195072,0.5833343771,19.5826377768\C,3.7522
752053,0.5897708684,18.2523726073\S,6.5294399303,0.0512898114,21.12228
53588\H,6.9713870009,1.3313224288,21.2691968299\H,2.7244876114,0.82552
92921,17.9769877875\H,3.6074630835,0.7890694841,20.4617816918\C,2.8198
780639,0.2833921402,12.3763452816\S,3.4117231902,-0.0191674804,10.7554
271403\C,1.8348192861,0.2717550493,10.0507593549\C,1.4734598931,0.5953
633972,12.3405024477\C,0.9227135445,0.5886007203,11.0405623711\O,-0.38
2610231,0.8670922424,10.7957552628\O,0.7399854872,0.8736222287,13.4473
582937\C,4.5652102144,0.1763153184,15.8947765243\S,3.0201901792,0.4968
406861,15.1468834881\C,3.6488302724,0.2017615109,13.5396967331\C,5.503
9761902,-0.137021625,14.9334269013\C,4.9907373991,-0.1206957026,13.612
4721742\O,5.7541998254,-0.4009307855,12.5250956588\O,6.7931912541,-0.4
420570508,15.2166930343\C,3.83696066,-1.021024196,5.5006682476\C,4.522
872706,-0.2708770288,6.6208177341\C,-1.1741941147,0.7850732826,11.9771
643284\C,-0.4962864814,1.501995101,13.1231930081\C,6.9518066917,-1.079
7107573,12.8880701046\C,7.621985534,-0.3934770225,14.0577354417\H,4.41
45426955,-0.9531427467,4.5701187355\H,3.7117136507,-2.0825796843,5.775
7980841\H,4.6359758393,0.7938742202,6.3512648065\H,5.5123041448,-0.698
9936122,6.8253683646\H,-1.3402928955,-0.2748054977,12.2379605953\H,-2.
136739906,1.2542743051,11.737260239\H,-1.1118152087,1.4591558596,14.03
06665247\H,-0.3149618126,2.5576231769,12.8554153111\H,7.5997216383,-1.
0598485485,12.0025746567\H,6.7201657375,-2.1282154201,13.1458225655\H,
7.8392625123,0.6589968804,13.8051414712\H,8.5568181736,-0.9016442397,1
4.3262404257\Au,0.0000067937,-0.0000040051,0.0000118574\Au,2.497617172
3,1.4419948978,-0.0000055593\Au,2.4976203166,-1.4420094518,-0.00000392
82\Au,-1.6650805523,0.0000011893,-2.3547796095\Au,0.8325398614,1.44200
20843,-2.3547787726\Au,0.8325417183,-1.442000627,-2.3547790085\Au,3.33
01697853,2.8840103719,-2.3547798482\Au,3.3301581834,-2.8840231464,-2.3
547787155\Au,4.94695385,-0.0000002357,22.9999927469\Au,2.4493574483,-1
.4419855803,22.9999871515\Au,2.4493624762,1.4420142891,22.9999845555\A
u,6.6120587799,-0.0000145725,25.3547808625\Au,4.1144929782,-1.44199586

69,25.3548012639\Au,4.1144214501,1.4419897024,25.3547797468\Au,1.61680
17077,-2.8839956374,25.3547858637\Au,1.6168180308,2.8840165883,25.3547
813935\\Version=ES64L-G09RevD.01\HF=-6410.2100228\RMSD=3.371e-09\RMSF=
5.588e-06\Dipole=0.5843582,-0.1539726,-0.2588008\Quadrupole=114.421268
4,32.4529041,-146.8741725,-4.6831525,45.0833956,14.0102494\PG=C01 [X(C
26H18Au16O6S7)]\\@

PEDOT4g.pbe0

1\1\GINC-R06-NODE24\FOpt\RPBE1PBE\Gen\C32H22Au16O8S8\GRYNOVA\10-Aug-20
16\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\DXN4g.pbe0.freq\\0,1\C,3
.5354465256,0.0120130107,13.5727818478\S,2.921337721,0.0967983718,15.2
121944852\C,4.5343194015,0.071030643,15.8950315308\C,4.9173398898,-0.0
323084737,13.5866412223\C,5.4752592946,-0.0000850585,14.8839614698\O,6
.8134594802,-0.0389611587,15.1085581976\O,5.6755527797,-0.0948861987,1
2.4615957525\C,6.7264285903,0.2222376844,20.7185952803\S,6.1700198698,
0.4648663388,22.356264089\C,7.8013895506,0.4124300393,22.9498053569\C,
8.104944409,0.0859346035,20.6782829938\C,8.7139619773,0.1912419973,21.
9458991316\S,8.2042650278,0.5265313347,24.6584061226\H,8.0882896264,1.
8733364849,24.8280245562\H,9.7852604544,0.1082520576,22.1260192606\H,8
.6532727111,-0.0874775975,19.7527431885\C,-1.5876593454,-0.4104630023,
3.0499911133\S,0.0435992652,-0.4644992227,3.6437811534\C,-0.5127865572
,-0.221099558,5.2813512047\C,-2.5001381178,-0.1883091581,4.0537471679\
C,-1.8911860486,-0.0835594959,5.3214486038\S,-1.9900170247,-0.52418077
7,1.3412456164\H,-1.876510827,-1.8712441212,1.1720522349\H,-2.43952916
61,0.0903984778,6.2468794569\H,-3.571348534,-0.1042916136,3.8735712058
\C,1.6790646039,-0.0708464909,10.1050777884\S,3.2920518164,-0.09660176
16,10.787921788\C,2.6779319981,-0.0115039774,12.4273197724\C,0.7381309
823,0.0006514498,11.1161193189\C,1.29605172,0.0330442511,12.413438631\
O,0.5378207639,0.0959390152,13.5384619087\O,-0.6000493662,0.039783176,
10.8914848447\C,0.3950492701,-0.1966862662,6.3918652919\S,-0.189264188
9,-0.1028293617,8.0360305017\C,1.4324780132,-0.1293514999,8.6968374302
\C,1.7737783987,-0.2515611859,6.3793195479\C,2.355701482,-0.2132290713
,7.6703493899\O,3.69846833,-0.2559890611,7.8687935376\O,2.506209614,-0
.3263277588,5.2433680117\C,4.7809305597,0.1293828694,17.3032748196\S,6
.4027305568,0.1035338689,17.9640031293\C,5.8184582679,0.1970996894,19.
6081963683\C,3.8577091268,0.2124025364,18.3298374425\C,4.4397034213,0.
2509485239,19.6208343599\O,3.7072123894,0.3250676652,20.7568237674\O,2
.5149389423,0.2543196425,18.1313888149\C,2.3542371177,0.6984616934,20.
5025364286\C,1.80005059,-0.0660604138,19.3208679656\C,7.5583837568,0.2
593021638,13.9323027628\C,7.0095702572,-0.5009855047,12.7451699985\C,-
0.7960307525,0.5024978983,13.2547618159\C,-1.3451069133,-0.2578852441,
12.0678102944\C,4.4133198798,0.0649584343,6.6794435023\C,3.8592988759,
-0.6993728958,5.4975743015\H,2.3047213401,1.783966709,20.3088940205\H,
1.7955536948,0.4676571073,21.4184004579\H,0.7539790974,0.209722934,19.
1367939958\H,1.8619058499,-1.152441021,19.5089041773\H,8.5950820962,-0
.034837693,14.1402371063\H,7.5203404891,1.3452620862,13.7361444274\H,7
.0317946369,-1.5861969108,12.9485478995\H,7.5961113302,-0.2903520862,1
1.8417598702\H,-0.8178209652,1.5876652235,13.0511010406\H,-1.382676243
8,0.2923268589,14.1582109151\H,-2.3816915452,0.0365834496,11.859773384
2\H,-1.3074731358,-1.3438068452,12.2642536426\H,5.459452181,-0.2106455
599,6.8634206471\H,4.3511969955,1.1513833631,6.4917498658\H,3.90912597
2,-1.7849113102,5.6909327334\H,4.4178974867,-0.4681815783,4.5817519269

\Au,0.0000127289,-0.000007036,0.0000097449\Au,2.4976240388,1.4419830046,0.0000040896\Au,2.4976224854,-1.4420056955,0.0000174189\Au,-1.6650793732,0.0000038213,-2.3547804432\Au,0.8325294388,1.4419930849,-2.3547879682\Au,0.8325242211,-1.4419937634,-2.3547893973\Au,3.3301730255,2.8840047598,-2.3547821393\Au,3.3301663826,-2.8840089451,-2.3547845131\Au,6.2145192919,-0.0000165202,25.9999900727\Au,3.7169166253,-1.4419668358,25.9999569728\Au,3.7169260679,1.4420031906,25.9999580612\Au,7.8796250448,0.0000009696,28.3547835038\Au,5.3820451054,-1.4419655092,28.3548135317\Au,5.3820562726,1.4419795298,28.3548088939\Au,2.8843683796,-2.8839898729,28.3547882168\Au,2.8843702646,2.8839858175,28.3547939548\\Version=ES64L-G09RevD.01\HF=-7189.3790049\RMSD=3.349e-09\RMSF=9.890e-06\Dipole=-0.0006338,0.0015707,0.0008736\Quadrupole=126.3617382,36.9056194,-163.2673576,5.0054658,19.9438636,23.8638518\PG=C01 [X(C32H22Au16O8S8)]\\@

PEDOT5g.pbe0

1\1\GINC-NODE07\FOpt\RPBE1PBE\Gen\C38H26Au16O10S9\GRYNOVA\01-Mar-2017\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\DXN5g.pbe0.freq\\0,1\C,3.3905815324,-0.7138464434,12.1819131285\S,3.8857787199,-0.2950336206,10.5539431052\C,2.3131686212,-0.6987503126,9.8942874372\C,2.0765076035,-1.1454777789,12.1805998625\C,1.475721681,-1.1370748535,10.9035879772\O,0.1911875033,-1.5231758091,10.6938254151\O,1.4125048429,-1.5319625058,13.3014621421\C,-0.1623255342,-0.4757015546,5.2198398501\S,0.2051729233,0.1118512144,3.6175499986\C,-1.4229973452,-0.1989960821,3.0988131812\C,-1.4747364825,-0.9148267252,5.2987169154\C,-2.1896562049,-0.7576965792,4.0933632154\S,-1.9686777956,0.0781107804,1.4506418403\H,-2.0831038853,1.4356332478,1.4753334735\H,-3.2322468684,-1.0402067131,3.9512722365\H,-1.9024615283,-1.3337028462,6.2091780283\C,8.1719383038,-0.3126536797,22.9132554674\S,6.6700701157,-0.7731808401,22.149080876\C,7.2664655601,-0.3683368334,20.5528718495\C,9.0730932858,0.1241079007,21.963938353\C,8.5653413692,0.0968638824,20.6420298745\C,8.3291350689,-0.3900993346,24.3372929932\O,9.2936979562,0.4983124071,19.5672192161\O,10.3275911488,0.5423430522,22.260431047\C,5.267355453,-0.5497840799,15.6323967865\S,3.7216685276,-0.9890947937,14.9356143953\C,4.2559970335,-0.5954894879,13.3147360402\C,6.131981277,-0.129786875,14.6382332992\C,5.5667883157,-0.1563483021,13.3425160149\O,6.2545632316,0.217928328,12.2320977575\O,7.4044319413,0.2823802493,14.8770692423\C,6.4635967815,-0.532121305,19.3809210632\S,7.0376802551,-0.1608553094,17.7669811907\C,5.5156895169,-0.6330753714,17.0388132031\C,5.1627477476,-0.9970878138,19.3245869377\C,4.6341111821,-1.0564094754,18.0169871779\O,3.3723378152,-1.4881064482,17.755649384\O,4.4507174623,-1.3559881082,20.4227787787\C,1.9811004336,-0.5463438747,8.5116805813\S,0.3713969987,-0.882230147,7.9085262394\C,0.8074468837,-0.4437082378,6.275270342\C,2.790981702,-0.1188618965,7.4752647691\C,2.132858739,-0.0630304969,6.2220066837\O,2.7521547339,0.3251302456,5.0822144678\O,4.095093266,0.2261466931,7.6337820446\C,3.9895124005,0.9857262438,5.3403040515\C,4.7866271105,0.2417261721,6.3889993765\C,-0.555925573,-1.5694844587,11.9048154023\C,0.2338305645,-2.2647625509,12.9916139362\C,7.4132692364,0.9748075407,12.5613234804\C,8.1814631488,0.3146662123,13.6857043518\C,2.5611102311,-1.4835098388,18.924182141\C,3.2953501176,-2.1162951071,20.0855240446\H,3.7896770408,2.0176294791,5.6773807073\H,4.5267596487,1.014084808,4.383798261\H,5.7456506662,0.7420870036,6.5739321449\H,4.9756111144,-0.794447707

3,6.0570710935\H,-1.4785313777,-2.1187851666,11.6775685653\H,-0.811397
8775,-0.5429139816,12.2212747504\H,0.504682183,-3.2851210273,12.667214
4583\H,-0.3478914388,-2.3232550008,13.9205033989\H,7.1176240997,1.9973
41567,12.8559796012\H,8.0214810755,1.0231967469,11.6489114661\H,9.0901
220686,0.882407585,13.924096065\H,8.4605947289,-0.7142045039,13.397009
6905\H,1.6572330063,-2.0544770951,18.6759776901\H,2.2786393753,-0.4460
653508,19.1763794414\H,3.5938009668,-3.1475301615,19.8272596517\H,2.66
55272042,-2.1360778321,20.9841276412\C,7.3861201976,-0.7971195781,25.2
67722007\C,7.8452189268,-0.7450923814,26.5999179682\C,9.1448745513,-0.
310120273,26.6882901393\S,9.817127693,0.0625304085,25.1269048863\S,10.
0996686018,-0.0222333885,28.1439170604\C,10.6829286009,0.5538154407,19
.8681980617\C,10.918144441,1.2647214319,21.182796338\H,6.3817627513,-1
.1148577086,24.9884888646\H,7.2457524659,-0.9914844607,27.4779202646\H
,10.6123611445,-1.271781444,28.3223849822\H,11.1578484299,1.0978485965
,19.041763817\H,11.094752544,-0.4700297236,19.9138211188\H,10.49135982
77,2.282088811,21.1444077199\H,11.9904730427,1.3301973376,21.406843526
4\Au,0.000029757,-0.0000011837,0.000055219\Au,2.4976194347,1.441990978
4,-0.0000092652\Au,2.4976183864,-1.4420127942,-0.0000074116\Au,-1.6650
750583,-0.0000012812,-2.3547834941\Au,0.8325302563,1.4420012126,-2.354
7827022\Au,0.8325302895,-1.4419975917,-2.3547849077\Au,3.3301701072,2.
8840098144,-2.3547800757\Au,3.3301599305,-2.8840201205,-2.3547799507\A
u,8.4999516241,0.0000104164,29.9999404085\Au,6.0023849329,-1.441998544
,29.9999977953\Au,6.0023831345,1.4420154291,29.999997449\Au,10.1650738
722,-0.0000013899,32.354784333\Au,7.6674746275,-1.441991496,32.3547903
785\Au,7.6674852959,1.4419859203,32.3547975639\Au,5.169826523,-2.88400
39776,32.3547824586\Au,5.1698368867,2.8840146076,32.3547822014\\Versio
n=ES64L-G09RevD.01\HF=-7968.5449339\RMSD=2.847e-09\RMSF=9.239e-06\Dipo
le=0.6449245,-0.024175,-0.2512798\Quadrupole=170.101205,56.4400271,-22
6.541232,13.5590619,33.6588641,-22.4959781\PG=C01 [X(C38H26Au16O10S9)]
\\@

PEDOT6g.pbe0

1\1\GINC-NODE01\FOpt\RPBE1PBE\Gen\C44H30Au16O12S10\GRYNOVA\01-Mar-2017
\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Em
piricalDispersion=GD3BJ pseudo=read Nosymm\\DXN6g.pbe0.freq\\0,1\C,2.4
203592105,0.1144485027,12.5086707515\S,3.0824320042,0.1646326258,10.88
63142426\C,1.4888407015,0.1577076569,10.1563189621\C,1.0386538736,0.09
46030583,12.4543157129\C,0.5190603031,0.1174363266,11.1415619315\O,-0.
8127986612,0.0976558583,10.8787538293\O,0.2456372355,0.0633993046,13.5
578271749\C,-0.5891347167,0.2792982363,5.2838504572\S,-0.000338246,0.5
011556929,3.6543377438\C,-1.6216828565,0.461153683,3.0311680127\C,-1.9
699058195,0.1582656704,5.2996086025\C,-2.5543938194,0.2586559326,4.020
4407736\S,-1.9949484307,0.5630013142,1.3158758365\H,-1.8590529424,1.90
62787889,1.1326958333\H,-3.6231382904,0.1855715674,3.8216800988\H,-2.5
368321955,-0.0006628784,6.2164521818\C,7.0113652228,-0.1258812924,23.3
409435466\S,5.4172409777,-0.1150399246,22.612143473\C,6.0778060206,-0.
0117144534,20.9917985714\C,7.9802586074,-0.0525006441,22.3567506341\C,
7.4593462841,0.0165164924,21.0461403155\C,7.2216564647,-0.1848171633,2
4.7545895252\O,8.2509820472,0.1023213989,19.9444596378\O,9.3125013628,
-0.0495080089,22.6184530384\C,4.1563632308,0.0642337414,16.0408636253\
S,2.5687760703,0.0555820439,15.299798639\C,3.2406192586,0.0955009501,1
3.6808465714\C,5.1331321912,0.096339611,15.0621021675\C,4.621522727,0.
1130894997,13.7448226507\O,5.4196816143,0.1377158238,12.6457300577\O,6

.46520193,0.1155213024,15.3323116296\C,5.2573682046,0.0142235391,19.81
98360747\S,5.9292239738,0.0518598695,18.2007879339\C,4.341759265,0.036
0598867,17.459689824\C,3.876526087,-0.0067141487,19.755819848\C,3.3650
311326,0.0026797633,18.4384336844\O,2.0329990165,-0.0210537669,18.1682
505572\O,3.0784833014,-0.0287499265,20.8550667112\C,1.2791449264,0.201
2281321,8.7420547882\S,-0.3273050104,0.1889357793,8.0439724123\C,0.295
2571189,0.2557859088,6.4123361915\C,2.2264729487,0.2608129257,7.735722
2103\C,1.6746504566,0.2921271064,6.431370459\O,2.4335681505,0.34412352
31,5.3114675298\O,3.5655172721,0.2882181185,7.9644533744\C,3.786062648
7,0.699188505,5.5926744492\C,4.3009381636,-0.0592374629,6.7960178888\C
,-1.5871752508,0.4221657107,12.0283793015\C,-1.0835846165,-0.329612255
8,13.240734249\C,6.7526293658,0.516119152,12.9679605002\C,7.2394604331
,-0.2303665698,14.1907441934\C,1.2584038363,0.3303508099,19.3079200095
\C,1.7457880241,-0.4094348304,20.5345586485\H,3.8485882047,1.786057499
5,5.7747471368\H,4.3619926957,0.448611584,4.6928190034\H,5.3473104213,
0.2013986798,6.99969931\H,4.2249450694,-1.1467642447,6.6195206724\H,-2
.6216236166,0.1402484074,11.7936557995\H,-1.5387308745,1.5099745928,12
.2117763728\H,-1.1149830989,-1.417084632,13.0500710682\H,-1.6939499251
,-0.0998039991,14.1235667419\H,6.7961697571,1.6047503595,13.1489857885
\H,7.3647784061,0.2708767806,12.0904730259\H,8.2768223176,0.0403537567
,14.4262526392\H,7.1783895156,-1.319298165,14.0160525855\H,0.221232304
2,0.0576550569,19.073872144\H,1.3186175096,1.4202391133,19.4766986219\
H,1.7028850282,-1.4990283431,20.3591786144\H,1.1334252827,-0.160102653
,21.4107558787\C,6.2750378973,-0.2662514273,25.7600341936\C,6.82643170
46,-0.2899238329,27.0647127063\C,8.2050071526,-0.230483022,27.08469310
49\S,8.8272927766,-0.1478271758,25.4537051115\C,9.089113281,-0.2466822
276,28.2135190722\C,9.5929304271,-0.2713513586,20.2295788379\C,10.0736
113353,0.3941879601,21.5001841843\O,4.9368650481,-0.3182203792,25.5302
642287\O,6.0679781269,-0.3586895317,28.1840032281\H,10.1939110106,0.05
03413665,19.3692963127\H,9.6603789768,-1.3692100915,20.3303853178\H,9.
9889855378,1.4912119237,21.4070900387\H,11.1172331501,0.1281523119,21.
7117047625\C,10.4679006232,-0.1047431772,28.1992066329\C,11.053553218,
-0.2063037036,29.4777737041\C,10.1236469678,-0.4295890906,30.465191025
9\S,8.5031738777,-0.4882777126,29.8412557517\S,10.4980934019,-0.538961
3303,32.1797474037\C,4.1943514516,0.012972469,26.6988966353\C,4.722434
5374,-0.7381441881,27.9010994503\H,11.0326636153,0.0691278135,27.28374
40317\H,12.1210931968,-0.1193719171,29.6774121009\H,10.3765747527,-1.8
848175098,32.3538255837\H,3.153162832,-0.2667730306,26.4939998474\H,4.
2497936782,1.1013810947,26.8776379441\H,4.6801673721,-1.8256263695,27.
7169133953\H,4.1413471603,-0.5000058427,28.8010247567\Au,0.0000234993,
-0.0000652909,-0.0000858319\Au,2.4976049593,1.4420160654,0.0000473757\
Au,2.49763721,-1.4419802072,0.0000597251\Au,-1.6650870745,0.0000062646
,-2.3547749987\Au,0.8325136402,1.4420198217,-2.3547771846\Au,0.8325007
507,-1.4419793108,-2.3548065469\Au,3.3301992505,2.8839593331,-2.354800
6856\Au,3.3301676884,-2.8840066834,-2.3547854366\Au,8.5000232755,-0.00
000002145,33.5000569328\Au,6.0023766059,-1.4419841228,33.4999865639\Au,
6.0023754764,1.4420021663,33.4999904585\Au,10.1650835796,-0.0000004826
,35.8547774689\Au,7.6674565826,-1.4420050892,35.8547756757\Au,7.667456
4276,1.4420058414,35.8547751603\Au,5.1698285131,-2.8840074246,35.85478
10514\Au,5.1698396153,2.8840193336,35.8547802721\\Version=ES64L-G09Rev
D.01\HF=-8747.7125775\RMSD=2.411e-09\RMSF=2.548e-06\Dipole=0.0014876,0
.0158061,-0.0069182\Quadrupole=180.0232094,61.0496584,-241.0728678,-6.
8576458,7.6734373,-29.9126754\PG=C01 [X(C44H30Au16O12S10)]\\@

