Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for:

Photoluminescent mechanism of ultra-small gold clusters

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Section 1.Schematic orbitals

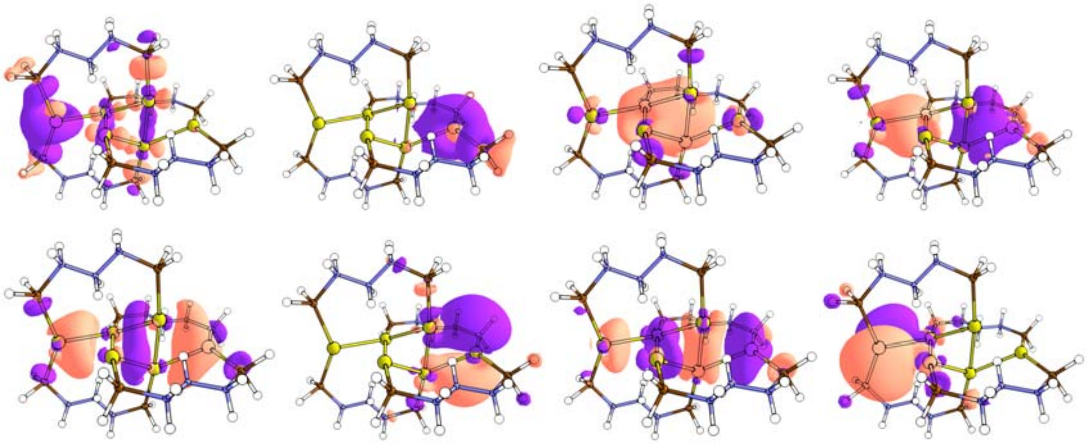


Figure S1.1 Molecular orbitals of 1 used in defining the active space for the CASSCF(8e/8o)/CASPT2 calculations.

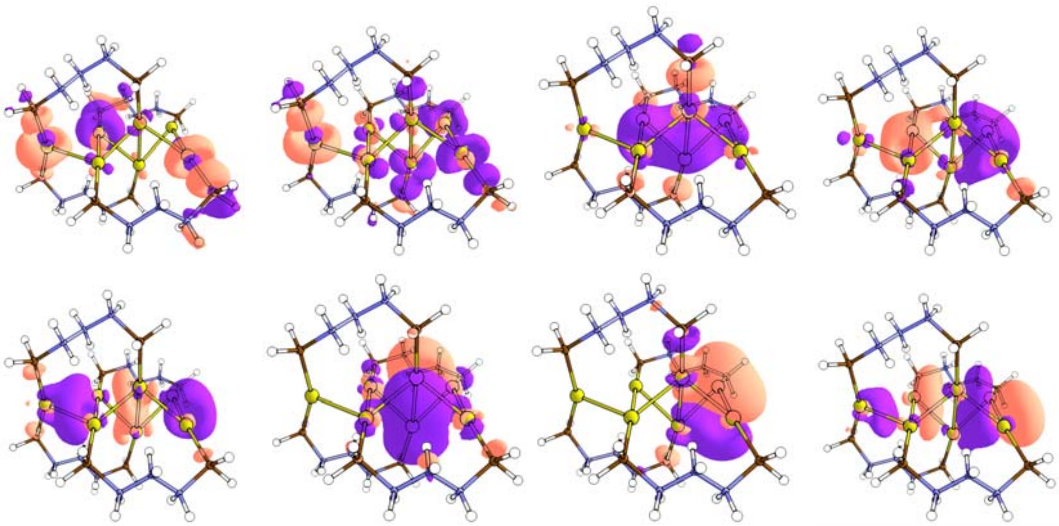


Figure S1.2 Molecular orbitals of 2 used in defining the active space for the CASSCF(8e/8o)/CASPT2 calculations.