Cp1g.pbe0

1\1\GINC-R01-NODE71\FOpt\RPBE1PBE\Gen\C15H14Au16S2\GRYNOVA\10-Feb-2017
\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) Empirica
lDispersion=GD3BJ pseudo=read Nosymm\\Cp1g.pbe0.freq\\0,1\C,1.57877546
71,-0.0190100653,9.1553814167\C,1.739474711,0.5863025952,7.7866431292\
C,0.6306020502,-0.0266281543,6.9757327294\C,0.498130498,-0.8591054698,
9.1197674722\C,-0.0784258173,-0.8611986953,7.7978814592\H,-0.946610077
,-1.4527433028,7.5062380797\H,0.1229887232,-1.4470931083,9.957797307\C
,0.4174976832,0.237590208,5.582268931\C,-0.6802544274,-0.372872139,4.7
516972841\C,-0.4466344813,0.2145632335,3.3902131695\C,1.1628528849,1.0
523652927,4.7716460878\C,0.6380782793,1.0273962212,3.4234822743\S,-1.4
327069811,-0.2140696739,1.9828912597\H,-2.1663942245,0.9263277097,1.87
62183769\H,1.0606798068,1.5539069192,2.5668143762\H,2.0338534924,1.631
4890592,5.0770829879\C,3.6503229976,0.0879489871,12.276292348\C,2.4310
375695,-0.447793326,11.5873126521\C,2.4663561281,0.2470668091,10.24908
679\C,4.2515888869,1.0171395437,11.4901266456\C,3.5273058155,1.1130335
861,10.2432850864\S,4.1921993149,-0.2861270668,13.9072292785\H,4.11913
13488,-1.6417736346,13.8400314222\H,3.8144317898,1.7614532977,9.416266
1145\H,5.1431990691,1.5884113016,11.7473621551\H,2.7291945868,0.357380
7853,7.3590387999\H,1.6532928978,1.6853915534,7.8172460542\H,-1.680766
9602,-0.1241716346,5.1433040304\H,-0.6129926539,-1.4742955212,4.733154
6771\H,1.526073108,-0.1923696046,12.1685690254\H,2.4429180565,-1.54587
41298,11.4892816792\Au,-0.0000138129,-0.0000018368,-0.0000252665\Au,2.
4976185472,1.4419925163,0.0000011896\Au,2.4976208475,-1.4420085321,0.0
000001828\Au,-1.6650814327,-0.0000059665,-2.354778987\Au,0.8325607946,
1.4420027973,-2.3547709362\Au,0.8325294154,-1.4420051697,-2.3547805761
\Au,3.3301684749,2.8840126415,-2.3547789216\Au,3.3301610412,-2.8840181
966,-2.3547807362\Au,2.3516010808,0.0000037175,15.5000398402\Au,-0.145
9610172,-1.4419882407,15.4999690365\Au,-0.1459630568,1.4420047074,15.4
999771349\Au,4.0167417214,0.0000042068,17.8547787827\Au,1.5191516745,-
1.4419982921,17.8547851726\Au,1.5191630612,1.4419940039,17.8547918235\
Au,-0.978519144,-2.8839941621,17.8547864659\Au,-0.9785081952,2.8840058
058,17.8547857948\\Version=ES64L-G09RevD.01\HF=-3547.8138502\RMSD=4.96
4e-09\RMSF=4.262e-06\Dipole=0.0416554,-0.0987297,0.2737209\Quadrupole=
46.0637351,19.0825291,-65.1462642,0.583946,43.969376,-8.7992897\PG=C01
[X(C15H14Au16S2)]\\@

Cp2g.pbe0

1\1\GINC-R02-NODE37\FOpt\RPBE1PBE\Gen\C20H18Au16S2\GRYNOVA\11-Feb-2017
\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) Empirica
lDispersion=GD3BJ pseudo=read Nosymm\\Cp2g.pbe0.freq\\0,1\C,1.09798887
96,-0.1384182508,8.8022876099\C,0.1352261512,0.576059265,7.8901553651\
C,0.3363373194,-0.0766356963,6.5468984937\C,1.7683110819,-1.0713466284
,8.0515415413\C,1.3060317197,-1.0344928802,6.6889022912\H,1.6781328443
,-1.681578553,5.8939793217\H,2.5365624787,-1.7494001113,8.423360337\C,
-0.4154778135,0.258491275,5.3741611285\C,-0.3265380033,-0.4599241241,4
.0485423998\C,-1.4198836053,0.1787190252,3.2434362029\C,-1.3804232945,
1.2260126774,5.2705758092\C,-1.9943128444,1.1764802321,3.9637686846\S,
-1.8719573786,-0.1844750514,1.5823466237\H,-1.8794287455,-1.5404447829
,1.6673878521\H,-2.8008409953,1.8246001308,3.6215655947\H,-1.676997823
2,1.9147249702,6.0608351228\C,3.7703738588,-0.1792822623,15.7562890799
\C,2.6768180275,0.4591394257,14.9512749327\C,2.7655952361,-0.259461946

3,13.6257614263\C,4.3446900521,-1.1771788389,15.0360512905\C,3.7305545
129,-1.2269658414,13.7293675324\S,4.222847252,0.1842056258,17.41720213
51\H,4.2299392134,1.5401627624,17.3319281377\H,4.027030462,-1.91579743
12,12.9391766814\H,5.1513085447,-1.8252085209,15.3782125118\C,2.013676
5467,0.0755680512,12.453060015\C,2.2148148817,-0.5771118306,11.1097903
048\C,1.2519531498,0.1372688691,10.1976858281\C,1.0439246305,1.0333689
211,12.3110659666\C,0.5816107296,1.0701770252,10.9484393837\H,-0.18668
01784,1.7481881522,10.5766234368\H,0.6718276037,1.6804661131,13.105981
141\H,0.3481879445,1.6573433191,7.8504582213\H,-0.9054128509,0.4706717
311,8.2379261578\H,3.2554356253,-0.4715326059,10.7620103814\H,2.002046
3926,-1.6584313775,11.1494503653\H,-0.4551259238,-1.5497463031,4.15406
75604\H,0.6491658864,-0.3008029042,3.554901447\H,1.7012215623,0.299990
9486,15.4451233777\H,2.8052702569,1.5489551834,14.8455358897\Au,-0.000
0601519,-0.0000001098,0.0000838962\Au,2.4976362291,1.44196189,-0.00006
75238\Au,2.4976290906,-1.4419942562,-0.0000606961\Au,-1.6650769198,0.0
000024892,-2.3547821781\Au,0.8325954114,1.4419873966,-2.3547681273\Au,
0.8325902714,-1.4419892617,-2.3547688037\Au,3.3301343659,2.8840717206,
-2.3547548024\Au,3.3301296766,-2.8840725216,-2.3547585583\Au,2.3514590
711,0.0000236564,18.999945017\Au,-0.1461132999,-1.442001604,19.0000230
252\Au,-0.1461178895,1.4420136547,19.0000180337\Au,4.0165971615,-0.000
007864,21.3547820071\Au,1.5189841178,-1.4420032995,21.3547759\Au,1.518
9913165,1.4419933914,21.354780977\Au,-0.9786655874,-2.884017643,21.354
7768797\Au,-0.9786528633,2.8840323608,21.3547749536\\Version=ES64L-G09
RevD.01\HF=-3740.5421238\RMSD=2.281e-09\RMSF=3.618e-06\Dipole=-0.00019
24,-0.0003492,0.0000919\Quadrupole=57.4151078,35.1910085,-92.6061164,-
3.2342205,52.9826542,10.5267773\PG=C01 [X(C20H18Au16S2)]\\@

Cp3g.pbe0

1\1\GINC-R06-NODE59\FOpt\RPBE1PBE\Gen\C25H22Au16S2\GRYNOVA\22-Feb-2017
\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(Loose,MaxStep=15) I
OP(2/17=4) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\Cp3g.pbe0.fre
q\\0,1\C,1.8587832958,-0.1164376509,8.781205441\C,0.8309043669,0.56698
18487,7.9153873777\C,0.9814405894,-0.0826073873,6.5631513149\C,2.52352
91473,-1.0247979129,7.9948904402\C,1.9907598305,-1.0053656662,6.656889
8305\H,2.3427285599,-1.6425461016,5.8447431836\H,3.3305321563,-1.67812
88992,8.3270328723\C,0.1434326243,0.2207319536,5.4397579434\C,0.143023
1197,-0.5120247696,4.117309284\C,-1.0345296395,0.0837716244,3.39959976
26\C,-0.8510353638,1.1636929815,5.401758874\C,-1.5711929391,1.07838236
,4.1532087591\S,-1.6418215916,-0.3302180609,1.7998885927\H,-1.51614923
29,-1.6799249394,1.8826047745\H,-2.4227894792,1.6987020433,3.874296841
4\H,-1.1001577229,1.8554243768,6.2055993877\C,5.2016670418,-0.10615265
71,19.5213541358\C,5.4864994717,-0.6789068272,18.1614227601\C,4.426147
2485,-0.0482066148,17.2895564266\C,4.1501207351,0.7458518139,19.445882
9489\C,3.6726103472,0.7809927518,18.0767384407\S,6.259926825,-0.339176
7213,20.9192682908\H,6.240480687,-1.7000886332,20.9561897052\H,2.82474
89089,1.3785512204,17.7427998481\H,3.7260327541,1.3032513528,20.281838
7725\C,2.8119099078,0.089610817,12.4322681459\C,3.0443019634,-0.527005
9161,11.0741079603\C,2.0437331964,0.155331454,10.1740641831\C,1.803720
7809,1.0120043521,12.3011024394\C,1.3423801843,1.0525376007,10.9413179
518\H,0.54532261,1.7028921806,10.5805577284\H,1.4036160304,1.628624175
2,13.1062441986\C,4.279928849,-0.3119146206,15.886601199\C,3.270948956
6,0.3516035062,14.9837941799\C,3.5302782925,-0.2481511931,13.623031793
1\C,5.0126003926,-1.1808620636,15.120504051\C,4.5591354126,-1.14684516

51,13.7555399315\H,4.9818223754,-1.7476097865,12.9501527004\H,5.824246
2325,-1.8128010198,15.4824933365\H,1.0121467706,1.6536953511,7.8637591
132\H,-0.1878361033,0.4344553014,8.3142932732\H,4.0773442517,-0.360547
6739,10.7263271208\H,2.8903803914,-1.618408568,11.0957092637\H,2.23887
17005,0.1559902142,15.3189901965\H,3.3977136364,1.4467226269,14.974215
7241\H,0.0593566091,-1.6038453754,4.2437060007\H,1.0679898022,-0.32762
52986,3.5408550755\H,6.5011602608,-0.4148896227,17.8212415608\H,5.4205
490296,-1.7805549113,18.1516819585\Au,-0.0000222582,-0.0000790213,-0.0
000291185\Au,2.4976091358,1.4420086927,-0.0000114914\Au,2.4976321472,-
1.4419892807,-0.0000036579\Au,-1.6650845849,0.0000135888,-2.3547768795
\Au,0.8325856821,1.4420255122,-2.3547486693\Au,0.83252511,-1.441993265
1,-2.354789642\Au,3.3301699203,2.8840103341,-2.3547798222\Au,3.3301517
438,-2.884033837,-2.3547745753\Au,4.9469553973,0.0000584633,23.0000370
273\Au,2.449370753,-1.4420090356,22.9999937156\Au,2.44935386,1.4419990
248,22.9999811608\Au,6.6120634652,-0.0000105087,25.3547773783\Au,4.114
4249816,-1.4420193382,25.3547629859\Au,4.1144843511,1.4420034951,25.35
47932617\Au,1.6168034425,-2.8839988381,25.3547845158\Au,1.6168168531,2
.8840150137,25.3547818107\\Version=ES64L-G09RevD.01\HF=-3933.269133\RM
SD=5.676e-09\RMSF=7.487e-06\Dipole=-0.1225383,-0.7852726,-0.004979\Qua
drupole=77.3602841,44.9164316,-122.2767157,-12.6004953,44.8749853,-16.
5181513\PG=C01 [X(C25H22Au16S2)]\\@

Cp4g.pbe0

1\1\GINC-R04-NODE41\FOpt\RPBE1PBE\Gen\C30H26Au16S2\GRYNOVA\10-Feb-2017
\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) Empirica
lDispersion=GD3BJ pseudo=read Nosymm\\Cp4g.pbe0.freq\\0,1\C,3.88662656
72,-0.3719805252,11.8747719611\C,2.940150639,0.2998399864,10.915276149
7\C,3.093270922,-0.4764943781,9.6337526152\C,4.5126595861,-1.391216458
4,11.1994028177\C,4.0290541809,-1.4580738083,9.8487671512\H,4.36061062
22,-2.1875014361,9.109446819\H,5.2584229379,-2.0645435163,11.622449951
4\C,0.9986802788,-0.9666760816,5.0080749667\C,-0.0580950042,-0.3411226
418,4.1331547629\C,-0.2376676364,-1.3501976442,3.0415795723\C,1.416159
6197,-2.1240459725,4.4058899226\C,0.6583176563,-2.3584843221,3.1940300
21\S,-1.3346731739,-1.1782387689,1.6806680335\H,-2.1320254371,-0.22244
85866,2.2200165623\H,0.7860784354,-3.2106602343,2.5270035413\H,2.17826
7041,-2.8015094668,4.789801456\C,6.8878883331,0.0462086452,22.66080060
34\C,7.2224002131,-0.5725210034,21.3361180223\C,6.2001879518,0.0281689
864,20.4078225295\C,5.8122763401,0.8617519457,22.5253861476\C,5.397842
7097,0.8654883488,21.1396867438\S,7.7583210393,-0.3615046642,24.145178
999\H,8.5511085401,0.7400164468,24.2510563112\H,4.559285319,1.44376716
02,20.7530447945\H,5.3264503427,1.4057687604,23.3364340443\C,4.7636528
498,0.0376483615,15.5118657947\C,4.9992870273,-0.6685159566,14.2027223
317\C,4.0467430064,-0.004230611,13.2434888968\C,3.7971506404,0.9906427
092,15.3048537882\C,3.3676478434,0.9694009282,13.9350716673\H,2.605914
8332,1.6270339131,13.5161919995\H,3.4071977882,1.6694528369,16.0637397
927\C,6.1172324436,-0.2644893732,19.0096866622\C,5.1493747921,0.383882
6207,18.0568009754\C,5.4436301876,-0.2643774613,16.7292728762\C,6.8656
666872,-1.1656567886,18.2980385399\C,6.4566291396,-1.1717351823,16.920
3812793\H,6.8943686298,-1.8039627026,16.1480328322\H,7.6539821838,-1.7
969043325,18.7093944513\C,2.3486616292,-0.2209610107,8.4436634762\C,2.
3803891805,-1.0844181524,7.2089310965\C,1.3863064387,-0.4404236361,6.2
797678918\C,1.462929921,0.8029271602,8.2164737567\C,0.8858923042,0.671
6305834,6.9071443551\H,0.1441462045,1.3533606433,6.4900243389\H,1.2202

482495,1.5977274749,8.9217002599\H,1.9009536032,0.2695976469,11.281047
4605\H,3.1971457454,1.3634669651,10.7784679574\H,4.8018481198,-1.74958
45209,14.2878493819\H,6.0442098849,-0.5629228723,13.8669836084\H,5.293
5512686,1.4762092097,18.0165374084\H,4.1036364131,0.2140308293,18.3619
281695\H,3.3881543699,-1.1111169352,6.7612072264\H,2.1077942911,-2.127
1099243,7.4385831936\H,-0.9906005753,-0.1301711285,4.6807204407\H,0.29
93690059,0.6123885454,3.7039647715\H,7.142642001,-1.672501031,21.37542
1775\H,8.2522234722,-0.3415054802,21.0164711281\Au,0.0000303401,0.0000
384273,0.0000586138\Au,2.4976167594,1.441995613,0.000002201\Au,2.49760
68532,-1.4420327696,0.0000036979\Au,-1.6650798504,0.0000050894,-2.3547
801058\Au,0.8325467361,1.4419418643,-2.3548132157\Au,0.8325247799,-1.4
419949318,-2.3547884843\Au,3.3301631828,2.8840218078,-2.3547751795\Au,
3.3301701084,-2.8840024924,-2.3547871471\Au,6.2144998367,0.0000004747,
25.9999689722\Au,3.7169363052,-1.4420009207,25.9999832363\Au,3.7169297
379,1.4420095461,25.9999876034\Au,7.879627891,0.000004418,28.354781491
3\Au,5.3820374523,-1.4419945173,28.3547930621\Au,5.382034625,1.4419900
152,28.3547948194\Au,2.8843702032,-2.8839930316,28.3547869271\Au,2.884
3850391,2.8840114077,28.3547835078\\Version=ES64L-G09RevD.01\HF=-4125.
9984894\RMSD=3.214e-09\RMSF=2.403e-06\Dipole=0.1547447,-0.3228737,-0.5
531738\Quadrupole=111.2876487,61.7579716,-173.0456203,-8.7976091,54.41
79588,5.5075817\PG=C01 [X(C30H26Au16S2)]\\@

TCp1g.pbe0

1\1\GINC-R01-NODE52\FOpt\RPBE1PBE\Gen\C13H10Au16S4\GRYNOVA\10-Feb-2017
\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) Empirica
lDispersion=GD3BJ pseudo=read Nosymm\\TCp1g.pbe0.freq\\0,1\C,1.0365799
414,-0.2355872485,6.2712437835\C,0.7343843432,0.0383903842,7.717044241
1\C,2.0585617873,-0.1381824357,8.4043762017\C,2.3663512482,-0.52413762
37,6.1592228737\C,2.9894589777,-0.4649331579,7.4608444449\H,4.04677220
21,-0.655532974,7.6463905065\H,2.8913878639,-0.764837298,5.234326106\C
,2.208356128,0.0235257545,9.8253392906\S,3.7214324402,-0.2491572566,10
.6423928123\C,3.0126164332,0.142595495,12.1802373482\C,1.2272790619,0.
3882328591,10.7310545463\C,1.6795841748,0.4509455861,12.067409258\S,3.
9764085307,0.0111285337,13.6558496429\H,4.3892672103,1.3049311684,13.7
507426325\H,1.0566899658,0.6891549263,12.9310246102\H,0.2002930315,0.6
004936346,10.4361943154\C,-1.2985748159,-0.3074438625,3.1523267582\S,0
.3634748187,-0.5552671139,3.5854446534\C,0.0221768637,-0.1857164189,5.
2535234572\C,-2.0632939708,0.0708159437,4.2294254089\C,-1.3126673836,0
.1375046942,5.4241864272\S,-1.8944521858,-0.4278333017,1.4992574276\H,
-1.8662272113,-1.7817461146,1.3611227842\H,-1.7363042384,0.4116943206,
6.3894380932\H,-3.1283410276,0.286185084,4.1520611321\H,-0.0212932798,
-0.6605947656,8.1117228529\H,0.3375677001,1.0570157795,7.8612552222\Au
,0.000072129,0.0000786985,-0.0000322329\Au,2.4976427827,1.4419505445,0
.0000658752\Au,2.4976145211,-1.4420194968,0.0000976818\Au,-1.665082186
2,-0.0000095629,-2.3547784542\Au,0.8324825559,1.4419439341,-2.35483464
22\Au,0.8324500979,-1.4420027307,-2.354810113\Au,3.3301879003,2.883978
9957,-2.3547926576\Au,3.3302049968,-2.8839420638,-2.3548118173\Au,2.35
15949648,-0.0000173282,15.4999955756\Au,-0.1459586439,-1.4419923489,15
.499994721\Au,-0.1459614228,1.442007536,15.4999923846\Au,4.016739763,0
.0000037208,17.8547801676\Au,1.5191562659,-1.4419933434,17.8547898262\
Au,1.5191421139,1.4420019442,17.8547795567\Au,-0.9785133525,-2.8840041
934,17.8547823706\Au,-0.978502486,2.8840156942,17.8547817578\\Version=
ES64L-G09RevD.01\HF=-4265.4323914\RMSD=4.232e-09\RMSF=1.459e-06\Dipole

=-0.4193341,-0.0410651,0.2547538\Quadrupole=44.5783801,11.448756,-56.0
271361,2.3600548,35.423838,9.2957716\PG=C01 [X(C13H10Au16S4)]\\@

TCp2g.pbe0

1\1\GINC-R04-NODE09\FOpt\RPBE1PBE\Gen\C18H14Au16S4\GRYNOVA\10-Feb-2017
\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) Empirica
lDispersion=GD3BJ pseudo=read Nosymm\\TCp2g.pbe0.freq\\0,1\C,1.1468245
991,-0.0967709331,8.7919620654\C,-0.0348609315,0.2659174677,7.93391978
26\C,0.3841563316,-0.1301936097,6.5436604787\C,2.1118641708,-0.6266549
593,7.975569015\C,1.6477972492,-0.6468060115,6.6118788953\H,2.22708423
99,-1.0220017906,5.7673430397\H,3.089491265,-0.9851735036,8.2971733226
\C,-0.4711898536,0.0294379784,5.3995223057\S,-0.0026125321,-0.49407158
57,3.8012846605\C,-1.5376092901,-0.0120939158,3.1485240226\C,-1.743204
8075,0.5761237814,5.3800928259\C,-2.3476301489,0.5538539202,4.10388337
13\S,-1.9743945387,-0.1637733466,1.4492453467\H,-2.1006846932,-1.51725
74824,1.3839083397\H,-3.3467817158,0.9282439357,3.8839948543\H,-2.2272
520106,0.9739336449,6.2710164988\C,3.8891431395,0.0119106908,15.851366
1592\S,2.3540842819,0.4937295311,15.1986251358\C,2.8227702149,-0.02954
05008,13.6003440242\C,4.6992662524,-0.5538123816,14.8959622933\C,4.094
8628812,-0.576049452,13.6197423532\S,4.3258455626,0.1635501896,17.5506
695938\H,4.4523413724,1.5170161444,17.6159726244\H,4.5789843657,-0.973
6989005,12.7287874342\H,5.6984665591,-0.9280840971,15.1158312509\C,1.9
674160282,0.1300567404,12.4562081638\C,2.386417756,-0.266081611,11.065
9630573\C,1.2047405037,0.096598163,10.2079217362\C,0.7037688902,0.6466
513749,12.3879939883\C,0.2396987771,0.6264852431,11.0243084085\H,-0.73
79320783,0.9849909035,10.7027014908\H,0.1244888463,1.0218612804,13.232
5282456\H,-0.261626635,1.3431957155,7.9964890684\H,-0.9442692819,-0.27
10325308,8.2501869564\H,3.2958333502,0.2708403492,10.7496713482\H,2.61
31628405,-1.3433666537,11.0034245346\Au,0.0000088663,0.0000085204,0.00
00702305\Au,2.4976162471,1.4419964979,-0.0000326904\Au,2.4976120795,-1
.4420237157,-0.000030896\Au,-1.6650766815,-0.0000022571,-2.3547823465\
Au,0.8325557342,1.4419980034,-2.3547756603\Au,0.8325522163,-1.44200239
58,-2.3547742142\Au,3.3301596695,2.8840278932,-2.3547726952\Au,3.33015
28538,-2.8840323772,-2.3547749471\Au,2.3514499388,-0.0000040569,18.999
9401856\Au,-0.1461171304,-1.4419949692,19.0000174516\Au,-0.1461155329,
1.4420177357,19.0000169314\Au,4.0165979006,0.0000012801,21.3547814845\
Au,1.5189882427,-1.4419963708,21.3547816011\Au,1.5189986682,1.44199847
42,21.3547804635\Au,-0.9786658832,-2.8840171306,21.3547770889\Au,-0.97
86571891,2.8840248684,21.3547780125\\Version=ES64L-G09RevD.01\HF=-4458
.1600092\RMSD=4.501e-09\RMSF=1.084e-06\Dipole=0.0000898,-0.00007,0.000
0036\Quadrupole=65.946944,25.8906357,-91.8375797,-1.8910081,54.7938632
,9.4402753\PG=C01 [X(C18H14Au16S4)]\\@

TCp3g.pbe0

1\1\GINC-R04-NODE34\FOpt\RPBE1PBE\Gen\C23H18Au16S4\GRYNOVA\10-Feb-2017
\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) Empirica
lDispersion=GD3BJ pseudo=read Nosymm\\TCp3g.pbe0.freq\\0,1\C,1.0891531
463,-0.0678099497,9.4772328255\C,1.5150032748,0.1111441687,8.041537413
6\C,0.2422416829,-0.0588031134,7.2538685329\C,-0.2607812848,-0.3096790
355,9.4853258188\C,-0.7707708472,-0.3030146062,8.1394184579\H,-1.81591
19417,-0.4708626839,7.8760720843\H,-0.868753239,-0.4824984926,10.37308
27202\C,0.1735917146,0.0338290921,5.818927428\S,-1.3376618847,-0.13233
64988,4.9627058015\C,-0.5569985199,0.1190330281,3.4281658832\C,1.20687

40735,0.2569001324,4.9234379615\C,0.7967404434,0.3009578171,3.5694581304\S,-1.5179095249,0.0366569644,1.9446565043\H,-1.8839721601,1.345523154,1.8634448901\H,1.4605871003,0.4488485162,2.7161030457\H,2.2417182818,0.3840443569,5.2398629608\C,6.071739474,-0.2516963935,19.6631488891\S,4.4253286925,-0.5122825408,19.1674308276\C,4.8148308865,-0.1071337853,17.5117166906\C,6.8621071499,0.1576854469,18.6154155783\C,6.1514180031,0.237842923,17.3983719444\S,6.6713059427,-0.4448515026,21.3093529887\H,6.5996901938,-1.800690525,21.4018518569\H,6.6046362189,0.5337170623,16.453293673\H,7.9229100445,0.3782459538,18.7293018977\C,2.8266633681,-0.0114529798,12.8245363632\C,1.5527104629,-0.1854883863,12.0379714223\C,1.9699343497,0.0084289479,10.6018104375\C,3.8344940519,0.2519535074,11.9311189053\C,3.318059547,0.2631120915,10.590108945\H,3.918851313,0.447846261,9.6993620167\H,4.8789797991,0.4263657915,12.1900272908\C,3.8518628364,-0.1641984527,16.4442176206\C,4.229979376,0.0612426484,15.0037019104\C,2.9400274772,-0.1180819819,14.2468473338\C,2.511217952,-0.4289406195,16.490925803\C,1.9567066116,-0.3998069937,15.1608230233\H,0.9074047654,-0.5810531353,14.9287119455\H,1.9362101629,-0.6333110169,17.3950840581\H,2.2733370218,-0.6344060608,7.7502045652\H,1.9639766361,1.1040508824,7.8734884039\H,1.1111605661,-1.1828875706,12.1984750141\H,0.7892002355,0.5505289163,12.3397836616\H,4.6479732904,1.0697031626,14.8479002917\H,4.9975367686,-0.6573426191,14.6725075114\Au,0.0002098908,0.0000965761,0.0002581852\Au,2.4976193192,1.4419911791,0.0000010394\Au,2.4975955529,-1.4420523438,-0.0000147518\Au,-1.66506814,-0.0000177981,-2.3547883863\Au,0.8324147241,1.4419615947,-2.3548478113\Au,0.8325179278,-1.4419905893,-2.3547935667\Au,3.3301768601,2.8839981181,-2.3547848507\Au,3.330168298,-2.8840056276,-2.3547858676\Au,4.9467976751,-0.0000639231,22.999749169\Au,2.449367357,-1.4420027428,23.0000135011\Au,2.4493790774,1.4420430434,23.0000177941\Au,6.6120528538,0.0000219882,25.3547850532\Au,4.1145139028,-1.4419737142,25.3548222265\Au,4.1144753217,1.4419864989,25.3548007564\Au,1.616805342,-2.8840019322,25.3547832936\Au,1.6168140373,2.8840096727,25.354784216\\Version=ES64L-G09RevD.01\HF=-4650.8888512\RMSD=7.778e-09\RMSF=1.391e-06\Dipole=0.4065544,-0.0262924,-0.3188042\Quadrupole=91.3966244,35.1841361,-126.5807605,-2.9746743,52.9554588,-15.5168091\PG=C01 [X(C23H18Au16S4)]\\@

TCp4g.pbe0

1\1\GINC-R03-NODE30\FOpt\RPBE1PBE\Gen\C28H22Au16S4\GRYNOVA\10-Feb-2017\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT IOP(2/17=4) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\TCp4g.pbe0.freq\\0,1\C,2.6641656301,-1.4601961081,12.3425320231\C,1.4094877121,-1.0510311866,11.6208595034\C,1.6662783539,-1.4305278139,10.1891245795\C,3.5151580312,-2.024045261,11.4241228292\C,2.9111580294,-2.0044614736,10.1211870977\H,3.3839141625,-2.3841147993,9.2151162393\H,4.5074932235,-2.4197272405,11.640659052\C,-0.2727641544,-1.0150055913,5.5140211729\S,-1.6464332453,-0.3454232515,4.679162999\C,-0.954414505,-0.7350648233,3.1343572144\C,0.6507252421,-1.5115538144,4.6081742427\C,0.270518578,-1.3441558596,3.2592596232\S,-1.7779837535,-0.2275770361,1.6604657919\H,-2.2972916393,-1.426525902,1.2786379126\H,0.8779437755,-1.6250083121,2.3975199646\H,1.5898530842,-1.9693220116,4.9163828746\C,6.9240137279,-0.2218016729,22.7379750208\S,7.5615617127,-0.9362482517,21.2874216486\C,6.0822108006,-0.6145438285,20.4261627324\C,5.6373614262,0.2274507476,22.566565968\C,5.1651656536,0.0119052701,21.2545395821\S,7.8780048907,-0.2412898895,24.2217707542\H,8.367687469,1.0287457731,24.1804610282\H,4.169093361,0.29

88674337,20.9201567202\H,5.0557810533,0.6685197335,23.3767909459\C,3.9
264081207,-1.120876777,15.8643600476\C,4.1657482732,-1.5892638318,14.4
553670394\C,2.8929531397,-1.2430820472,13.7312871251\C,2.6619649368,-0
.5900534083,15.9240943224\C,2.0364087257,-0.6637539165,14.6349141758\H
,1.0320669322,-0.3034620392,14.4125263669\H,2.1957326685,-0.1667464912
,16.8139263319\C,5.8991520815,-0.9716915737,19.0494336157\C,4.62325192
98,-0.6826094624,18.3107519731\C,4.8751724935,-1.206246299,16.92432921
67\C,6.7607451657,-1.5900904176,18.1866376852\C,6.14167442,-1.73312497
18,16.8946869449\H,6.6189657779,-2.1910720096,16.0286961247\H,7.769423
1811,-1.9265446383,18.429723725\C,0.7599421968,-1.1801357529,9.1180840
221\C,1.057651586,-1.471505543,7.6732188902\C,-0.1610570128,-0.9805483
629,6.9433367136\C,-0.487355081,-0.6127040872,9.1875295389\C,-1.044333
0379,-0.493630961,7.8664191547\H,-2.0228123598,-0.0658703338,7.6442016
995\H,-0.9871727381,-0.2879279811,10.0996725007\H,0.5247496996,-1.5711
325982,12.0243332379\H,1.2170428068,0.029129114,11.7242131238\H,4.3691
839034,-2.6724413885,14.4186808636\H,5.0374283771,-1.0877450608,14.004
300125\H,4.3965912247,0.3960601096,18.2999401231\H,3.7623644859,-1.185
303264,18.7818008318\H,1.9686198449,-0.951228891,7.3354391218\H,1.2237
198892,-2.548589544,7.5040542103\Au,-0.0000000731,-0.0000026931,0.0000
15976\Au,2.497617599,1.4419941584,-0.0000076283\Au,2.4976202004,-1.442
0096526,-0.0000101474\Au,-1.6650794448,-0.0000001916,-2.3547803926\Au,
0.8325439066,1.442001444,-2.3547777347\Au,0.8325459548,-1.4419997393,-
2.3547780545\Au,3.3301682151,2.8840130916,-2.3547787379\Au,3.330156254
8,-2.8840264868,-2.3547773518\Au,6.2145413971,0.0000019905,25.99998634
75\Au,3.7169309583,-1.4419916598,25.9999999494\Au,3.7169309999,1.44201
17318,26.0000001738\Au,7.8796285449,-0.0000005438,28.3547810289\Au,5.3
820132001,-1.4419982025,28.354782232\Au,5.3820133169,1.4419960178,28.3
547836112\Au,2.8843792727,-2.8840087403,28.3547805143\Au,2.8843896973,
2.8840194757,28.354780214\\Version=ES64L-G09RevD.01\HF=-4843.6180177\R
MSD=3.501e-09\RMSF=1.564e-06\Dipole=-0.0805036,-0.5530986,-0.1212971\Q
uadrupole=93.2811994,42.2705391,-135.5517384,-2.0293026,41.3062566,3.7
62198\PG=C01 [X(C28H22Au16S4)]\\@

THIO1g.pbe0

1\1\GINC-LCMD47\FOpt\RPBE1PBE\Gen\C12H8Au16S5\ROOT\17-Apr-2016\0\\#PBE
1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(MaxCyc=250,MaxStep=10) IOP(
2/17=4) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\1TG\\0,1\Au,0.00
00409923,-0.0000012204,0.0000675269\Au,2.497617823,1.44199377,-0.00000
86645\Au,2.4976168673,-1.442015425,-0.0000102563\Au,-1.6650789696,0.00
00011646,-2.3547807286\Au,0.8325313284,1.4419956953,-2.3547857015\Au,0
.8325296908,-1.4419934091,-2.3547876803\Au,3.3301701525,2.884009736,-2
.3547801078\Au,3.3301602285,-2.8840196042,-2.3547801616\Au,2.351609542
3,-0.0000042806,15.499934685\Au,-0.145957001,-1.4419951942,15.50000214
99\Au,-0.1459588369,1.4420120144,15.5000005613\Au,4.0167373846,0.00000
11076,17.8547818494\Au,1.519139165,-1.4419889709,17.8547935283\Au,1.51
91365438,1.4419939924,17.854789527\Au,-0.9785126358,-2.8840054346,17.8
547818638\Au,-0.9785022753,2.884016059,17.8547816089\C,1.905382065,0.6
425815088,8.526863722\S,0.2866266872,0.8566859526,7.932346047\C,0.7882
345654,0.5908675761,6.2895730493\C,2.7708350547,0.3492067093,7.4934524
293\C,2.1401706615,0.32062333,6.2292244309\H,2.6646953599,0.1328233587
,5.2920339907\H,3.8380966155,0.1872319435,7.6443015525\C,-0.1848914135
,0.6511771196,5.2236924583\S,0.1276977191,-0.1079591492,3.6902293875\C
,-1.4369509796,0.354220627,3.1024244852\C,-1.4328136271,1.2426315239,5

.2415119665\C,-2.1464887277,1.0734537083,4.0331683752\S,-1.9820170794,
0.0262921826,1.4598682972\H,-2.1494733041,-1.3206626762,1.5589217568\H
,-3.1452268091,1.465141892,3.8437930899\H,-1.8153018905,1.7917310225,6
.1017642556\C,3.0687658501,0.5331242484,12.2476011887\S,3.5012816241,-
0.0712374659,10.6789200082\C,2.1653734619,0.760654204,9.9438016301\C,1
.9420852958,1.3168567735,12.2019588443\C,1.4363668463,1.4543550139,10.
8899142046\S,3.9904072944,0.0201633863,13.6640022894\H,4.648854277,1.1
843575588,13.9122531778\H,0.5599220917,2.0514862564,10.6381793705\H,1.
4900365341,1.7529024105,13.0937258356\\Version=ES64L-G09RevD.01\HF=-46
24.1946723\RMSD=5.202e-09\RMSF=1.447e-06\Dipole=-0.1980089,0.4530593,0
.1543181\Quadrupole=45.1496112,10.6830388,-55.83265,1.6003656,41.07087
82,13.8040795\PG=C01 [X(C12H8Au16S5)]\\@

THIO2g.pbe0

1\1\GINC-LCMD40\FOpt\RPBE1PBE\Gen\C16H10Au16S6\ROOT\17-Apr-2016\0\\#PB
E1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(MaxCyc=250,MaxStep=10) IOP
(2/17=4) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\1TG\\0,1\Au,0.0
00040017,0.0000021106,0.0000682973\Au,2.4976304666,1.4419718712,0.0000
128598\Au,2.4976289413,-1.4419945133,0.0000131618\Au,-1.6650862741,-0.
000000071,-2.3547755635\Au,0.8325154188,1.4419858964,-2.3547973274\Au,
0.8325100372,-1.4419895502,-2.3547969926\Au,3.3301787199,2.8839948967,
-2.3547861659\Au,3.3301709468,-2.8840010399,-2.3547877404\Au,2.3514699
95,-0.0000022808,18.9999317213\Au,-0.1461205207,-1.4419717775,18.99998
70181\Au,-0.1461189642,1.4419944736,18.9999868011\Au,4.0165962844,0.00
000000739,21.3547755563\Au,1.5189946494,-1.4419858255,21.3547973949\Au,
1.5190000187,1.4419895314,21.3547970239\Au,-0.9786687723,-2.8839948059
,21.354786203\Au,-0.9786609637,2.8840010105,21.3547877524\C,1.25277520
39,0.005850247,10.2166766854\S,2.8278728577,-0.159109043,10.9368296318
\C,2.1729288773,-0.0676555605,12.5468290683\C,0.2856877464,0.139781998
3,11.1943049962\C,0.8037512955,0.0975800139,12.5062574382\H,0.18943423
3,0.1675901528,13.4042241445\H,-0.7737296305,0.2575839395,10.966777993
1\C,3.0484768976,-0.1605602162,13.6907409492\S,2.5270198339,0.38811128
62,15.2582924204\C,4.0635500633,-0.0182618892,15.9528970909\C,4.342003
917,-0.6429704731,13.7389037757\C,4.9192291928,-0.5632898749,15.026521
4224\S,4.4243624772,0.1595374865,17.6678380359\H,4.5318976845,1.515200
5,17.7202326364\H,5.9266969359,-0.8953753694,15.2746284586\H,4.8524447
609,-1.0549461407,12.868558541\C,-1.7120272886,0.0182859418,3.04714044
8\S,-0.175591008,-0.3884799551,3.741724367\C,-0.6969674101,0.160101256
8,5.3093357077\C,-2.5676297027,0.5633321013,3.9735755079\C,-1.99041237
71,0.6427402251,5.2612116001\S,-2.0728482599,-0.1592483978,1.332175673
8\H,-2.1806768817,-1.5148829778,1.2796396817\H,-2.5008094151,1.0546751
447,6.1316020323\H,-3.5750368697,0.8956224646,3.7254973252\C,0.1785372
781,0.0668923419,6.4532540796\S,-0.4763519663,0.1588649803,8.063247900
6\C,1.0986530497,-0.0069076561,8.7834156601\C,1.547630195,-0.099046437
7,6.4938436149\C,2.0656715046,-0.1414143189,7.8057989355\H,3.125017360
3,-0.2598320147,8.0333383182\H,2.1619128782,-0.1694921398,5.5958873862
\\Version=ES64L-G09RevD.01\HF=-5175.7261048\RMSD=7.346e-09\RMSF=1.798e
-06\Dipole=-0.0000428,-0.0001351,0.000058\Quadrupole=61.6167389,16.818
4577,-78.4351966,-0.2427382,55.2619523,8.8135622\PG=C01 [X(C16H10Au16S
6)]\\@

THIO3g.pbe0

1\1\GINC-R07-NODE01\FOpt\RPBE1PBE\Gen\C20H12Au16S7\GRYNOVA\10-Aug-2016

\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Em
piricalDispersion=GD3BJ pseudo=read Nosymm\\THIO3g.pbe0.freq\\0,1\C,4.
8697884205,0.331966938,17.2989690984\C,4.2716341659,0.4988549582,19.55
46287025\C,3.8469722775,0.5282454529,18.2068436149\C,5.6223318008,0.28
64678873,19.6720229726\S,6.3873360867,0.1093219261,18.1207032455\H,2.8
091147956,0.671591384,17.9062608088\H,3.6168554333,0.6061843181,20.421
0549817\C,-1.3281181279,0.2831301227,3.1552679189\C,2.0294192395,0.657
1161878,8.5745302144\C,0.9162119214,0.5386266789,6.3316706223\C,2.8791
036899,0.256236109,7.5623265725\C,2.25144507,0.1908855508,6.2978681701
\C,-0.0531478919,0.595836912,5.2636245975\C,-1.2991753203,1.1926686688
,5.2850986487\C,-2.02561119,1.0130140562,4.0867610244\C,3.223006924,0.
7860515779,12.3052651263\C,2.288954729,0.8516873277,9.9795163195\C,2.0
814291742,1.5553119218,12.1936856506\C,1.5561405071,1.5921800614,10.88
6080571\C,4.7901193972,0.3047262775,15.8576260213\C,4.0080310658,0.520
6931415,13.4848380428\C,5.7138826499,-0.140454928,14.9342662736\C,5.27
44468111,-0.0185708241,13.5974874101\S,-1.9104186287,-0.0628871899,1.5
306289878\S,0.2450449448,-0.1735508362,3.7299862767\S,0.425919232,0.92
54085297,7.9560788474\S,3.6385870942,0.0831773021,10.7665066847\S,3.35
59686179,0.8814007933,15.0577487786\S,6.5693779309,0.0879068158,21.151
747726\H,2.7679919893,-0.0819035164,5.3772422066\H,3.9346698983,0.0427
316159,7.7290110951\H,-2.0183316041,-1.4159029737,1.6284488042\H,-3.02
69264187,1.4014957471,3.9050512623\H,-1.6739157286,1.7470516892,6.1451
893979\H,6.9693740234,1.3791077916,21.3136246337\H,0.6750355432,2.1663
652226,10.6002551334\H,1.6506446842,2.0961865678,13.0361727945\H,5.870
515825,-0.3105030099,12.7330927983\H,6.6814356549,-0.5542933117,15.218
5958065\Au,-0.0000996687,-0.0000220734,-0.0001690884\Au,2.4976264484,1
.4419788231,0.0000214089\Au,2.4976281404,-1.441995891,0.0000232572\Au,
-1.6650819505,0.0000032697,-2.3547786207\Au,0.8325630219,1.4420201011,
-2.354759543\Au,0.832563007,-1.442007374,-2.3547673449\Au,3.3301710738
,2.8840081404,-2.354780759\Au,3.3301580169,-2.8840234344,-2.3547785982
\Au,4.9472273188,0.0001782877,23.0001744851\Au,2.4493647136,-1.4419981
741,23.0000493391\Au,2.4492970726,1.4419009229,23.0000909121\Au,6.6120
786764,-0.000022398,25.3547667923\Au,4.1143324755,-1.4421296583,25.354
6624219\Au,4.1143077792,1.4419927603,25.3547376206\Au,1.6168161498,-2.
8840206492,25.3547756528\Au,1.6168877248,2.8841373472,25.3547320642\\V
ersion=ES64L-G09RevD.01\HF=-5727.3126148\RMSD=5.914e-09\RMSF=6.463e-06
\Dipole=-0.1940602,0.369333,0.1726002\Quadrupole=73.1406105,21.2870907
,-94.4277013,0.3597638,49.8078739,19.0989927\PG=C01 [X(C20H12Au16S7)]\
\@