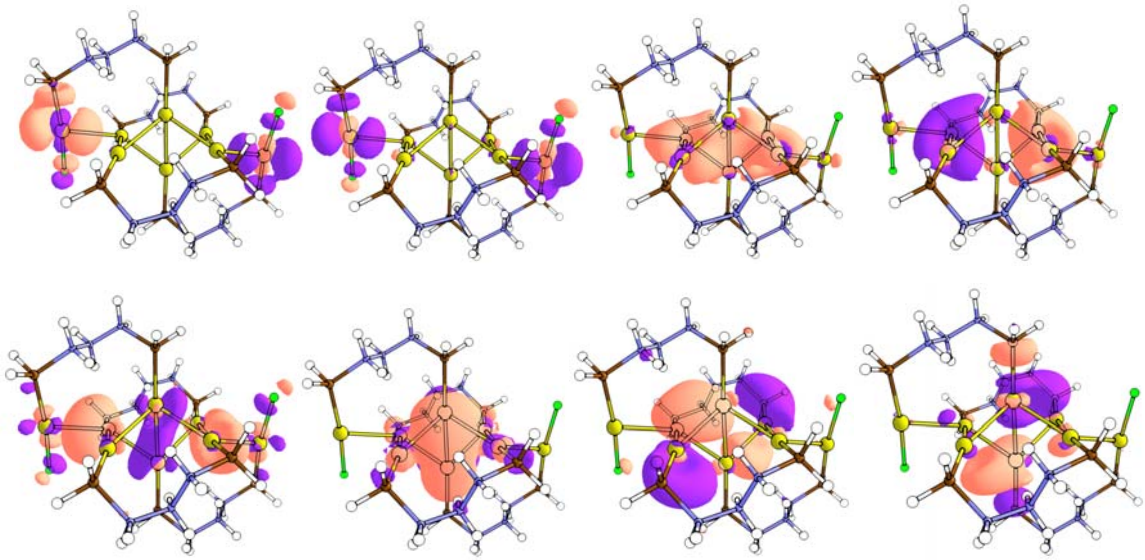


Figure S1.3 Molecular orbitals of 3 used in defining the active space for the CASSCF(8e/8o)/CASPT2 calculation.

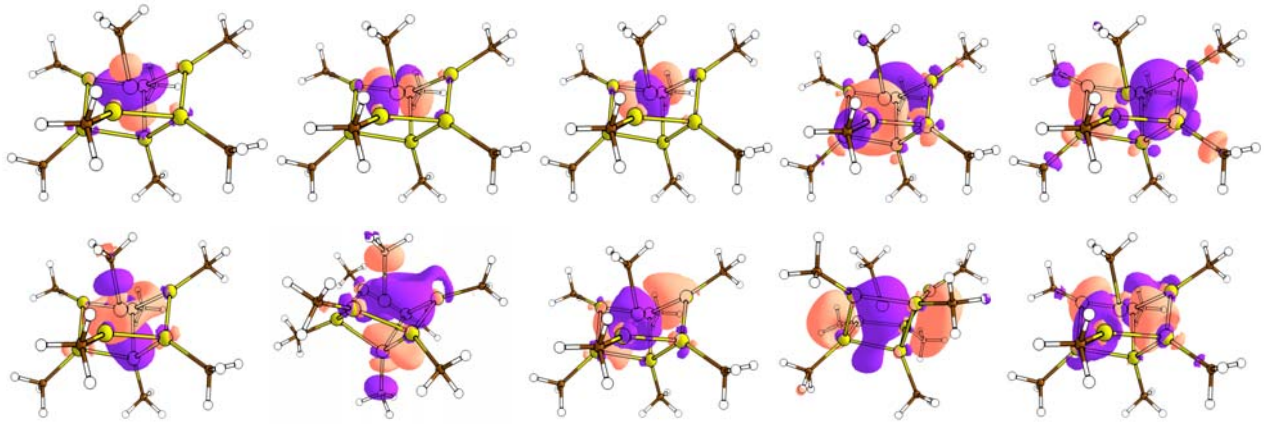


Figure S1.4 Molecular orbitals of 4 used in defining the active space for the CASSCF(10e/10o)/CASPT2 calculation.