THIO4g.pbe0

1\1\GINC-R07-NODE01\FOpt\RPBE1PBE\Gen\C24H14Au16S8\GRYNOVA\09-Aug-2016
\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Em
piricalDispersion=GD3BJ pseudo=read Nosymm\\THIO4g.pbe0.freq\\0,1\C,7.
7628111614,0.0094770234,22.9076387766\C,6.6332128953,-0.206880978,20.7
068911539\C,8.5847991369,-0.5263633173,21.9462430156\C,7.9421105823,-0
.6491457444,20.6938410079\S,6.1771946978,0.3534760709,22.2912752731\H,
8.4171045297,-1.0613527556,19.8039196934\H,9.614290874,-0.8213367985,2
2.1457802126\C,2.6755691425,0.1048824401,12.4297564018\C,1.7234210054,
0.2292350138,10.1114743894\C,1.3650920546,0.540639156,12.3962691187\C,
0.830600074,0.6114291116,11.093438947\C,-0.4214485803,0.2244915846,5.2
911240585\C,-1.5513418139,0.0080552625,3.0905539863\C,-1.728561258,0.6
720843617,5.3029146126\C,-2.3713929458,0.5493076989,4.0505871867\C,4.4

890517594,-0.207973484,15.886321225\C,3.5374540844,-0.0808598998,13.56
79373077\C,5.3846262656,-0.581345987,14.9034732948\C,4.8504732461,-0.5
089449303,13.6006068659\C,5.7041738644,-0.1568429639,19.6038850305\C,4
.6886931017,-0.1574569291,17.3121671808\C,4.3296242418,-0.0369626944,1
9.6164139912\C,3.7570076033,-0.037233282,18.3254905864\C,1.5231531952,
0.1756060921,8.6858277486\C,0.5073464998,0.1732869711,6.3942831033\C,2
.4541951979,0.0489398776,7.6727038156\C,1.8813948681,0.0477416926,6.38
18757688\S,3.2460805014,-0.2334905839,10.8183239426\S,0.032660186,-0.3
410817329,3.708087066\S,-2.0036234465,-0.2144315928,1.4037010082\S,8.2
149283953,0.2303190253,24.5947071228\S,2.9636958711,0.2472534486,15.18
03504536\S,6.2972960162,-0.2435095272,17.9696071604\S,-0.0851942649,0.
2665095576,8.02842296\H,-0.1811171787,0.9499248719,10.8705399606\H,0.8
091935033,0.8098811569,13.2942529121\H,-2.0583374144,-1.5740713753,1.3
763166986\H,-3.3995944246,0.8481162509,3.8501032923\H,-2.2020717892,1.
0881365016,6.1918358193\H,8.2616254509,1.5901639012,24.6255429591\H,5.
408879915,-0.7703837302,12.7018750899\H,6.3984347885,-0.9140159968,15.
125645539\H,2.6853842695,0.0240390446,18.1370477994\H,3.7505597195,0.0
231377775,20.5382256882\H,2.4600677629,-0.0170090637,5.4601326968\H,3.
5255868679,-0.0160786436,7.8611993921\Au,0.0000291046,-0.000016134,0.0
000461155\Au,2.4976231766,1.4419844979,-0.0000027971\Au,2.4976183542,-
1.4420128505,-0.0000086817\Au,-1.6650833843,0.0000041642,-2.3547776069
\Au,0.8325360832,1.4420045626,-2.3547785908\Au,0.8325288852,-1.4419956
78,-2.3547865763\Au,3.3301695882,2.8840107133,-2.3547797088\Au,3.33016
14062,-2.8840175645,-2.3547809943\Au,6.2145276955,0.0000316297,25.9999
517633\Au,3.7169265602,-1.441984042,26.0000084017\Au,3.7169367752,1.44
2021735,26.0000189712\Au,7.879632947,-0.0000079713,28.3547779162\Au,5.
3819994475,-1.4420145719,28.3547673457\Au,5.3820182909,1.4419916785,28
.3547880272\Au,2.8843854704,-2.884019475,28.3547761318\Au,2.8843895993
,2.884019306,28.3547802833\\Version=ES64L-G09RevD.01\HF=-6278.8493881\
RMSD=5.933e-09\RMSF=6.506e-06\Dipole=-0.0009422,0.0120448,-0.0005714\Q
uadrupole=98.9963667,25.5314041,-124.5277708,-0.9600287,59.9473701,13.
1941644\PG=C01 [X(C24H14Au16S8)]\\@

THIO5g.pbe0

1\1\GINC-NODE05\FOpt\RPBE1PBE\Gen\C28H16Au16S9\GRYNOVA\28-Feb-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Empiri
calDispersion=GD3BJ pseudo=read Nosymm\\THIO5g.pbe0.freq\\0,1\C,3.5325
058949,0.8083483598,12.1919866219\S,4.035367513,0.4120598097,10.571419
4667\C,2.4529313635,0.7540806187,9.9274658338\C,2.1976894464,1.1642318
859,12.2102014804\C,1.5917500395,1.1333727345,10.9382878147\H,0.552119
1176,1.4046673795,10.7551690257\H,1.6798491765,1.4610712135,13.1220327
411\C,-0.0184809728,0.301305181,5.2906608599\S,0.3399191609,0.65993716
05,3.6249653993\C,-1.3062139458,0.3495766768,3.1680780311\C,-1.3443164
769,-0.053494603,5.449170285\C,-2.0768014624,-0.0266278102,4.241373551
\S,-1.8871055957,0.4193993705,1.5066345671\H,-1.8931265441,1.770301322
9,1.3405907492\H,-3.1331063084,-0.2773420089,4.151699033\H,-1.76794530
95,-0.3387261545,6.4118014065\C,8.2450210817,0.0974999087,22.860448547
7\S,6.6881090138,0.303213287,22.109651936\C,7.3909994895,0.3742917767,
20.5186079147\C,9.2440565434,0.085917395,21.9089113352\C,8.7641533797,
0.2423883003,20.5899190032\H,9.4055139325,0.2678144151,19.7092012197\H
,10.296978122,-0.0435803773,22.159643893\C,5.4445701724,0.6789598954,1
5.6049953044\S,3.8412687571,0.7800285898,14.932283778\C,4.4490531194,0
.7320623412,13.3006161867\C,6.3850399812,0.585346716,14.5977541422\C,5

.8251148985,0.6150147854,13.3017143765\H,6.4138662543,0.5746656696,12.
3853766858\H,7.4550147847,0.5194347683,14.7946272891\C,6.5474391661,0.
5521313757,19.3638496316\S,7.1536351133,0.2691831116,17.7547018145\C,5
.6266677108,0.6978229877,17.0337535552\C,5.2218050262,0.9363564683,19.
319909004\C,4.7044653436,1.0185677279,18.0111947976\H,3.6847835007,1.3
262712518,17.7803873673\H,4.6470034964,1.1743010775,20.214902193\C,2.1
674693575,0.617590668,8.5211309189\S,0.5142795562,0.5608443235,7.98090
2061\C,0.9939955247,0.4062883909,6.3148219828\C,3.0309539263,0.5196631
969,7.4472514487\C,2.3692217758,0.4009644851,6.2041144465\H,2.88425158
73,0.300526613,5.2483694747\H,4.1148218213,0.5432507384,7.5582646262\C
,8.3420836729,-0.0372079385,24.2948627167\C,7.3385355836,-0.3363435074
,25.1963589873\C,7.7798344787,-0.391070762,26.5381301014\C,9.124690627
7,-0.1431490091,26.6558578922\S,9.857442197,0.1967718278,25.1162241439
\H,6.3090334341,-0.5257146015,24.8925979056\H,7.1424710065,-0.59468791
12,27.4000184505\S,10.0964166557,-0.0490975556,28.1293517793\H,10.4636
290603,-1.3569886954,28.2202562217\Au,0.0000038493,0.0000012606,0.0000
038452\Au,2.4976195436,1.4419907905,0.000000351\Au,2.4976194004,-1.442
0110385,-0.0000001421\Au,-1.6650794893,-0.0000001481,-2.3547803611\Au,
0.8325377908,1.4419991289,-2.3547813145\Au,0.8325391285,-1.4419990765,
-2.3547808737\Au,3.3301705305,2.8840090812,-2.3547803751\Au,3.33016011
25,-2.8840198051,-2.3547800796\Au,8.4999881375,-0.0000304292,30.000035
1221\Au,6.0023749911,-1.4419813247,29.9999931298\Au,6.0023888495,1.442
0253285,29.9999885184\Au,10.1651205034,0.0000337425,32.354751362\Au,7.
6674436211,-1.44198801,32.3547815517\Au,7.6674331842,1.4419580163,32.3
547962292\Au,5.1698342066,-2.8840172862,32.3547770253\Au,5.1698456403,
2.8840297696,32.3547760114\\Version=ES64L-G09RevD.01\HF=-6830.3862684\
RMSD=7.467e-09\RMSF=4.948e-06\Dipole=-0.1672735,0.2140441,0.0919858\Qu
adrupole=109.0647206,27.86727,-136.9319905,-8.5962598,50.9709419,-13.1
190896\PG=C01 [X(C28H16Au16S9)]\\@

THIO6g.pbe0

1\1\GINC-NODE01\FOpt\RPBE1PBE\Gen\C32H18Au16S10\GRYNOVA\25-Feb-2017\0\
\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Empir
icalDispersion=GD3BJ pseudo=read Nosymm\\THIO6g.pbe0.freq\\0,1\C,2.572
9472192,-0.3387610644,12.4968773091\S,3.1415658162,0.1376028986,10.920
0077934\C,1.6890683835,-0.4385576989,10.1504928949\C,1.310836421,-0.89
37745523,12.4077433637\C,0.8147149116,-0.9498960945,11.0893644159\H,-0
.1522269453,-1.3761091839,10.8223835076\H,0.7693328065,-1.2683302808,1
3.2761992551\C,-0.3924001386,-0.3432701633,5.305473367\S,0.0464769258,
0.2961157736,3.7460106451\C,-1.5215977245,-0.0880301156,3.1077066234\C
,-1.6808544448,-0.8423100897,5.2922689708\C,-2.3234366332,-0.696528927
3,4.0425111652\S,-1.9834062165,0.1820244312,1.4308365201\H,-2.04617227
94,1.5414304663,1.4440345459\H,-3.3392657303,-1.0250807629,3.826178552
\H,-2.1422849122,-1.3078161642,6.1628095398\C,6.8452575261,0.482402937
9,23.3521955394\S,5.3711274849,-0.0387530394,22.5845703213\C,5.9556052
266,0.415232687,21.0069659837\C,7.7378632192,0.9583972122,22.411868071
\C,7.2384587973,0.9206554999,21.0940443179\H,7.7919149642,1.275353785,
20.2247959705\H,8.7206309984,1.3476541795,22.6775162706\C,4.2019226402
,0.0673051823,16.0352035221\S,2.6966736997,-0.3404423447,15.2586559227
\C,3.3810243082,-0.1286726423,13.6699774542\C,5.1683748003,0.355369463
5,15.0908151098\C,4.707443947,0.2444931808,13.7621126459\H,5.331909366
9,0.4234993341,12.8869412474\H,6.1865032972,0.639506156,15.356535683\C
,5.1376499219,0.238413325,19.8351861143\S,5.8375737934,0.3791230693,18

.2455642379\C,4.3075196081,0.0726140819,17.4711169677\C,3.7898696956,-0.0486887684,19.7452176044\C,3.3235266766,-0.1421574966,18.4169870434\H,2.2867360297,-0.3502108638,18.1529041347\H,3.1533233245,-0.1705947379,20.62148375\C,1.5100315648,-0.3354550734,8.7244267342\S,-0.0829933526,-0.4833930007,8.0407297054\C,0.5228592838,-0.290914977,6.4199767609\C,2.4449313567,-0.1159350985,7.7310499549\C,1.8881692932,-0.0914078983,6.4329068087\H,2.4738951062,0.0432852086,5.5232365464\H,3.5088650421,-0.0025946702,7.9378780027\C,7.020674405,0.3765045754,24.7784928641\C,6.0787443702,0.1901621836,25.7720473686\C,6.6337095962,0.1523115699,27.0706337618\C,8.0046205069,0.308539949,27.0837368152\S,8.6173045956,0.4755306171,25.4627728795\H,5.0118029251,0.1102746219,25.5650522417\H,6.0435156987,0.039973161,27.9804490384\C,8.9199401289,0.3385364561,28.1990304731\C,10.2204413281,0.8051782877,28.213175019\C,10.8568556369,0.6469833703,29.4646087359\C,10.0384493796,0.0610752462,30.3995176784\S,8.4627611674,-0.2865244699,29.7589917486\S,10.4887490656,-0.2136228962,32.0788512224\H,10.6945303498,1.2574907122,27.3424833143\H,11.8799029917,0.9514501453,29.6822157073\H,10.5271923808,-1.5739529978,32.069141729\Au,0.0000096767,0.0000019754,0.0000238811\Au,2.4976197341,1.4419904606,-0.0000036974\Au,2.4976191163,-1.4420115305,-0.000004599\Au,-1.6650776083,-0.0000013681,-2.3547816912\Au,0.832537177,1.4419988958,-2.3547816742\Au,0.8325366237,-1.4419988508,-2.3547818974\Au,3.3301696956,2.8840105273,-2.3547797847\Au,3.3301600081,-2.884019986,-2.3547800057\Au,8.4999952312,-0.0000062003,33.4999686035\Au,6.0023812014,-1.4419920805,33.5000140157\Au,6.0023844671,1.4420177368,33.5000099125\Au,10.1650773555,0.0000008432,35.8547818699\Au,7.6674548901,-1.4419956696,35.8547808452\Au,7.6674560928,1.4419998609,35.8547787038\Au,5.1698345013,-2.8840177966,35.854776817\Au,5.1698418374,2.8840231824,35.8547787008\\Version=ES64L-G09RevD.01\HF=-7381.9225504\RMSD=5.450e-09\RMSF=5.294e-06\Dipole=-0.0003813,0.0108134,0.0059288\Quadrupole=131.566163,39.9190094,-171.4851724,4.2372336,70.888455,-13.3663669\PG=C01 [X(C32H18Au16S10)]\\@

THIA1g.pbe0

1\1\GINC-R03-NODE39\FOpt\RPBE1PBE\Gen\C8H4Au16S5\GRYNOVA\29-Jan-2017\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\THIA1g.pbe0.freq\\0,1\S,-0.7967322747,1.870216293,6.999118628\C,1.2584539794,0.3114164734,6.495901109\S,2.7058378617,-0.4530707674,7.0535874618\C,2.5231366577,0.3096999542,8.6217518438\C,0.6916930726,1.1093759141,7.4942953264\C,1.4100341286,1.1065659063,8.7123215175\S,3.6675757916,-0.091877905,9.9072916282\H,4.3445273051,1.0867533478,9.9457738282\H,1.1148407804,1.6161798773,9.630360079\C,-0.9661949733,0.2973908432,3.3070436368\S,0.5723891626,-0.417065348,3.7391897281\C,0.4819848018,0.3169727654,5.3054021982\C,-1.4960025741,1.0951141063,4.2917183807\C,-0.6623068901,1.1088906661,5.4354822633\S,-1.7289842634,0.0688399567,1.7344338266\H,-1.9855193494,-1.2635474151,1.8287692479\H,-2.4435357036,1.620962876,4.1895932204\Au,0.0000231355,-0.0000238476,0.0000320099\Au,2.4976167027,1.4419957109,0.0000018268\Au,2.4976215587,-1.4420073003,0.000002579\Au,-1.6650772921,0.0000053022,-2.3547819146\Au,0.832532872,1.4419975176,-2.3547840402\Au,0.8325270019,-1.4419864496,-2.3547928925\Au,3.3301733337,2.884004226,-2.3547823573\Au,3.3301606921,-2.8840188013,-2.3547804893\Au,2.3516201439,0.000011769,11.9999662249\Au,-0.1459637694,-1.4419834707,12.0000162421\Au,-0.1459616487,1.4420071435,12.0000187467\Au,4.0167414608,-0.00

00104761,14.3547789668\Au,1.5191453109,-1.4419998175,14.3547818034\Au,
1.5191054456,1.4419901933,14.3547737887\Au,-0.9785048699,-2.8840188854
,14.3547765215\Au,-0.9784900776,2.8840371859,14.354772984\\Version=ES6
4L-G09RevD.01\HF=-4469.5714595\RMSD=8.671e-09\RMSF=1.516e-05\Dipole=-0
.3400018,0.2425002,0.3410685\Quadrupole=32.3509842,3.3189086,-35.66989
28,2.1171791,31.3659939,6.7841901\PG=C01 [X(C8H4Au16S5)]\\@

THIA2g.pbe0

1\1\GINC-R04-NODE22\FOpt\RPBE1PBE\Gen\C10H4Au16S6\GRYNOVA\29-Jan-2017\
0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Emp
iricalDispersion=GD3BJ pseudo=read Nosymm\\THIA2g.pbe0.freq\\0,1\C,0.7
960334319,0.2153294892,8.054020854\S,-0.8402825259,0.6540102729,7.6441
08374\C,-0.5286348576,0.2751235115,5.9660844427\C,0.7785370162,-0.1632
399896,5.7414331643\S,1.0347050843,-0.542232888,4.0643118633\C,-0.6379
72289,-0.1527021397,3.7015302643\C,-1.3379041623,0.2815393774,4.803569
208\S,-1.3854618698,-0.3144482283,2.1040812301\H,-1.4005682753,-1.6717
625299,2.0406538301\H,-2.389069301,0.561900293,4.766003779\C,2.9763741
513,0.1762017388,11.2951808831\S,1.3028745271,0.5622877749,10.93261125
3\C,3.6764251194,-0.2587795575,10.1934565564\S,3.7242437258,0.34251260
11,12.8917830598\H,3.7212708216,1.6995932253,12.9598722435\H,4.7282329
97,-0.5367346186,10.2308328623\C,2.8665638446,-0.2553137758,9.03128094
55\S,3.1780734113,-0.6348557797,7.3533346227\C,1.5414695104,-0.1971263
541,6.9433624668\C,1.5590564066,0.1820484463,9.2558307501\Au,0.0000541
126,0.0000445955,0.0000648767\Au,2.4976088936,1.4420092376,-0.00001290
31\Au,2.4976121318,-1.4420236277,-0.0000128505\Au,-1.6650803836,-0.000
0074357,-2.3547797283\Au,0.8325059444,1.4419938999,-2.3547957697\Au,0.
8325588452,-1.4420139684,-2.3547647755\Au,3.3301684849,2.8840126248,-2
.3547789291\Au,3.3301547256,-2.8840291342,-2.3547762704\Au,2.351581618
,-0.0000498255,14.9999513229\Au,-0.1459557128,-1.4419974239,14.9999880
935\Au,-0.1459547119,1.4420191579,14.9999932677\Au,4.0167333478,0.0000
070561,17.3547847039\Au,1.519166082,-1.4419875731,17.3547968261\Au,1.5
19132888,1.4419996234,17.3547777052\Au,-0.9785168259,-2.8839981767,17.
3547848272\Au,-0.9784994396,2.88402097,17.3547796034\\Version=ES64L-G0
9RevD.01\HF=-4943.7644803\RMSD=6.671e-09\RMSF=1.333e-05\Dipole=-0.0072
055,0.0112872,0.0041283\Quadrupole=42.0342887,10.5797282,-52.6140169,1
.4486913,39.7250306,8.592046\PG=C01 [X(C10H4Au16S6)]\\@

THIA3g.pbe0

1\1\GINC-R09-NODE44\FOpt\RPBE1PBE\Gen\C12H4Au16S7\GRYNOVA\30-Jan-2017\
0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Emp
iricalDispersion=GD3BJ pseudo=read Nosymm\\THIA3g.pbe0.freq\\0,1\S,-2.
1932039385,0.6592821274,7.0581472528\C,-1.6295197736,0.2545381836,5.45
7289964\C,0.3171383145,-0.0425533003,6.714536122\C,-0.2756538828,-0.09
36581504,5.4238660071\S,0.2309106026,-0.4980780264,3.815136834\C,-1.39
93943675,-0.2408576514,3.2256631474\C,-2.2735141044,0.1714241292,4.201
8396611\S,-1.8681137641,-0.4322064922,1.5372503265\H,-1.8058244345,-1.
7891341279,1.4596117504\H,-3.3239889257,0.3836124713,4.011209318\C,2.7
710845001,0.1162053103,12.5909956784\S,3.4107001323,-0.2850195999,11.0
055444242\C,1.4457072629,0.4687959392,12.5680010621\C,0.9386887262,0.4
318294722,11.2485540537\S,3.818260716,-0.0455634765,14.0079338436\H,4.
2826740208,1.232684979,14.0611288619\H,0.8818290285,0.7129237158,13.47
00596099\S,1.8996966296,-0.3659087974,7.376850599\C,-0.0319103778,0.38
48752285,8.9857879354\C,-0.6034170373,0.3472374697,7.6913033797\S,-0.6

363121334,0.7634575773,10.5733781213\C,1.8740180325,0.0465018872,10.28
29719661\C,1.3169503436,0.0205180378,8.9766931271\Au,-0.0000389816,-0.
0000233045,-0.0000638923\Au,2.497621215,1.4419878955,0.0000050707\Au,2
.4976239998,-1.4420030721,0.0000065194\Au,-1.6650813366,0.0000034618,-
2.3547790549\Au,0.8325518503,1.4420153013,-2.3547664399\Au,0.832550924
4,-1.4420015389,-2.3547751952\Au,3.3301698118,2.8840103259,-2.35477986
7\Au,3.3301574332,-2.8840244458,-2.3547781851\Au,2.351653083,0.0000259
669,16.0000526777\Au,-0.1459606495,-1.4419888751,15.9999995417\Au,-0.1
459650029,1.4420013346,15.9999995624\Au,4.0167421121,-0.000004538,18.3
547785065\Au,1.5191145411,-1.4420101185,18.3547648024\Au,1.5191371525,
1.4420005212,18.3547786741\Au,-0.9785083897,-2.8840127892,18.354778861
3\Au,-0.9784977629,2.8840238748,18.3547784181\\Version=ES64L-G09RevD.0
1\HF=-5417.9768203\RMSD=6.151e-09\RMSF=1.833e-05\Dipole=-0.4332683,-0.
0947932,0.3483989\Quadrupole=39.2011036,5.8008987,-45.0020023,2.408823
4,39.4826888,7.9874505\PG=C01 [X(C12H4Au16S7)]\\@

THIA4g.pbe0

1\1\GINC-R09-NODE51\FOpt\RPBE1PBE\Gen\C14H4Au16S8\GRYNOVA\30-Jan-2017\
0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Emp
iricalDispersion=GD3BJ pseudo=read Nosymm\\THIA4g.pbe0.freq\\0,1\C,1.8
60827145,0.1280910846,8.6700482533\S,2.3085763472,0.4091121052,7.00874
89944\C,-0.0516970054,0.2216130464,5.2913077608\S,0.3495785616,0.50055
97797,3.6302479736\C,-1.334125443,0.3131208222,3.1860215867\C,-1.41690
72491,-0.0293518836,5.4561634603\C,-2.1530544626,0.0194825833,4.249746
9908\S,-1.8927771184,0.4168277515,1.5172427221\H,-1.8671309707,1.77031
00945,1.3743289735\H,-3.2252368596,-0.1407685243,4.1513825548\C,3.6905
904469,-0.3085396332,14.3162896783\S,2.0072160723,-0.4977414161,13.871
5671327\C,2.4088120317,-0.219399667,12.2105231697\C,4.5097367275,-0.01
54040687,13.2525817919\C,3.7739616596,0.0320757407,12.0458826581\S,4.2
479946812,-0.4098270327,15.9856803853\H,4.2272919541,-1.7633808882,16.
128826869\H,5.5817600073,0.1457652834,13.3512046799\C,1.7080200574,-0.
1835089613,10.978213149\S,0.0488000395,-0.4075672442,10.492920918\C,0.
4966614009,-0.1268073376,8.8316283607\S,4.2160839173,0.319943805,10.38
05204084\C,-0.1993622698,-0.0940084779,7.5986042057\S,-1.8588238701,-0
.3176624302,7.1214728625\C,0.6493230159,0.1850984924,6.5234865976\C,2.
5567838568,0.0955046951,9.9031360486\Au,0.0000043833,-0.0000361094,-0.
0000457063\Au,2.4976283102,1.4419756171,0.0000699638\Au,2.4976379299,-
1.4419789539,0.0000536381\Au,-1.6650744238,0.0000017867,-2.3547839429\
Au,0.8324954364,1.4419857479,-2.3548044858\Au,0.8324988747,-1.44195682
22,-2.354820986\Au,3.330194492,2.8839675764,-2.3547973206\Au,3.3301742
641,-2.8839952946,-2.3547900864\Au,2.3516049923,0.0000354078,17.500047
0066\Au,-0.1459683881,-1.4419754817,17.4999298623\Au,-0.145977824,1.44
19791375,17.499946235\Au,4.0167348855,-0.0000018502,19.8547836166\Au,1
.5191847182,-1.4419862113,19.854804255\Au,1.5191812534,1.4419577865,19
.8548204391\Au,-0.9785345502,-2.8839674761,19.8547973617\Au,-0.9785143
537,2.8839951396,19.8547901498\\Version=ES64L-G09RevD.01\HF=-5892.1805
713\RMSD=5.857e-09\RMSF=1.076e-05\Dipole=0.0017498,0.0032105,0.000762\
Quadrupole=52.6846785,12.2317326,-64.916411,-2.9163928,52.4707974,-13.
4859911\PG=C01 [X(C14H4Au16S8)]\\@

PYR1g.pbe0

1\1\GINC-R01-NODE01\FOpt\RPBE1PBE\Gen\C14H8Au16N2S5\GRYNOVA\10-Aug-201
6\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) E

mpiricalDispersion=GD3BJ pseudo=read Nosymm\\THIOPYR1g.pbe0.freq\\0,1\
C,1.7569899658,0.3426362807,8.5309408507\S,0.2052251091,0.7244887623,7
.8695237697\C,0.631765811,0.2797202585,6.2539373364\C,1.9555607036,-0.
1660227105,6.2294077186\C,-0.3151619294,0.3661658813,5.180345155\S,0.0
65730366,-0.2226064909,3.5839350733\C,-1.5311984302,0.1744926246,3.038
4413695\C,-1.60422832,0.8711536805,5.2379875133\C,-2.2982448698,0.7632
341072,4.0155518532\S,-2.0380710894,-0.0572551405,1.3678261264\H,-2.17
3493873,-1.411727234,1.3748470413\H,-3.3212358521,1.0989946215,3.85131
37055\H,-2.033509813,1.3032172786,6.1420277251\C,2.9622534752,0.452438
4003,12.2230898689\S,3.5068786727,-0.0570665371,10.6546151109\C,2.0251
247938,0.5038355511,9.9310964601\C,1.7135738115,1.0246069211,12.187758
8233\C,1.1860596282,1.0609141629,10.8826613182\S,3.9574013932,0.116588
1184,13.6440951354\H,4.4521554254,1.3671873037,13.8513101795\H,0.20642
94803,1.4743994826,10.6421400483\H,1.1928252305,1.3690451881,13.082429
2485\C,2.589995648,-0.133012589,7.5152918763\N,3.8746313829,-0.5368017
331,7.6917751456\C,4.4768903142,-0.9487316656,6.6044057555\C,3.8441736
126,-0.9784775464,5.3170996195\N,2.60670072,-0.5986693534,5.1189924363
\H,5.5141607064,-1.2833460221,6.70070266\H,4.4055024483,-1.3316641722,
4.4468545524\Au,0.0001361647,0.0000118102,0.0002501569\Au,2.4976092304
,1.4420086337,-0.0000363837\Au,2.4976065894,-1.4420332033,-0.000041263
6\Au,-1.6650725898,-0.000000415,-2.3547852394\Au,0.8325120767,1.441973
5132,-2.3548060792\Au,0.8325110846,-1.4419770903,-2.3548042406\Au,3.33
01688172,2.8840120493,-2.3547791629\Au,3.3301596778,-2.8840205582,-2.3
54779772\Au,2.3514540215,-0.0000148223,15.4997775616\Au,-0.1459495933,
-1.4420080154,15.5000154845\Au,-0.1459555592,1.4420176851,15.500013332
5\Au,4.0167325225,0.0000022104,17.8547852874\Au,1.519193296,-1.4419679
413,17.8548184523\Au,1.5191827493,1.4419824188,17.8548058642\Au,-0.978
5153193,-2.8840007867,17.8547837613\Au,-0.9785031686,2.8840145118,17.8
547822406\\Version=ES64L-G09RevD.01\HF=-4809.7737844\RMSD=2.790e-09\RM
SF=1.207e-05\Dipole=-0.1034482,0.1858342,0.1364832\Quadrupole=50.21556
94,11.7853872,-62.0009565,-0.8566737,38.4141417,11.9570469\PG=C01 [X(C
14H8Au16N2S5)]\\@

PYR2g.pbe0

1\1\GINC-R04-NODE69\FOpt\RPBE1PBE\Gen\C20H10Au16N4S6\GRYNOVA\09-Aug-20
16\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\THIOPYR2g.pbe0.freq\\0,1
\C,1.2648808106,0.0792400797,10.2030261148\S,2.8255262689,-0.063232339
2,10.9532540288\C,2.2072920627,0.1502881464,12.5598266934\C,0.28903759
05,0.2919503103,11.1909257115\C,0.8215224949,0.3325279584,12.518176903
7\N,0.0291631251,0.5285403026,13.6018273048\N,-1.03319337,0.4469106428
,10.9443637751\C,3.0681643465,0.1324503566,13.7062576226\S,2.463270080
6,0.4593119207,15.3124122244\C,4.0597301173,0.2920182979,15.9696080615
\C,4.4317524741,-0.1184544229,13.726237479\C,4.9956629783,-0.030987201
,15.0147360317\S,4.4006322837,0.4260754415,17.6932645335\H,4.331374928
1,1.7796706951,17.8177609557\H,6.0483056411,-0.1935180156,15.242649726
1\H,5.0033511395,-0.3575136523,12.8294631175\C,-1.7211574123,-0.210750
8311,3.0307153008\S,-0.1273535959,-0.3945486825,3.6894493115\C,-0.7297
2533,-0.0567994827,5.2942450107\C,-2.6543276061,0.1248290884,3.9838924
246\C,-2.0905585408,0.2085905639,5.2727185012\S,-2.0610883422,-0.34737
87931,1.3066049387\H,-2.0360371126,-1.7036665817,1.194249887\H,-2.6599
232795,0.4568112905,6.1684342017\H,-3.7047458524,0.2993735675,3.754595
4729\C,0.1304479582,-0.0797888373,6.441146662\S,-0.4876962841,0.134198

5478,8.0476546887\C,1.072448047,-0.0119532354,8.798157794\C,1.51553871
04,-0.2669049146,6.4831473458\C,2.0479099518,-0.2275343058,7.810465437
9\N,3.3696603628,-0.3860991127,8.0572492764\N,2.3074416014,-0.46581182
49,5.399690846\C,-1.2467107686,0.6745270031,13.3367560605\C,-1.7780098
642,0.6340923257,12.0088449517\C,4.114064006,-0.5760310733,6.992967557
7\C,3.5828104615,-0.6156259283,5.6649904311\H,-1.919578465,0.832960286
7,14.1847758731\H,-2.8531455596,0.7632599342,11.8534250611\H,5.1887904
311,-0.7082888918,7.1486164635\H,4.2552473764,-0.7766160379,4.81710822
04\Au,0.0000151216,-0.0000161811,0.0000290426\Au,2.4976158556,1.441997
1775,-0.0000065261\Au,2.4976199496,-1.4420100869,-0.0000051351\Au,-1.6
6507932,0.0000047109,-2.3547804808\Au,0.8325381911,1.4420015468,-2.354
7796922\Au,0.8325371887,-1.4419944677,-2.3547843814\Au,3.3301707657,2.
8840086737,-2.3547805415\Au,3.3301582456,-2.8840230388,-2.3547787594\A
u,2.3514544532,0.000013013,18.9999717797\Au,-0.1461166094,-1.441995872
,19.0000051402\Au,-0.1461197999,1.4420103461,19.0000048153\Au,4.016599
479,-0.0000038713,21.3547803684\Au,1.5189924454,-1.4420006149,21.35478
04879\Au,1.5190036045,1.4419952448,21.3547841859\Au,-0.9786707727,-2.8
840086616,21.3547805464\Au,-0.9786587982,2.8840220816,21.3547791502\\V
ersion=ES64L-G09RevD.01\HF=-5546.8481949\RMSD=3.096e-09\RMSF=4.195e-05
\Dipole=-0.0129863,0.0435701,0.0061884\Quadrupole=72.4054415,19.513777
4,-91.9192189,-0.0431872,46.8747602,15.4401609\PG=C01 [X(C20H10Au16N4S
6)]\\@

PYR3g.pbe0

1\1\GINC-R05-NODE46\FOpt\RPBE1PBE\Gen\C26H12Au16N6S7\GRYNOVA\10-Aug-20
16\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\THIOPYR3g.pbe0.freq\\0,1
\C,3.6769302252,0.0962288575,13.534873574\S,3.0786419717,0.4135867727,
15.1373236061\C,4.6053393064,0.1056380484,15.8998577536\C,5.0408802415
,-0.2398721479,13.6045176917\C,5.5617999622,-0.2348412464,14.937590586
4\N,6.857984857,-0.5380687846,15.1995116634\N,5.8093343345,-0.54673487
92,12.5347920067\C,4.756029092,0.2052011069,17.3215091791\S,6.27596928
73,-0.1200577452,18.1139236191\C,5.5695903773,0.219422097,19.665401387
1\C,3.7796919539,0.5463895981,18.246037118\C,4.2386106842,0.5499419382
,19.577812298\S,6.5420804218,0.0288973697,21.1298780588\H,6.9795830772
,1.3118009852,21.2582752098\H,3.6226425233,0.7630780334,20.452781023\H
,2.7534881405,0.7818993041,17.9636861836\C,-1.5244630629,-0.227074723,
3.0738970335\S,0.0996638527,-0.4663161861,3.6358103189\C,-0.3800989202
,-0.0419097939,5.2605615592\C,-2.3757599863,0.1911221764,4.0699905529\
C,-1.7248278869,0.2949327401,5.3148883518\S,-1.986849528,-0.4000857061
,1.3838076848\H,-1.9379716732,-1.7569936463,1.2851899589\H,-2.22134223
85,0.603310031,6.2347979638\H,-3.4296624937,0.4086101156,3.9013734539\
C,1.8631257143,0.1290495667,10.0483655775\S,3.4246614069,-0.1528810137
,10.7682603729\C,2.8541775424,0.1703895254,12.3828355155\C,0.927982714
9,0.4694560463,11.0431974012\C,1.4854520751,0.4939782677,12.3546921647
\N,0.7420406215,0.7977596556,13.4421526408\N,-0.3754269718,0.747683816
,10.8162233714\C,0.5445278035,-0.0765701982,6.3538047439\S,0.026876742
8,0.2529385258,7.9755286649\C,1.6076351013,0.0091759683,8.659153357\C,
1.9126690406,-0.3675965723,6.3360241764\C,2.5134318215,-0.3205084409,7
.6340425428\N,3.8280261156,-0.5750073143,7.8251067076\N,2.6312037998,-
0.6687734786,5.2252696497\C,7.5810644048,-0.8318437008,14.1451895541\C
,7.0593865508,-0.8367134922,12.8143044215\C,-0.521483168,1.0659416722,
13.198719733\C,-1.079519909,1.0406958213,11.886877666\C,4.5017359746,-

0.8627340367,6.7349654781\C,3.9035482043,-0.9086330555,5.4369922309\H,
8.6328550544,-1.0828948237,14.3130715092\H,7.7151921991,-1.0909923688,
11.9764571478\H,-1.1554897929,1.3165065331,14.0542657953\H,-2.13899529
17,1.272144476,11.7430430703\H,5.5692408394,-1.074193829,6.8459764676\
H,4.5181605246,-1.152989125,4.5653529965\Au,-0.0000322102,-0.000010038
2,-0.0000578816\Au,2.497623219,1.4419844234,0.0000090879\Au,2.49762177
04,-1.4420069325,0.0000098986\Au,-1.665080071,0.0000021033,-2.35477994
97\Au,0.8325466013,1.4420082644,-2.3547726044\Au,0.8325458959,-1.44200
03022,-2.3547777301\Au,3.3301705327,2.8840090773,-2.3547803767\Au,3.33
01600394,-2.8840199318,-2.3547800279\Au,4.9470763434,0.0000503262,23.0
000457529\Au,2.4493608434,-1.441991461,23.0000301507\Au,2.4493403173,1
.4419758984,23.0000395608\Au,6.6120657542,-0.0000038777,25.3547759313\
Au,4.1143791704,-1.4420329421,25.3547383012\Au,4.1143978969,1.44200203
23,25.3547638624\Au,1.6168202066,-2.8840276782,25.3547727821\Au,1.6168
436903,2.8840610384,25.3547632424\\Version=ES64L-G09RevD.01\HF=-6283.9
22206\RMSD=6.022e-09\RMSF=4.696e-06\Dipole=-0.126303,-0.0669743,0.1252
141\Quadrupole=92.0943611,24.3768983,-116.4712594,-2.642711,38.8326725
,15.462063\PG=C01 [X(C26H12Au16N6S7)]\\@

PYR4g.pbe0

1\1\GINC-R09-NODE18\FOpt\RPBE1PBE\Gen\C32H14Au16N8S8\GRYNOVA\10-Aug-20
16\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\THIOPYR4g.pbe0.freq\\0,1
\C,2.7042875929,0.0157602859,12.4348553668\S,3.3031323332,-0.128293683
8,10.8016414746\C,1.7090841663,-0.0554841472,10.0994659046\C,1.2982138
055,0.1185793646,12.4240011946\C,0.7404068314,0.0786060335,11.11287521
08\N,-0.5919216955,0.1620230688,10.9007628263\N,0.527415499,0.24223739
4,13.5257286401\C,-0.4747599214,-0.227146686,5.2800449337\S,0.06961001
98,-0.500162934,3.6422036947\C,-1.5636066495,-0.4046428833,3.063319255
1\C,-1.849585522,-0.0458652797,5.3277219385\C,-2.4683865961,-0.1435185
103,4.0660598741\S,-1.9823821269,-0.5270811927,1.3568109826\H,-1.85635
55013,-1.8738197086,1.200266968\H,-3.5373503133,-0.0304300436,3.889804
5751\H,-2.3885011502,0.1522259717,6.2541096877\C,7.8006379913,0.410094
0267,22.9512539364\S,6.1691921096,0.5106641323,22.3685822562\C,6.71789
09819,0.2483865226,20.7303444845\C,8.7083251538,0.1566102447,21.949279
836\C,8.0929207681,0.0683162313,20.6851038783\S,8.2118037624,0.5187758
939,24.6608400678\H,8.0970543917,1.8657753857,24.8248382468\H,8.634464
8493,-0.1230692943,19.7588261042\H,9.7767998072,0.0419693006,22.127448
1913\C,4.5395460748,0.0922063649,15.9074576089\S,2.9457812015,0.166714
0633,15.2047981815\C,3.5451101834,0.0233905319,13.5716925616\C,5.50855
5113,-0.0409575685,14.8942674019\C,4.9511598388,-0.0795041199,13.58287
48686\N,5.7222524829,-0.2024965282,12.4812661699\N,6.8407855653,-0.125
1512645,15.106788628\C,5.8092192441,0.2427378288,19.6235162685\S,6.374
8154189,0.0936976595,17.9894296662\C,4.7776263623,0.1638754996,17.3016
030426\C,4.4145798908,0.3494167677,19.640661656\C,3.8308863017,0.30363
44955,18.3353810612\N,2.4954514634,0.3896075927,18.144947549\N,3.65781
12832,0.4821803294,20.7588295808\C,1.4700205415,-0.1299106126,8.705640
315\S,-0.1279556185,-0.0630562575,8.0193520892\C,0.43602428,-0.2162985
698,6.3850744658\C,2.4157778585,-0.2713927661,7.6712046422\C,1.8307221
79,-0.3214330373,6.3666129189\N,2.5863820168,-0.4569024861,5.247994178
4\N,3.7514794068,-0.3557222105,7.8605103195\C,3.8792143416,-0.53519968
08,5.4587430443\C,4.4619537741,-0.4848753513,6.7627432558\C,-1.3237380
966,0.281968891,11.9871071353\C,-0.7656472136,0.3221129073,13.29723566

21\C,7.0152113865,-0.2830643953,12.7101749996\C,7.5728786763,-0.244357
2061,14.0205353022\C,1.7838844581,0.5161630454,19.2422936247\C,2.36527
20004,0.5621784138,20.5470602363\H,4.5230218988,-0.643301224,4.5806290
425\H,5.5479001625,-0.5558005505,6.8733242814\H,-2.4075973619,0.352349
6226,11.8560022561\H,-1.4228905126,0.4230198161,14.1657995258\H,7.6727
444832,-0.3834928954,11.8417752048\H,8.6566704783,-0.3153194609,14.151
8879479\H,0.6981170861,0.5882719489,19.1307330212\H,1.7206842519,0.668
1174529,21.4248699456\Au,0.0000559934,0.0000147399,0.0001050988\Au,2.4
976123296,1.4420032849,-0.0000140466\Au,2.4976133414,-1.4420215317,-0.
00001732\Au,-1.6650754063,-0.0000028773,-2.3547832482\Au,0.8325280454,
1.4419815288,-2.3547955369\Au,0.832527028,-1.4419946064,-2.3547878888\
Au,3.3301696522,2.8840106026,-2.3547797539\Au,3.3301608902,-2.88401845
81,-2.3547806295\Au,6.2144953095,-0.000014383,25.9999000335\Au,3.71693
64545,-1.4420011788,26.0000134029\Au,3.7169357787,1.4420200079,26.0000
168322\Au,7.8796270255,0.0000025554,28.3547821033\Au,5.3820215286,-1.4
419836344,28.354794097\Au,5.382022265,1.4419961563,28.3547866897\Au,2.
884380519,-2.884010899,28.3547796329\Au,2.8843892454,2.884018693,28.35
47805336\\Version=ES64L-G09RevD.01\HF=-7020.9974438\RMSD=4.280e-09\RMS
F=1.901e-05\Dipole=0.0069944,0.0028725,0.0057828\Quadrupole=120.479367
5,31.9196729,-152.3990405,3.2189204,39.0237752,23.3381812\PG=C01 [X(C3
2H14Au16N8S8)]\\@

THIOQ1g.pbe0

1\1\GINC-R06-NODE40\FOpt\RPBE1PBE\Gen\C16H8Au16N2S5\GRYNOVA\04-Feb-201
7\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(Loose) IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\THIOQ1g.pbe0.freq\\0,1\
S,-0.6477883044,-2.6624907849,8.4651279873\C,0.4647504039,-1.781562259
,9.5064792915\C,0.8977634466,-0.5877973455,8.8566288473\C,0.3697867763
,-0.4084627374,7.6106990872\C,-0.5036074302,-1.4558482505,7.1923238187
\C,0.8456139996,-2.238494215,10.7521915015\C,0.418031222,-3.4149633384
,11.4363791962\C,1.0111928504,-3.6054706115,12.6501271955\C,1.97149512
48,-2.5929230953,12.9791346947\S,2.0339129376,-1.3717425192,11.7264977
53\C,-1.1435623289,-1.5709942079,5.9739570888\C,-1.9662800076,-2.63468
07335,5.5015610964\C,-2.4159912427,-2.4718847461,4.2231744736\C,-1.990
7581953,-1.2435214843,3.6209600581\S,-0.9868304831,-0.3299129476,4.729
0439715\C,-2.2990798186,-0.7941098848,2.3576743919\C,-3.0800191898,-1.
5451403917,1.4528130887\S,-1.5700174369,0.7023651096,1.750071112\N,-3.
7251188002,-2.1185593256,0.6684310008\C,2.76814107,-2.5479071696,14.09
72449545\S,3.8185440676,-1.1462510124,14.3749106293\C,2.6772644621,-3.
5127010219,15.1237120169\N,2.6385098301,-4.2949138486,15.9878427886\H,
1.5904506836,0.1074066941,9.330928568\H,0.5945427782,0.4442171087,6.97
00125425\H,-0.3196062961,-4.0934829465,11.0070806717\H,0.8167000731,-4
.4414728225,13.3209350293\H,-2.1977883142,-3.5012421042,6.1215641487\H
,-3.0443196978,-3.1802575077,3.6846358506\H,-2.6407075883,1.1195845242
,1.0270937925\H,4.7085191819,-1.7803908873,15.1788224853\Au,-0.0000461
526,0.0000155195,-0.0000550869\Au,2.49762621,1.4419792435,0.000000089\
Au,2.4976209473,-1.4420083593,-0.0000002984\Au,-1.6650816158,0.0000029
309,-2.3547788574\Au,0.8325603649,1.4420057866,-2.3547692552\Au,0.8325
550857,-1.4420165716,-2.3547645172\Au,3.3301649865,2.8840186837,-2.354
7764548\Au,3.3301586969,-2.884022257,-2.3547790786\Au,2.3516464576,-0.
000063488,16.0000649243\Au,-0.1459769228,-1.4419606867,16.0000040288\A
u,-0.1459618731,1.4420067558,16.0000004297\Au,4.0167437933,0.000006010
2,18.3547773176\Au,1.5191219029,-1.4419944259,18.3547770149\Au,1.51914

38195,1.4420597388,18.3547375106\Au,-0.9784966269,-2.8840331641,18.354
7705425\Au,-0.9785090734,2.8840042835,18.3547916913\\Version=ES64L-G09
RevD.01\HF=-4885.8333073\RMSD=7.486e-09\RMSF=2.025e-05\Dipole=-0.03340
99,-0.103156,0.2541409\Quadrupole=45.6726842,25.5142211,-71.1869052,1.
9150638,29.7884759,-13.4068655\PG=C01 [X(C16H8Au16N2S5)]\\@

THIOQ2g.pbe0

1\1\GINC-R05-NODE65\FOpt\RPBE1PBE\Gen\C20H10Au16N2S6\GRYNOVA\03-Feb-20
17\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(Loose) IOP(2/17=4
) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\THIOQ2g.pbe0.freq\\0,1
\C,1.4894825885,-0.0855710127,10.5858580013\S,0.8391105038,-1.33070123
46,11.6426417265\C,1.8839088996,-0.835671021,12.9654500249\C,2.4758068
132,0.6700385999,11.2730465519\C,2.6908210402,0.2649536155,12.56347901
26\H,3.4105528262,0.7292303032,13.2375021959\H,3.0046137841,1.49633326
96,10.7977583892\C,1.8769724474,-1.474229443,14.1929965162\S,2.9415040
912,-0.9661674047,15.5031097705\C,2.3351167064,-2.2304873184,16.551741
5783\C,1.087846405,-2.5830819082,14.6068220672\C,1.3247082169,-2.99534
00311,15.8877492297\C,2.795860814,-2.4137170086,17.8349599109\C,2.2676
062459,-3.4200112509,18.6702805902\H,0.8202895668,-3.8225355465,16.385
4631878\H,0.3626174297,-3.0528311559,13.941765157\C,0.0998008047,2.281
1078861,3.3536382117\S,-0.473081882,0.9962937613,4.3954237247\C,0.6190
140163,1.4899949263,5.6879261202\C,1.1263060923,3.0372369747,4.0026050
938\C,1.3966764594,2.6058493274,5.2706609878\C,-0.4003089398,2.4841799
073,2.0884577402\S,-1.5531738994,1.3247696143,1.407300271\H,2.13709141
88,3.0673233003,5.9246403108\H,1.6155053561,3.8737154122,3.5051669882\
C,0.633128225,0.8390043448,6.9088283984\S,1.6924074616,1.3249543456,8.
2236909323\C,1.0489298849,0.0762883773,9.2806513088\C,-0.1683648036,-0
.2652991945,7.3113804626\C,0.0581126479,-0.6771745283,8.597511786\H,-0
.467228111,-1.5052948626,9.0734380119\H,-0.894714649,-0.725534225,6.64
16953003\N,1.8541090099,-4.2568251865,19.3709255869\S,3.9204238224,-1.
240263744,18.5389614693\C,0.1007728557,3.5022145078,1.2506662516\N,0.4
907892921,4.349736614,0.5495335312\H,4.4778463302,-2.0771206866,19.449
377121\H,-2.070382259,2.1519667139,0.4654428812\Au,0.0003085195,-0.000
3204865,0.0004088663\Au,2.4975406836,1.4421274288,0.0001035189\Au,2.49
75688035,-1.4420986631,0.0000388059\Au,-1.6650689407,-0.0000111524,-2.
3547878183\Au,0.8323289695,1.4419965179,-2.3548568071\Au,0.8325339055,
-1.4415966887,-2.3550293007\Au,3.3302632685,2.8838484291,-2.3548459745
\Au,3.3301509983,-2.8840355892,-2.3547736353\Au,2.3513449812,0.0002699
338,19.9996930903\Au,-0.1459161127,-1.4420660305,19.9999038748\Au,-0.1
459311886,1.4420598934,19.999966526\Au,4.0167412848,-0.0000063837,22.3
547790923\Au,1.519315635,-1.4420240168,22.3548274331\Au,1.5191749009,1
.4417283796,22.3549587827\Au,-0.9785820391,-2.8838852144,22.3548309478
\Au,-0.9785036694,2.8840136428,22.3547825977\\Version=ES64L-G09RevD.01
\HF=-5437.364493\RMSD=5.440e-09\RMSF=5.823e-05\Dipole=0.0758552,0.0009
812,-0.1450689\Quadrupole=75.4523181,35.8480371,-111.3003552,6.0211789
,56.8519107,-1.9530842\PG=C01 [X(C20H10Au16N2S6)]\\@

THIOQ3g.pbe0

1\1\GINC-R07-NODE10\FOpt\RPBE1PBE\Gen\C24H12Au16N2S7\GRYNOVA\05-Feb-20
17\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(Loose) IOP(2/17=4
) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\THIOQ3g.pbe0.freq\\0,1
\C,0.1333780048,-1.6731075572,14.7574637223\S,-0.1860975148,-2.7840438
436,16.0794346146\C,0.88093988,-1.9009054781,17.1606311494\C,1.0211688

155,-0.6570116928,15.1828849809\C,1.4303004672,-0.7792842321,16.488071
9897\H,2.1179553594,-0.0906039813,16.9784790827\H,1.3487067572,0.14097
84027,14.5164351756\C,1.1348465214,-2.3093156945,18.463748387\S,2.2712
25866,-1.4343086695,19.488083003\C,2.058661103,-2.5811927625,20.793552
9803\C,0.614124123,-3.4301857173,19.1619077129\C,1.1017527168,-3.57981
712,20.4326934654\C,2.7554363102,-2.4959791257,21.9795384978\C,2.56988
99027,-3.425857286,23.0239275317\H,0.8240439752,-4.3754325062,21.12280
58859\H,-0.1083340647,-4.1079485984,18.7060834999\C,-1.6583590669,-1.0
308041372,7.2432534859\S,-2.0751613533,-2.1530425817,8.5284542419\C,-1
.1358406028,-1.2490386505,9.7059391889\C,-0.8231270243,-0.0033887227,7
.7503524603\C,-0.5393226218,-0.1255209168,9.0888258722\C,-2.103219717,
-1.1806911928,5.9343856195\C,-2.9163043914,-2.1990227701,5.3761869482\
H,0.0902555942,0.5716830001,9.641784405\H,-0.4445660312,0.7993850614,7
.1180398514\C,-1.0234017426,-1.6408107407,11.0408982549\S,-0.048288527
3,-0.728621047,12.1791398951\C,-0.4154092839,-1.8411210322,13.48550282
3\C,-1.6053627865,-2.7546552941,11.6883199121\C,-1.2752465229,-2.86295
3592,13.0214126775\H,-1.6296504185,-3.6618101156,13.6728081923\H,-2.25
24852457,-3.4567183463,11.1626070788\N,2.456995798,-4.1876803708,23.90
07882294\S,3.7751112664,-1.0834463809,22.3057660796\S,-1.6534933126,-0
.0176549721,4.6895048559\H,4.70606183,-1.7254306506,23.0566628904\C,-3
.1489169142,-2.0630469611,4.0314323847\C,-2.5361235814,-0.9057742687,3
.4641558311\C,-2.5872921619,-0.4852055319,2.1495128082\C,-3.2755850293
,-1.1854892033,1.138021038\N,-3.8284596093,-1.7063904601,0.2516226783\
S,-1.5936556437,0.8888569775,1.6380365516\H,-3.3120507069,-3.016563571
9,5.9796951285\H,-3.7406262747,-2.748724416,3.4263496135\H,-2.50408663
43,1.4663956193,0.8124897717\Au,-0.0000107014,0.0000097145,-0.00000884
16\Au,2.4976248714,1.4419815626,-0.0000039287\Au,2.4976204164,-1.44200
92787,-0.000000943\Au,-1.6650803746,0.000000765,-2.3547797351\Au,0.832
5479013,1.4419989053,-2.3547778769\Au,0.8325405674,-1.4420100763,-2.35
47736292\Au,3.3301656118,2.8840176006,-2.3547768971\Au,3.330160742,-2.
8840187148,-2.3547805247\Au,2.3516129176,0.0000021136,24.0000048929\Au
,-0.1459592468,-1.4419913046,23.9999987729\Au,-0.1459623121,1.44200599
54,24.0000003569\Au,4.0167397154,-0.0000009797,26.3547802012\Au,1.5191
401073,-1.4420011667,26.3547793234\Au,1.5191402959,1.442002674,26.3547
784672\Au,-0.978510888,-2.884008462,26.3547806279\Au,-0.9784996236,2.8
840206519,26.3547797339\\Version=ES64L-G09RevD.01\HF=-5988.8934018\RMS
D=4.765e-09\RMSF=1.845e-05\Dipole=-0.3298167,-0.1851118,0.2417079\Quad
rupole=84.7205051,67.531466,-152.2519711,7.8903581,37.9593526,-23.1482
003\PG=C01 [X(C24H12Au16N2S7)]\\@

THIOQ4g.pbe0

1\1\GINC-R07-NODE07\FOpt\RPBE1PBE\Gen\C28H14Au16N2S8\GRYNOVA\04-Feb-20
17\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(Loose) IOP(2/17=4
) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\THIOQ4g.pbe0.freq\\0,1
\C,1.3437673385,-0.8682266944,18.9796421436\S,0.733457692,-2.021506830
1,20.1496370476\C,1.7379115094,-1.3525642169,21.4231648934\C,2.2761335
598,-0.0048747478,19.5891775781\C,2.4930119544,-0.2662779153,20.924400
0529\H,3.1822974079,0.297853676,21.5522050446\H,2.7748548888,0.7924358
195,19.0380066153\C,1.7603295755,-1.8828061063,22.710971734\S,2.815874
2343,-1.212706904,23.9493713596\C,2.2953302394,-2.4105709547,25.114402
0354\C,1.0358874863,-2.9826325815,23.2303587893\C,1.3140339936,-3.2726
967246,24.5421536876\C,2.8051602139,-2.4684713591,26.3956964589\C,2.36
50265088,-3.4333251432,27.3238542338\H,0.8596502951,-4.0782801046,25.1

172399554\H,0.3256610889,-3.544324654,22.6228462112\C,0.5295838777,0.5
252144781,11.3980077206\S,-0.1924057065,-0.5847174927,12.5449140343\C,
0.7494958185,0.0723501446,13.8672846444\C,1.4582349117,1.3585578391,12
.0496330953\C,1.5773197547,1.110275857,13.4035440046\C,0.1821249323,0.
5271412419,10.0398833911\C,-0.7510930571,-0.2858149294,9.3676372349\H,
2.2491263043,1.6576955429,14.064580105\H,2.0234576465,2.1250089664,11.
5197719747\C,0.6474699019,-0.4258569005,15.176112577\S,1.603385101,0.2
491424955,16.4779966257\C,0.9332124804,-0.8772881628,17.6396976175\C,-
0.1542511785,-1.4760778325,15.6581708212\C,0.0028685071,-1.7251763175,
17.009706621\H,-0.5341913538,-2.5036254919,17.5514276003\H,-0.82934489
98,-2.0362736405,15.0112898323\N,2.0297004351,-4.2359071713,28.1028111
522\S,3.8803709352,-1.1855079438,26.9709093399\S,0.9301546076,1.643288
082,8.9152354362\H,4.5843114046,-1.9422999153,27.8498433979\C,-0.85976
00843,-0.0178932396,8.0182335243\C,-0.01001886,1.0197779894,7.57300220
44\C,0.1265138683,1.5402699365,6.2871399269\S,-0.8263657549,0.94302742
53,4.9324939021\C,0.9898911217,2.5747266007,5.8574689195\H,-1.32939708
13,-1.0530999725,9.8826384199\H,-1.5311006299,-0.5477207727,7.34287540
59\C,0.899351595,2.8670923009,4.5205003003\C,-0.0651021599,2.073689476
3,3.8338250278\C,-0.385294192,2.1620360266,2.4909737224\C,0.2826711176
,3.0796423321,1.6579984011\S,-1.4541410781,0.9711368681,1.7363982458\N
,0.8337085958,3.8391545035,0.9607620439\H,1.6654838155,3.0855066334,6.
5443000708\H,1.4846402228,3.6255201066,4.0027814266\H,-2.1842372942,1.
8354563216,0.9848916303\Au,-0.000008952,0.0000432628,-0.000064357\Au,2
.4976236394,1.441983696,0.0000065925\Au,2.4976196404,-1.4420106228,0.0
000038628\Au,-1.6650858737,-0.0000054323,-2.3547758466\Au,0.8325469602
,1.4419997435,-2.3547776962\Au,0.8325419734,-1.442034349,-2.3547582672
\Au,3.3301665383,2.8840159958,-2.3547775522\Au,3.3301621467,-2.8840162
82,-2.3547815179\Au,2.3516004664,-0.0000312525,28.5000613712\Au,-0.145
9584869,-1.4419926208,28.4999850164\Au,-0.1459654289,1.4420005972,28.4
999960589\Au,4.0167459053,0.0000068752,30.8547758242\Au,1.519136797,-1
.4419986311,30.8547797059\Au,1.5191565941,1.442033343,30.8547654479\Au
,-0.9785097119,-2.884010499,30.8547797963\Au,-0.9785022079,2.884016176
,30.8547815611\\Version=ES64L-G09RevD.01\HF=-6540.4258156\RMSD=6.501e-
09\RMSF=3.787e-05\Dipole=-0.3928732,-0.0598634,0.798235\Quadrupole=110
.6119594,74.6855241,-185.2974835,10.5073741,71.8008434,-6.4522759\PG=C
01 [X(C28H14Au16N2S8)]\\@

TCLO1g.pbe0

1\1\GINC-R05-NODE27\FOpt\RPBE1PBE\Gen\C12H8Au16Cl2S5\GRYNOVA\10-Aug-20
16\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\TCLO1g.pbe0.freq\\0,1\C,
2.0093883636,-0.1649987576,8.5092895488\S,0.3362963328,0.0355674994,7.
8742758954\C,0.8538041723,-0.4910446535,6.2315532936\C,2.8260072601,-0
.5897824673,7.51025967\C,2.1833257201,-0.7696018379,6.241469394\H,2.71
26510984,-1.108370728,5.3508418813\H,3.8886144688,-0.774083392,7.66721
01676\C,-0.1465075176,-0.5163490034,5.2075548813\S,0.2872908455,-0.620
0974217,3.5270191776\C,-1.3860481484,-0.6410741968,3.0755796652\C,-1.5
16889204,-0.4654937647,5.3797221216\C,-2.2238366848,-0.5317647461,4.15
99517837\S,-1.9169363233,-0.6835004598,1.3938814827\H,-1.7298999049,-2
.010717161,1.1587214954\H,-3.3089639341,-0.5106574315,4.070951607\H,-1
.9931664924,-0.4132695682,6.358531721\C,3.0736598077,0.2120293677,12.2
201152715\S,3.6148482864,-0.5004040102,10.7353747711\C,2.2145250841,0.
0983585821,9.9018364556\C,1.8682405358,0.8572156822,12.0800268511\C,1.

3843111841,0.8009886937,10.7557832049\S,4.0170818979,-0.0398559839,13.
6932817409\H,4.5256394957,1.2160141839,13.8107318749\H,0.4588456265,1.
2741093508,10.4276973039\H,1.3487347988,1.3243396558,12.9173785371\Cl,
-0.1555544278,-2.1348022568,8.440157848\Cl,0.7744543363,2.2222677911,7
.3321577419\Au,0.0000326447,0.0000140391,0.0000576706\Au,2.4976234717,
1.4419839831,-0.0000175665\Au,2.4976215266,-1.4420073521,-0.0000131557
\Au,-1.6650866926,-0.00000399,-2.3547752672\Au,0.8325383899,1.44200314
25,-2.3547786434\Au,0.8325331063,-1.4420127617,-2.3547746215\Au,3.3301
676241,2.8840141148,-2.3547783203\Au,3.3301605902,-2.8840189781,-2.354
7804174\Au,2.3515729034,-0.000006878,15.4999263374\Au,-0.1459602945,-1
.4419894899,15.5000141541\Au,-0.145960794,1.4420086246,15.5000147236\A
u,4.0167410849,0.0000037297,17.8547792328\Au,1.5191408989,-1.441994542
6,17.8547836598\Au,1.5191513433,1.4419980868,17.8547851816\Au,-0.97850
74026,-2.8840144989,17.8547781633\Au,-0.9784984003,2.8840227705,17.854
778869\\Version=ES64L-G09RevD.01\HF=-5544.3067045\RMSD=6.640e-09\RMSF=
8.035e-06\Dipole=0.4334651,-0.4639582,-0.297033\Quadrupole=48.6388082,
1.4697455,-50.1085537,0.2891939,49.7659889,7.8313321\PG=C01 [X(C12H8Au
16Cl2S5)]\\@

TCLO2g.pbe0

1\1\GINC-R05-NODE32\FOpt\RPBE1PBE\Gen\C16H10Au16Cl4S6\GRYNOVA\10-Aug-2
016\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\TCLO2g.pbe0.freq\\0,1\C
,1.1339754207,-0.3663987578,10.2106070255\S,2.7572614116,-0.3802037902
,10.9781127373\C,2.0128150709,-0.3343338923,12.620372789\C,0.167175703
2,-0.2845763972,11.1666591135\C,0.6589888605,-0.2659681112,12.50907495
96\H,0.0059470551,-0.231867989,13.3809986964\H,-0.894171149,-0.2909887
514,10.9189657467\C,2.9038067308,-0.3321080663,13.7396861079\S,2.40127
18862,0.2684573958,15.2928782851\C,3.9760363814,-0.0384460297,15.94453
31445\C,4.2175289737,-0.7630689033,13.7594220418\C,4.8281027894,-0.597
1222744,15.0201380559\S,4.3887963627,0.2532157958,17.6328442124\H,4.36
99496003,1.6130310089,17.6091590162\H,5.8560934865,-0.8715911998,15.25
18897744\H,4.7060468543,-1.2127462586,12.8951894125\C,-1.709095381,-0.
3551667288,3.0091949227\S,-0.118166077,-0.6254570202,3.639112822\C,-0.
6905385598,-0.3546010621,5.2601045317\C,-2.6159672984,-0.0334871897,3.
991745923\C,-2.0368451243,-0.0375594003,5.2774636651\S,-2.0709223069,-
0.3947131491,1.2840945112\H,-2.0478298961,-1.7437472906,1.1103952863\H
,-2.5921620742,0.1568625217,6.1946343648\H,-3.6626750031,0.183282358,3
.7842652865\C,0.1784227917,-0.4823992867,6.3872147661\S,-0.47578872,0.
0110422006,7.9948464506\C,1.0553988633,-0.4716815976,8.7984086328\C,1.
4599732253,-0.9182046234,6.528690225\C,1.9503732049,-0.9115935528,7.87
07331508\H,2.9389564171,-1.2768390282,8.148160458\H,2.052083146,-1.268
1680291,5.6833266752\Cl,2.7240551564,-2.6995128415,11.0156014468\Cl,2.
856086206,1.8856083905,10.9423657156\Cl,-1.3188591766,-2.1212613503,8.
3064889886\Cl,0.2876257504,2.1262106057,7.6899041742\Au,0.0000309523,0
.0000027578,0.0000656682\Au,2.4976168102,1.4419955249,-0.0000104944\Au
,2.497617807,-1.4420137984,-0.0000119419\Au,-1.6650782632,-0.000000449
2,-2.3547812281\Au,0.832533331,1.4419936677,-2.3547862355\Au,0.8325334
116,-1.4419965119,-2.3547844653\Au,3.330169845,2.8840102685,-2.3547798
904\Au,3.3301594805,-2.8840208997,-2.3547796327\Au,2.3514383366,0.0000
013418,18.9999340445\Au,-0.1461163299,-1.4419963567,19.0000107279\Au,-
0.1461175674,1.4420142134,19.0000114602\Au,4.0165979696,-0.0000010424,
21.3547814357\Au,1.5189961672,-1.4419945617,21.3547855105\Au,1.5190073

972,1.4419952849,21.3547855025\Au,-0.9786698358,-2.8840102844,21.35477
98839\Au,-0.9786595119,2.8840208454,21.3547796549\\Version=ES64L-G09Re
vD.01\HF=-7015.9086626\RMSD=3.074e-09\RMSF=8.120e-06\Dipole=-0.03605,-
0.1758721,-0.048759\Quadrupole=49.6636845,-8.488052,-41.1756325,-2.520
2495,54.60551,11.7688279\PG=C01 [X(C16H10Au16Cl4S6)]\\@

TCLO3g.pbe0

1\1\GINC-R05-NODE35\FOpt\RPBE1PBE\Gen\C20H12Au16Cl6S7\GRYNOVA\09-Aug-2
016\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\TCLO3g.pbe0.freq\\0,1\C
,2.0471203248,0.3378069785,8.6260955148\S,0.3726113991,0.3919526734,7.
9807995158\C,0.989671215,0.2989330257,6.289367519\C,2.937523033,0.2119
058412,7.6018667559\C,2.3465935174,0.1893328432,6.3002778107\H,2.93103
12972,0.1212595272,5.3829116403\H,4.0139310133,0.1879286261,7.77148468
49\C,0.0079185657,0.3015390912,5.2498348056\S,0.3445121835,-0.36029020
68,3.6761748392\C,-1.2796852889,-0.0340448717,3.1705474457\C,-1.289473
3251,0.7735673146,5.3387693881\C,-2.0237773278,0.581533069,4.150943656
1\S,-1.8727024018,-0.3720702473,1.5467758601\H,-1.7643506885,-1.727365
9534,1.5753634276\H,-3.0630008657,0.8746310341,4.0102203284\H,-1.67985
7815,1.2668649426,6.2287551886\C,5.7262304053,0.2686918746,19.70219112
66\S,6.5014039961,-0.0200912264,18.1779773215\C,5.0295127345,0.3416622
106,17.3276840825\C,4.3998768635,0.5988785509,19.559793073\C,4.0052810
532,0.6473487987,18.2065306368\S,6.6325715146,0.0306463769,21.20375774
19\H,7.0721614641,1.3087374659,21.3596224362\H,3.0024750078,0.92182861
43,17.8795658127\H,3.7453754063,0.7821143479,20.4137892701\C,3.1844148
068,0.4618998563,12.391943334\S,3.7625887943,-0.0728241113,10.77352098
16\C,2.2149640012,0.4619873316,10.0274736591\C,1.9111384232,0.94159088
68,12.3030769073\C,1.3705493456,0.9409570421,10.985203621\H,0.38751382
01,1.3426951191,10.7409825631\H,1.3834915045,1.3446356175,13.167141205
6\C,4.9674532641,0.3112226843,15.9002820206\S,3.3312171947,0.389220188
6,15.14658576\C,4.0555362065,0.3469324697,13.5032168107\C,5.9164789894
,0.2166178837,14.9281912238\C,5.4104703741,0.234837141,13.5926414604\H
,6.0485488736,0.218186565,12.709179931\H,6.9802718978,0.1602570994,15.
1572878827\Cl,0.4720509883,2.708553377,7.8979738938\Cl,0.2054062433,-1
.8674355616,8.056820778\Cl,4.6713669807,2.0284293639,10.3970175763\Cl,
2.933870042,-2.1461515127,11.1104717611\Cl,3.446926982,2.7013837107,15
.1439735183\Cl,3.178120485,-1.8723817641,15.1966848564\Au,0.0000301641
,0.0000071282,0.0000455645\Au,2.4976179144,1.4419936123,-0.0000059896\
Au,2.4976196756,-1.4420105619,-0.0000060553\Au,-1.6650811546,-0.000001
1347,-2.3547791835\Au,0.8325325039,1.4419951776,-2.3547856034\Au,0.832
5337935,-1.4420010211,-2.3547815691\Au,3.3301700507,2.8840099122,-2.35
47800358\Au,3.3301602501,-2.8840195668,-2.3547801768\Au,4.9468712538,-
0.0000363223,22.9999661968\Au,2.4493589166,-1.4419881213,22.9999507491
\Au,2.4493731151,1.4420327139,22.9999421037\Au,6.6120545159,-0.0000030
333,25.3547838779\Au,4.1145296238,-1.4419661972,25.3548323832\Au,4.114
4866872,1.4419872966,25.3548042847\Au,1.616789198,-2.8839739693,25.354
7947098\Au,1.6167934919,2.8839740869,25.3547987438\\Version=ES64L-G09R
evD.01\HF=-8487.5119805\RMSD=4.888e-09\RMSF=8.205e-06\Dipole=0.3794908
,-0.1392311,-0.2850995\Quadrupole=71.489453,-18.8553506,-52.6341024,-2
.1292738,72.2187264,12.9475518\PG=C01 [X(C20H12Au16Cl6S7)]\\@

TCLO4g.pbe0

1\1\GINC-R05-NODE38\FOpt\RPBE1PBE\Gen\C24H14Au16Cl8S8\GRYNOVA\10-Aug-2

016\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\TCLO4g.pbe0.freq\\0,1\C
,2.9556091489,0.7514918937,12.3806785238\S,3.4188537352,0.0077347877,1
0.8092231266\C,2.0086065453,0.785140635,10.0091000506\C,1.7997990627,1
.4641553625,12.243596999\C,1.2711390472,1.4819228069,10.9215786455\H,0
.3856746401,2.0494925393,10.6366358764\H,1.3596234336,2.0178564673,13.
0726139491\C,-0.1251987106,0.6336140935,5.1954843209\S,0.158076727,-0.
1690013197,3.6785360241\C,-1.3899752231,0.3415799889,3.0967599962\C,-1
.3459920274,1.2849698355,5.208607764\C,-2.0674760085,1.1179818185,4.00
90784685\S,-1.967716696,-0.0231580918,1.4735316047\H,-2.0601030411,-1.
3743241501,1.5982675826\H,-3.0512397245,1.541494213,3.8128292186\H,-1.
6898627507,1.8823216231,6.0528929462\C,7.8135276008,0.0688132613,22.94
91628686\S,6.2908254629,0.6584221582,22.3733914292\C,6.7008292366,0.19
10287241,20.7482008871\C,8.5702090397,-0.5006460197,21.9510678915\C,7.
9371831039,-0.4289376372,20.6940260618\S,8.2682630816,0.1110603387,24.
6505582199\H,8.4402841419,1.4547821195,24.771418871\H,8.3845858842,-0.
7874902953,19.7674320397\H,9.5522580727,-0.9368326565,22.1266911408\C,
4.7233954817,0.4484316208,15.8753045708\S,3.1271434131,0.8323267508,15
.1415557528\C,3.7950179839,0.5348003084,13.4977431893\C,5.6134863073,0
.0825424329,14.9073452651\C,5.0960079956,0.1308484929,13.582283876\H,5
.6963374456,-0.0758031842,12.6965756447\H,6.6494496959,-0.1645957323,1
5.1373549407\C,5.8328588198,0.4734220678,19.6512566547\S,6.2758537869,
-0.2314140727,18.051227296\C,4.8738213544,0.5772784788,17.2762333104\C
,4.6859696391,1.1998363747,19.5323760945\C,4.1510184444,1.2583748246,1
8.2111038287\H,3.2698534935,1.8428915507,17.9469984327\H,4.2349340745,
1.7178957778,20.378334147\C,1.8324600259,0.5955649438,8.6169943865\S,0
.2037736602,0.8909064508,7.9237321896\C,0.8209507849,0.556454174,6.262
7466568\C,2.7038169078,0.2393266989,7.6304844512\C,2.1389710689,0.2182
064131,6.3191979129\H,2.7161205261,-0.0218792006,5.4264347833\H,3.7566
933844,0.0431692044,7.8332706241\Cl,-0.3607161391,-1.2922104891,8.1647
083279\Cl,0.7085960307,3.1389586531,7.6665599076\Cl,2.1972739779,-1.83
35171328,11.2687821373\Cl,4.7207023429,1.8620000559,10.3088792956\Cl,2
.4814517477,-1.3234977691,15.3225375938\Cl,3.7383852017,3.0647088052,1
4.9902267516\Cl,5.0376394552,-2.0785256988,18.4952760082\Cl,7.59565980
63,1.6183185156,17.6115917066\Au,0.0000307416,-0.0000091275,0.00004866
11\Au,2.4976162581,1.4419964808,-0.0000046588\Au,2.4976182202,-1.44201
30825,-0.0000038702\Au,-1.6650782061,0.0000032052,-2.3547812684\Au,0.8
325328885,1.4419959845,-2.354784973\Au,0.8325289719,-1.441992677,-2.35
47883829\Au,3.3301715211,2.8840073653,-2.3547810756\Au,3.3301607247,-2
.8840187448,-2.3547805124\Au,6.2145224332,0.0000061237,25.9999464066\A
u,3.7169349209,-1.4419985227,26.0000103869\Au,3.7169326695,1.442014623
2,26.0000089505\Au,7.8796277247,-0.0000016609,28.3547816088\Au,5.38201
47903,-1.4419962027,28.3547840188\Au,5.3820151697,1.4419939425,28.3547
85537\Au,2.8843799239,-2.8840098681,28.3547800538\Au,2.8843912477,2.88
40221611,28.3547791177\\Version=ES64L-G09RevD.01\HF=-9959.1141705\RMSD
=3.606e-09\RMSF=4.839e-06\Dipole=0.0257281,0.0279574,0.0130517\Quadrup
ole=63.7762305,-26.0806591,-37.6955715,-14.6556976,79.16255,19.6267871
\PG=C01 [X(C24H14Au16Cl8S8)]\\@

TDOA1g.pbe0

1\1\GINC-NODE06\FOpt\RPBE1PBE\Gen\C8H4Au16O2S5\GRYNOVA\03-Mar-2017\0\\
#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Empiri
calDispersion=GD3BJ pseudo=read Nosymm\\TDOA1g.pbe0.freq\\0,1\S,-0.816

8218667,1.9304039102,7.081779703\C,1.2725550804,0.4202173029,6.5411491
35\S,2.7122912151,-0.367814614,7.0532552227\C,2.57217054,0.3530356251,
8.6430586619\C,0.7449325469,1.1912719101,7.5577591952\C,1.4633626335,1
.1595739018,8.7636618365\S,3.7162003513,-0.0916567869,9.9138273061\H,4
.3985280262,1.0827117207,9.9740492399\H,1.1777573047,1.6547979746,9.69
29653306\C,-0.9716025801,0.3635074125,3.3306825541\S,0.5832764236,-0.3
011661654,3.7784508273\C,0.4593410387,0.4171078635,5.3384418427\C,-1.5
274774824,1.1404122642,4.3243166003\C,-0.6980077012,1.1608668942,5.459
6481284\S,-1.7198784454,0.1121900748,1.7535368794\H,-1.9781027464,-1.2
177549665,1.8701988624\H,-2.48810467,1.6437054203,4.2313704733\O,-0.70
07648488,3.3917052049,6.9669888157\O,-1.9099388801,1.3277692712,7.8625
558148\Au,0.0000663463,-0.0000050984,0.0000827324\Au,2.4976188559,1.44
19919811,-0.0000068859\Au,2.4976157382,-1.4420173807,-0.0000085867\Au,
-1.6650788358,0.0000008192,-2.3547808232\Au,0.8325235985,1.4419949026,
-2.3547889192\Au,0.8325211327,-1.4419896297,-2.3547930195\Au,3.3301709
556,2.8840083448,-2.3547806757\Au,3.3301616253,-2.884017185,-2.3547811
492\Au,2.3515446952,0.0000122329,11.9999283419\Au,-0.1459571879,-1.441
9948701,12.0000046803\Au,-0.1459603691,1.4420093606,12.0000023842\Au,4
.0167385839,0.0000001506,14.3547810013\Au,1.5191544692,-1.4419975801,1
4.3547865963\Au,1.5191630272,1.4419929447,14.3547924595\Au,-0.97851160
84,-2.8840072142,14.3547811374\Au,-0.9785010268,2.8840182216,14.354780
7261\\Version=ES64L-G09RevD.01\HF=-4619.7728594\RMSD=8.810e-09\RMSF=3.
669e-05\Dipole=0.6741946,-0.7025925,-0.6685861\Quadrupole=38.4821642,2
.8475379,-41.3297021,5.2740276,44.3004127,-6.3517453\PG=C01 [X(C8H4Au1
6O2S5)]\\@

TDOA2g.pbe0

1\1\GINC-NODE07\FOpt\RPBE1PBE\Gen\C10H4Au16O4S6\GRYNOVA\03-Mar-2017\0\
\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Empir
icalDispersion=GD3BJ pseudo=read Nosymm\\TDOA2g.pbe0.freq\\0,1\C,0.856
5092381,0.2168912618,8.0554651701\S,-0.8153710509,0.7821659901,7.64901
22362\C,-0.5541495029,0.3574319968,5.9181840744\C,0.7139541689,-0.1582
893645,5.7255199868\S,0.9605845548,-0.6151198484,4.080714914\C,-0.6821
82742,-0.1594241349,3.6859969964\C,-1.364798021,0.361299816,4.77016302
92\S,-1.4147813176,-0.3396878457,2.0855622693\H,-1.3944681782,-1.69650
76924,2.0317223045\H,-2.3998797276,0.6946290675,4.7243650204\C,3.03182
94281,0.1533092481,11.3112520562\S,1.3888282471,0.6085022785,10.916833
672\C,3.7144482462,-0.367036586,10.2269317346\S,3.7650196863,0.3341489
016,12.9113799371\H,3.7458879408,1.6910243809,12.9642006057\H,4.749615
101,-0.7001256499,10.2724855048\C,2.9036175544,-0.3632848787,9.0790339
817\S,3.1647587105,-0.7882187804,7.3482814065\C,1.492282321,-0.2245055
426,6.9421729197\C,1.6353322162,0.1518503899,9.2719006268\O,-1.8056660
538,-0.1163060377,8.257671721\O,-0.8967942008,2.2368818212,7.834706613
3\O,3.2480247924,-2.2428795467,7.163106248\O,4.1536413085,0.1113224594
,6.7388629833\Au,0.0005644615,-0.0000570369,0.000640454\Au,2.497603653
4,1.4420183049,-0.0000256198\Au,2.4976061144,-1.4420340385,-0.00001956
85\Au,-1.6650732276,0.0000234217,-2.3547847906\Au,0.832386567,1.441969
2124,-2.3548530497\Au,0.8323246598,-1.441965277,-2.3548773461\Au,3.330
1834446,2.883986713,-2.3547895055\Au,3.3301816152,-2.8839825608,-2.354
7952878\Au,2.3508912878,0.0000368535,14.9993694404\Au,-0.1461024519,-1
.4420203891,15.0000184859\Au,-0.1461014588,1.4420421011,15.0000084552\
Au,4.0165926463,-0.0000419006,17.354785204\Au,1.5191925445,-1.44194908
36,17.3548827034\Au,1.5191759354,1.4419788414,17.3548551173\Au,-0.9786

835183,-2.8839865856,17.3547895568\Au,-0.9786822732,2.883981424,17.354
7957508\\Version=ES64L-G09RevD.01\HF=-5244.1544059\RMSD=5.179e-09\RMSF
=1.340e-05\Dipole=-0.0009613,-0.0028126,-0.0003473\Quadrupole=24.69741
25,-0.4406826,-24.2567299,5.3324989,44.7166119,8.1205532\PG=C01 [X(C10
H4Au16O4S6)]\\@

TDOA3g.pbe0

1\1\GINC-NODE05\FOpt\RPBE1PBE\Gen\C12H4Au16O6S7\GRYNOVA\04-Mar-2017\0\
\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Empir
icalDispersion=GD3BJ pseudo=read Nosymm\\TDOA3g.pbe0.freq\\0,1\S,-0.59
30262027,1.2426393313,7.3627916789\C,-0.328953731,0.6019029548,5.70450
49064\C,1.6609795896,0.0139535228,6.817834618\C,0.911839229,-0.0011787
24,5.5841799806\S,1.110809278,-0.6961420056,4.0143090429\C,-0.52217872
28,-0.2391929007,3.5836367806\C,-1.1622437673,0.466580122,4.5860267484
\S,-1.2977477999,-0.6006711798,2.044042731\H,-1.0090750251,-1.92619887
9,1.9977925473\H,-2.1871426275,0.8257183789,4.5126398394\C,4.906957925
6,0.0413972799,12.4525868195\S,5.2339999471,-0.5455709379,10.833508999
8\C,3.6653921698,0.6300722462,12.5642465517\C,3.0001055032,0.608428952
9,11.3284264096\S,6.0995934421,-0.2213591947,13.7367542727\H,6.7032631
581,0.9948390916,13.6694495521\H,3.2714700285,1.0149444363,13.50795655
65\S,3.2940886279,-0.5789336352,7.3534984989\C,1.7713695753,0.63826203
48,9.0884272238\C,1.0298104706,0.6117939134,7.861752321\S,1.4011034517
,1.206531734,10.7766679038\C,3.7023713482,0.0186780196,10.2912449659\C
,2.9921822892,0.0492864756,9.0333123782\O,3.3189768489,-2.0461817295,7
.3683997118\O,4.3484497877,0.2014410927,6.6960460566\O,0.3176213683,0.
3873545474,11.3320371709\O,1.3570113139,2.6720682956,10.8184447623\O,-
0.5698008501,2.708968854,7.3742662591\O,-1.6584676189,0.4841520435,8.0
272814253\Au,0.0000454328,0.0000101812,0.0000335847\Au,2.4976189525,1.
4419918145,0.000001952\Au,2.4976122563,-1.4420234102,0.0000045608\Au,-
1.6650796763,0.0000030656,-2.354780229\Au,0.8325182876,1.441991673,-2.
3547927713\Au,0.8325316987,-1.4419993242,-2.354783348\Au,3.330171445,2
.8840074973,-2.3547810217\Au,3.3301649948,-2.8840113499,-2.3547835308\
Au,4.9469450273,0.0000010102,15.9999721882\Au,2.4493634127,-1.44199591
08,15.9999992073\Au,2.449359008,1.442008282,15.9999982882\Au,6.6120597
721,0.00000538,18.3547801611\Au,4.1144315308,-1.441995657,18.354779665
7\Au,4.1144706302,1.442002442,18.3547893323\Au,1.6168102573,-2.8840104
457,18.354779818\Au,1.6168169701,2.8840147521,18.3547821426\\Version=E
S64L-G09RevD.01\HF=-5868.5482883\RMSD=4.148e-09\RMSF=2.905e-05\Dipole=
0.9518006,-0.9560593,-1.1238625\Quadrupole=48.0082787,-2.3407805,-45.6
674981,4.8500538,60.8992692,-8.9917401\PG=C01 [X(C12H4Au16O6S7)]\\@

TDOA4g.pbe0

1\1\GINC-NODE06\FOpt\RPBE1PBE\Gen\C14H4Au16O8S8\GRYNOVA\05-Mar-2017\0\
\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Empir
icalDispersion=GD3BJ pseudo=read Nosymm\\TDOA4g.pbe0.freq\\0,1\C,3.735
2463567,0.3085889746,8.621702243\S,3.7290610847,1.0177549835,6.9462957
035\C,1.3039518921,0.0900446226,5.4435806472\S,1.2392530205,0.82829205
91,3.8824839467\C,-0.32159317,0.0996410619,3.5838525632\C,0.2042692725
,-0.7273422216,5.6544643904\C,-0.7398051941,-0.7192391114,4.6188636539
\S,-1.2647202273,0.3380363695,2.116632954\H,-1.2280415143,1.6948905279
,2.0929581267\H,-1.6895328023,-1.2511087603,4.6219851704\C,6.554946213
7,-0.1196866773,13.9156259461\S,4.9275205132,-0.7008573788,13.65110209
71\C,4.9490013359,-0.0736786583,12.0416068046\C,7.0587675575,0.5819498

566,12.8335120168\C,6.1344594381,0.5947662963,11.7805778039\S,7.482019
5511,-0.3878645398,15.3900447728\H,7.3873004347,-1.7420864408,15.42603
67751\H,8.0580558492,1.0125643455,12.8069869923\C,4.0491646776,-0.0846
194192,10.919312742\S,2.5018404387,-0.9559415317,10.5540942244\C,2.613
6670696,-0.4408525565,8.8125840974\S,6.167067159,1.2287716646,10.09670
92422\C,1.7047872214,-0.4575795113,7.7075502773\S,0.195933498,-1.38967
67861,7.3277074624\C,2.1255841978,0.238020963,6.6140921653\C,4.5205742
231,0.5285605565,9.7978104954\O,-0.9560221362,-0.8526321814,8.06024619
47\O,0.5170820154,-2.8212968338,7.3455600852\O,1.3569324493,-0.2811590
593,11.1729234188\O,2.7356346811,-2.3946683755,10.7115696279\O,3.59130
46901,2.4738307517,7.0479640036\O,4.7381762391,0.389776936,6.088157762
2\O,6.1178424078,2.6941405362,10.0980321909\O,7.1450672632,0.493951803
7,9.2850669047\Au,0.0000171886,-0.0000042207,0.0000143657\Au,2.4976173
927,1.4419945159,0.0000015943\Au,2.4976209758,-1.44200831,0.0000019003
\Au,-1.6650792183,-0.0000034676,-2.3547805528\Au,0.8325466872,1.441996
058,-2.35478005\Au,0.8325208014,-1.4419972524,-2.3547884696\Au,3.33017
01464,2.8840097465,-2.3547801035\Au,3.3301615431,-2.8840173274,-2.3547
810911\Au,6.2145341665,0.0000001203,17.4999911034\Au,3.7169287974,-1.4
419879172,17.4999983793\Au,3.7169314626,1.4420125334,17.4999990388\Au,
7.8796295209,-0.00000443,19.8547803388\Au,5.3820311162,-1.4420049817,1
9.8547844146\Au,5.3820020639,1.4419998907,19.854777262\Au,2.8843772222
,-2.8840051888,19.8547819641\Au,2.8843901335,2.8840202312,19.854779905
6\\Version=ES64L-G09RevD.01\HF=-6492.938343\RMSD=7.455e-09\RMSF=1.221e
-05\Dipole=-0.0779193,0.0368997,-0.1060612\Quadrupole=27.9311972,-20.7
649709,-7.1662263,-11.676592,58.894396,-8.8881691\PG=C01 [X(C14H4Au16O
8S8)]\\@

TDO1g.pbe0

1\1\GINC-LCMD55\FOpt\RPBE1PBE\Gen\C12H8Au16O2S5\STUDENT1\16-Apr-2016\0
\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(MaxCyc=250,MaxStep=10
) IOP(2/17=4) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\1TG\\0,1\A
u,0.,0.,0.\Au,2.49762,1.44199,0.\Au,2.49762,-1.44201,0.\Au,-1.66508,0.
,-2.35478\Au,0.83254,1.442,-2.35478\Au,0.83254,-1.442,-2.35478\Au,3.33
017,2.88401,-2.35478\Au,3.33016,-2.88402,-2.35478\Au,2.35166,0.,15.5\A
u,-0.14596,-1.44199,15.5\Au,-0.14596,1.44201,15.5\Au,4.01674,0.,17.854
78\Au,1.51912,-1.442,17.85478\Au,1.51912,1.442,17.85478\Au,-0.97851,-2
.88401,17.85478\Au,-0.9785,2.88402,17.85478\C,2.1745890576,0.555248772
1,8.5468959557\S,0.5007308005,0.8145786207,7.9140651769\C,0.9998135627
,0.4597758256,6.2136978692\C,2.9658369065,0.1858118222,7.5141414807\C,
2.3127742781,0.1337602703,6.2154007207\O,-0.3910417538,-0.2485739327,8
.4073605597\O,0.0952731131,2.2288647564,8.0580046395\H,2.8617791402,-0
.1368324589,5.3122905777\H,4.0254069428,-0.0469234813,7.6273090871\C,0
.0005068826,0.5176326522,5.1912003057\S,0.2620066922,-0.1818837732,3.6
193583297\C,-1.3376481716,0.2655631991,3.12854873\C,-1.256444622,1.087
9103991,5.2919843413\C,-2.0182689963,0.943497518,4.112337136\S,-1.9531
042214,-0.0365739353,1.5046251341\H,-2.0736456763,-1.3896616683,1.5825
659424\H,-3.0329983751,1.3170092589,3.9816616859\H,-1.5991966897,1.601
0975891,6.1896964473\C,3.2000472648,0.5855464257,12.2911476702\S,3.762
8064251,0.0055107445,10.7578406233\C,2.3865096686,0.7011684071,9.95485
36477\C,2.0120339743,1.2687237115,12.185661577\C,1.5533089023,1.344276
4295,10.8540630537\S,4.0874399269,0.1561928405,13.7579804799\H,4.59584
0588,1.3845322536,14.0441131214\H,0.6411020286,1.8541059497,10.5453594
446\H,1.4822669789,1.6670632426,13.051785026\\Version=ES64L-G09RevD.01

\HF=-4774.3909819\RMSD=3.426e-09\RMSF=1.848e-06\Dipole=0.7681864,0.070
9057,-0.4391013\Quadrupole=49.6556472,8.0092348,-57.664882,2.1371619,5
5.2315272,9.5231475\PG=C01 [X(C12H8Au16O2S5)]\\@

TDO2g.pbe0

1\1\GINC-LCMD55\FOpt\RPBE1PBE\Gen\C16H10Au16O4S6\STUDENT1\16-Apr-2016\
0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(MaxCyc=250,MaxStep=1
0) IOP(2/17=4) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\1TG\\0,1\
Au,0.,0.,0.\Au,2.49762,1.44199,0.\Au,2.49762,-1.44201,0.\Au,-1.66508,0
.,-2.35478\Au,0.83254,1.442,-2.35478\Au,0.83254,-1.442,-2.35478\Au,3.3
3017,2.88401,-2.35478\Au,3.33016,-2.88402,-2.35478\Au,2.35151,0.,19.\A
u,-0.14611,-1.44199,19.\Au,-0.14611,1.44201,19.\Au,4.01659,0.,21.35478
\Au,1.51897,-1.442,21.35478\Au,1.51897,1.442,21.35478\Au,-0.97866,-2.8
8401,21.35478\Au,-0.97865,2.88402,21.35478\C,1.2266494493,0.0376462026
,10.2036838346\S,2.8394670849,-0.1399176007,10.9878547734\C,2.13324072
41,0.0340285946,12.6444244933\C,0.2907863319,0.2405198264,11.166614412
9\C,0.7985114766,0.2392259619,12.5232103094\O,3.6891929054,1.021581368
9,10.6711233141\O,3.3681260697,-1.5022382119,10.7809554215\H,0.1373655
237,0.3840570006,13.3786829858\H,-0.7659373679,0.3868485105,10.9431576
758\C,3.0132438476,-0.0278442732,13.7678503943\S,2.4957753392,0.444947
8889,15.3616793559\C,4.0696416199,0.1066816494,15.9979333943\C,4.33332
64064,-0.4466347759,13.7650091785\C,4.9330415545,-0.3713016242,15.0397
589157\S,4.4511994971,0.2654682406,17.7116915259\H,4.4746497918,1.6237
167354,17.7859169371\H,5.9624480129,-0.6528843107,15.2571151224\H,4.83
45289352,-0.8088830274,12.8681879012\C,-1.7183516387,-0.1068162736,3.0
019592499\S,-0.1444934786,-0.4450885255,3.6382308544\C,-0.6620364445,0
.0275089543,5.2320931753\C,-2.5818362433,0.3709274223,3.9601762701\C,-
1.9821669094,0.4461505145,5.2349539004\S,-2.0998087995,-0.2653815171,1
.2881559689\H,-2.1233555977,-1.6236210953,1.2137878138\H,-2.4834326158
,0.8082365883,6.1318052594\H,-3.6112609526,0.6524473506,3.7428247983\C
,0.2179562855,-0.0343709032,6.3555265121\S,-0.4882883416,0.1394895582,
8.0120977335\C,1.1245342993,-0.0380116317,8.7962719355\C,1.5526949454,
-0.239507655,6.4767424623\C,2.0604130674,-0.2408099056,7.8333403547\O,
-1.3379567805,-1.0220627197,8.328783532\O,-1.0170176816,1.5017770298,8
.2190392215\H,3.1171451838,-0.3870771816,8.0567973561\H,2.2138530474,-
0.3842848111,5.6212699909\\Version=ES64L-G09RevD.01\HF=-5476.1195862\R
MSD=2.128e-09\RMSF=4.197e-06\Dipole=-0.0000294,0.0000676,-0.000028\Qua
drupole=42.5085439,1.5237545,-44.0322984,0.703846,54.2447511,12.303228
7\PG=C01 [X(C16H10Au16O4S6)]\\@

TDO3g.pbe0

1\1\GINC-R02-NODE56\FOpt\RPBE1PBE\Gen\C20H12Au16O6S7\GRYNOVA\10-Aug-20
16\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\TDO3g.pbe0.freq\\0,1\C,5
.134358413,0.3130092414,17.3484978562\C,4.4499174451,0.5444383186,19.5
67407189\C,4.0745129617,0.5533995475,18.2083397142\C,5.7932631768,0.30
75465083,19.735820134\S,6.617287705,0.074872675,18.2279477732\H,3.0541
865978,0.7030237854,17.8571189747\H,3.7685505876,0.681698669,20.408765
842\C,-1.288493866,0.0661146802,3.141353881\C,2.1540684781,0.454861279
7,8.5745824576\C,1.0335063043,0.3443661573,6.2270486543\C,2.9828766021
,0.1055035167,7.5558554191\C,2.3563537796,0.0426531468,6.2514373652\C,
0.0448406125,0.3700808351,5.1982180325\C,-1.2358259295,0.8886460498,5.
3040310489\C,-1.9947170581,0.7136543069,4.1289578313\C,3.3620093884,0.

5995495607,12.3551459439\C,2.3630166652,0.6112718471,9.9614959123\C,2.
0787250077,1.0445223269,12.2691325344\C,1.524103269,1.0531961899,10.93
77090553\C,5.0735822515,0.2467509674,15.9236612838\C,4.1972356942,0.41
48459384,13.4772139465\C,5.949219435,-0.1489958529,14.9660132188\C,5.4
634326789,-0.061620358,13.6046334518\O,-0.3996766068,-0.3739723722,8.3
907450014\O,0.0800118705,2.1056244642,8.0623496226\O,5.0092788194,1.06
27397076,10.2564482517\O,4.1464383232,-1.3057008806,10.6205645697\O,2.
421973605,-0.0663544943,15.4464199965\O,3.4170271929,2.2720040002,15.2
683633535\S,-1.9085358584,-0.2572782035,1.5247813831\S,0.3328079948,-0
.3094482661,3.6203178539\S,0.4945409312,0.6959767726,7.9169065016\S,3.
9412872456,0.1509225652,10.7053266229\S,3.5583879781,0.8139867082,15.1
143360823\S,6.6800703225,0.1365321898,21.2575591353\H,2.9235631264,-0.
2226216374,5.3583700217\H,4.0435679775,-0.0993474477,7.7018480657\H,-1
.8802596469,-1.6164617276,1.5682216113\H,-3.0259132204,1.040124889,4.0
028499245\H,-1.5978637796,1.3830797334,6.2045671906\H,7.0179294471,1.4
434005967,21.4291230879\H,0.5092719204,1.3938918081,10.7329431501\H,1.
5042657458,1.3628846106,13.1388346131\H,6.0659171209,-0.3738533265,12.
7516179215\H,6.9475439844,-0.5259719746,15.190605818\Au,-0.0000034197,
0.0000024939,-0.0000050537\Au,2.4976203275,1.4419894328,0.0000007648\A
u,2.4976199039,-1.4420101664,0.0000006728\Au,-1.6650799841,-0.00000065
31,-2.3547800113\Au,0.832540465,1.4419991408,-2.3547803617\Au,0.832541
2361,-1.4420003834,-2.3547793282\Au,3.3301698717,2.8840102222,-2.35477
99093\Au,3.3301601516,-2.8840197373,-2.3547801072\Au,4.9469741421,-0.0
000047859,23.0000101656\Au,2.4493601018,-1.4419901762,22.9999922668\Au
,2.4493621728,1.4420137632,22.999991393\Au,6.6120602114,0.0000006763,2
5.3547798505\Au,4.1144468328,-1.4419981827,25.3547835286\Au,4.11444465
35,1.442000375,25.3547814156\Au,1.6168072498,-2.8840052365,25.35478194
47\Au,1.6168160838,2.8840132172,25.354782769\\Version=ES64L-G09RevD.01
\HF=-6177.9088458\RMSD=2.823e-09\RMSF=8.787e-06\Dipole=0.6909153,-0.24
20831,-0.4560029\Quadrupole=69.4003753,0.3533383,-69.7537136,-0.947253
3,78.9037974,7.3090261\PG=C01 [X(C20H12Au16O6S7)]\\@

TDO4g.pbe0

1\1\GINC-R03-NODE15\FOpt\RPBE1PBE\Gen\C24H14Au16O8S8\GRYNOVA\09-Aug-20
16\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4)
EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\TDO4g.pbe0.freq\\0,1\C,7
.8004464838,0.175350755,22.9807878485\C,6.6365416004,-0.043066011,20.8
147617835\C,8.6371721213,-0.2689573974,21.983014457\C,7.9756664288,-0.
3925128125,20.743863342\S,6.178263829,0.4206777654,22.4293740647\H,8.4
465194727,-0.7388874428,19.8247495525\H,9.689981844,-0.4926520191,22.1
486777628\C,2.6478944642,-0.2124266485,12.4573590723\C,1.656229035,-0.
2268717443,10.0621496145\C,1.307254035,0.0191836954,12.3876243759\C,0.
7559316032,0.012285123,11.0555858759\C,-0.4414904562,-0.2382218541,5.1
871137347\C,-1.5936931838,-0.3455958133,3.0063016299\C,-1.7816040826,0
.1052666128,5.2687186947\C,-2.43635246,0.0450395572,4.0213967386\C,4.5
198568017,-0.227966241,15.9511033383\C,3.5240688285,-0.2758528036,13.5
580249061\C,5.4176384442,-0.48547398,14.9600287659\C,4.8640851238,-0.5
106060128,13.6290466983\C,5.7000468304,-0.0409234156,19.7391425146\C,4
.6820193631,-0.1216509314,17.3474270549\C,4.3525356178,0.109810642,19.
6799244661\C,3.7831025906,0.0624905212,18.3510999097\C,1.4984339834,-0
.2973104522,8.6630280304\C,0.4899978939,-0.2894653318,6.2657393919\C,2
.4008847535,-0.4483624397,7.6569680799\C,1.8368313924,-0.4466685666,6.
3250537196\O,4.1902677742,0.6307658988,10.4034938557\O,3.7286945818,-1

.8644996419,10.6201515336\O,1.9829409157,-1.0868329315,15.6263819644\O
,2.449864875,1.4039339809,15.3734131232\O,7.1180281522,0.9747337145,17
.6843741765\O,6.910998847,-1.5587514533,17.843949641\O,-0.9381012243,-
1.3778534863,8.2759078308\O,-0.7263498977,1.1594303398,8.2105418229\S,
3.2879997457,-0.4690134216,10.7902496618\S,0.0259092755,-0.6173443402,
3.5530672761\S,-2.0455361826,-0.4495109581,1.3063208999\S,8.2610282637
,0.3708788165,24.6704768062\S,2.8871385761,0.00517191,15.2224233604\S,
6.3352538097,-0.2163839289,18.0550879528\S,-0.1518162675,-0.1753040488
,7.9526117707\H,-0.3002326272,0.1985037511,10.8619325038\H,0.693132057
9,0.2014298408,13.2694150729\H,-1.9764282612,-1.8005460731,1.162565027
4\H,-3.4885580652,0.2758645088,3.8618270277\H,-2.2579450042,0.40351793
73,6.2017219875\H,8.2010523074,1.7283545077,24.7381397215\H,5.47656090
58,-0.7061200038,12.7489394211\H,6.4741869657,-0.6687082099,15.1544978
56\H,2.711169106,0.1515142587,18.1743661814\H,3.7285305439,0.245368106
9,20.5641400664\H,2.4644652425,-0.5506458323,5.4391327952\H,3.47217499
18,-0.5433197696,7.8344912627\Au,0.0000258614,-0.0000005876,0.00005852
58\Au,2.497614844,1.4419989298,-0.0000112426\Au,2.4976176594,-1.442014
0533,-0.0000119052\Au,-1.6650773162,0.0000003962,-2.3547818977\Au,0.83
25359406,1.4419931141,-2.3547856517\Au,0.832536583,-1.4419957425,-2.35
47838151\Au,3.3301695961,2.8840106997,-2.3547797143\Au,3.3301584838,-2
.8840226262,-2.3547789279\Au,6.2145403434,0.0000051003,25.9999269442\A
u,3.716937388,-1.442002795,26.0000279698\Au,3.7169349238,1.4420185266,
26.0000340004\Au,7.8796248438,-0.0000000949,28.3547836459\Au,5.3819973
551,-1.442000651,28.354775131\Au,5.3819972863,1.4419952765,28.35477839
77\Au,2.8843868026,-2.8840217825,28.3547751898\Au,2.8843994049,2.88403
62896,28.3547733498\\Version=ES64L-G09RevD.01\HF=-6879.6445735\RMSD=6.
546e-09\RMSF=4.807e-06\Dipole=0.0108598,-0.0129447,-0.0251613\Quadrupo
le=57.2473505,-12.2887054,-44.9586451,2.5952563,71.3072487,19.9457526\
PG=C01 [X(C24H14Au16O8S8)]\\@

TDO5g.pbe0

1\1\GINC-NODE05\FOpt\RPBE1PBE\Gen\C28H16Au16O10S9\GRYNOVA\28-Feb-2017\
0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=Loose IOP(2/17=4) Emp
iricalDispersion=GD3BJ pseudo=read Nosymm\\TDO5g.pbe0.freq\\0,1\C,3.98
34217186,-1.0825932187,12.0979569118\S,4.5074920481,-0.7248692942,10.4
079927218\C,2.8407770884,-1.0021343195,9.7712981594\C,2.6539100782,-1.
3837767591,12.0959593837\C,2.0197534317,-1.3412541869,10.8042554675\O,
4.8759963596,0.6950351184,10.2739157224\O,5.4279239405,-1.7664887421,9
.9184840414\H,0.9610080383,-1.5613670465,10.6696036184\H,2.1054619943,
-1.6382204947,13.0028828133\C,0.2791660021,-0.5696184323,5.1502835514\
S,0.5098543514,0.154012743,3.5827563146\C,-1.1461301825,-0.1498945736,
3.1783966757\C,-1.0123574025,-1.0475198074,5.30753926\C,-1.8236376592,
-0.8068755126,4.1803894658\S,-1.8379508834,0.2546018305,1.609620958\H,
-1.7599367033,1.6094899194,1.7017127085\H,-2.8710094999,-1.0933807975,
4.0980162701\H,-1.3441690044,-1.5607205386,6.2092773347\C,8.7046059975
,-0.1671548973,22.9122204147\S,7.1152694395,-0.5254847857,22.125104786
\C,7.8465218196,-0.5094973253,20.4781702448\C,9.6554682938,-0.09173395
33,21.9469692631\C,9.1808758943,-0.2752077606,20.5921293832\C,8.734399
074,-0.0521188235,24.3345241573\H,9.8468459707,-0.2208273429,19.730844
5464\H,10.706361156,0.1068297246,22.1599239371\C,5.9258652116,-0.90471
95979,15.5462552967\S,4.2878789671,-1.1973434212,14.8507120087\C,4.896
8578334,-0.9889203929,13.1656556463\C,6.8057871086,-0.6818699435,14.52
94996838\C,6.2338737093,-0.7270913883,13.2066524556\O,3.8657079817,-2.

590804922,15.0789321363\O,3.3779287924,-0.0949827987,15.2087669404\H,6
.8299821883,-0.5601960752,12.3095611687\H,7.8619948034,-0.4732478042,1
4.6993939586\C,7.0135492727,-0.7055463537,19.3576292407\S,7.6940575653
,-0.5882027235,17.6895554902\C,6.0800171412,-0.9035268673,16.946184170
8\C,5.6791619355,-0.9664138565,19.2770505415\C,5.1613291193,-1.0783305
961,17.9377171924\O,8.1271903858,0.7917698553,17.4078840833\O,8.615472
1617,-1.7080611556,17.4288021118\H,4.1085371881,-1.276896233,17.737543
5432\H,5.0445359301,-1.0791611716,20.1557853947\C,2.5623397466,-0.8212
196655,8.4014788489\S,0.8606956706,-0.9795642463,7.8322447433\C,1.3218
847328,-0.613825256,6.122622765\C,3.3504964722,-0.4932598603,7.3425452
538\C,2.6578760658,-0.3756537473,6.0775208741\O,0.3963652761,-2.373647
6256,7.9702564381\O,0.0394958679,0.1152239362,8.3769573892\H,3.1866493
176,-0.1185159707,5.1588763554\H,4.4249158859,-0.3329480326,7.43361482
66\C,7.640104988,0.0685242575,25.1761714405\C,7.9955836519,0.169100805
4,26.5371081359\C,9.3570263508,0.1341402849,26.7238085711\S,10.2243946
216,-0.0518239594,25.2341378414\S,10.2371954321,0.1374987642,28.259490
6382\H,6.6154614248,0.1043001509,24.8076601283\H,7.2917859663,0.257318
3737,27.3664928872\H,10.4711979786,1.4756042548,28.3415354601\O,6.6695
246009,-1.8853115811,22.4734556259\O,6.1858297215,0.6090648218,22.2813
51223\Au,-0.0000067476,-0.0000031048,-0.0000135781\Au,2.4976203241,1.4
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0S9)]\\@

TDO6g.pbe0

1\1\GINC-NODE05\FOpt\RPBE1PBE\Gen\C32H18Au16O12S10\GRYNOVA\03-Mar-2017
\0\\#PBE1PBE/gen SCF=Tight INT(grid=finegrid) OPT=(MaxStep=15,Loose) I
OP(2/17=4) EmpiricalDispersion=GD3BJ pseudo=read Nosymm\\TDO6g.pbe0.fr
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1740237845,-0.4525043434,12.5520496377\C,0.6874750446,-0.4845537606,11
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69,-0.5867408687,3.1044632227\C,-1.6924028873,-0.2262546517,5.37665131
22\C,-2.3243354428,-0.3526557338,4.1233541642\S,-1.8849470033,-0.74181
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Geometry of the gold slab Au_{30}:

Au	1.66508	0.00000	-4.70956
Au	4.16270	1.44200	-4.70956
Au	4.16270	-1.44200	-4.70956
Au	6.66032	2.88401	-4.70956
Au	6.66032	0.00000	-4.70956
Au	6.66032	-2.88401	-4.70956
Au	-0.83254	1.44200	-4.70956
Au	-0.83254	-1.44200	-4.70956

Au	1.66508	2.88401	-4.70956
Au	1.66508	-2.88401	-4.70956
Au	0.00000	0.00000	-7.06434
Au	2.49762	1.44200	-7.06434
Au	2.49762	-1.44200	-7.06434
Au	4.99524	2.88401	-7.06434
Au	4.99524	0.00000	-7.06434
Au	4.99524	-2.88401	-7.06434
Au	-2.49762	1.44200	-7.06434
Au	-2.49762	-1.44200	-7.06434
Au	0.00000	2.88401	-7.06434
Au	0.00000	-2.88401	-7.06434
Au	-1.66508	0.00000	-9.41912
Au	0.83254	1.44200	-9.41912
Au	0.83254	-1.44200	-9.41912
Au	3.33016	2.88401	-9.41912
Au	3.33016	0.00000	-9.41912
Au	3.33016	-2.88401	-9.41912
Au	-4.16270	1.44200	-9.41912
Au	-4.16270	-1.44200	-9.41912
Au	-1.66508	2.88401	-9.41912
Au	-1.66508	-2.88401	-9.41912