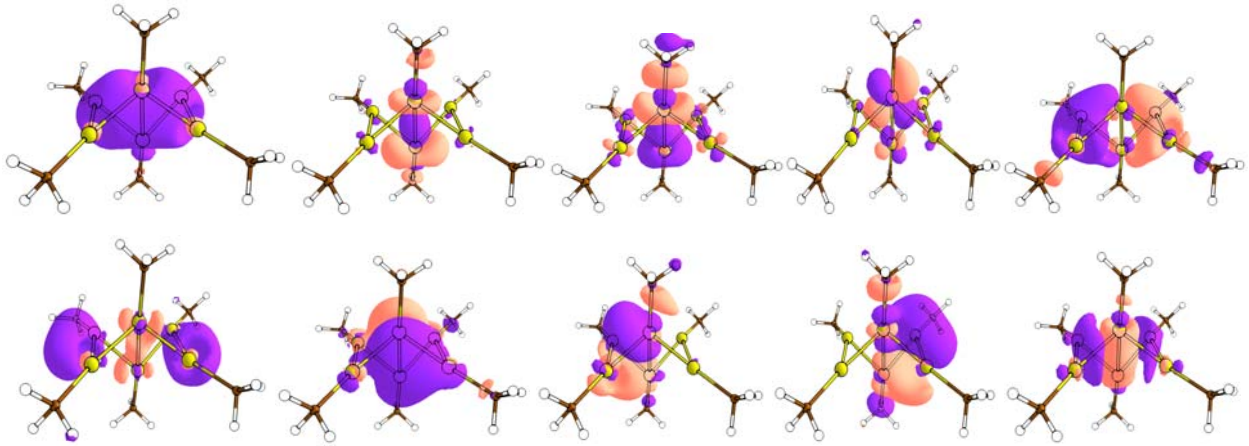


Figure S1.5 Molecular orbitals of 5 used in defining the active space for the CASSCF(10e/10o)/CASPT2 calculation.

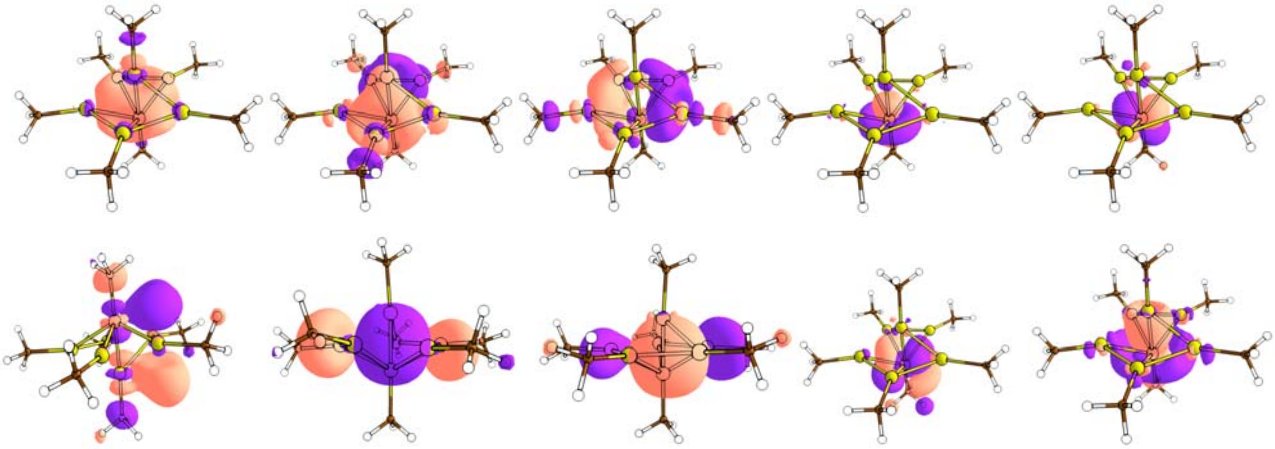


Figure S1.6 Molecular orbitals of 6 used in defining the active space for the CASSCF(10e/10o)/CASPT2 calculation.

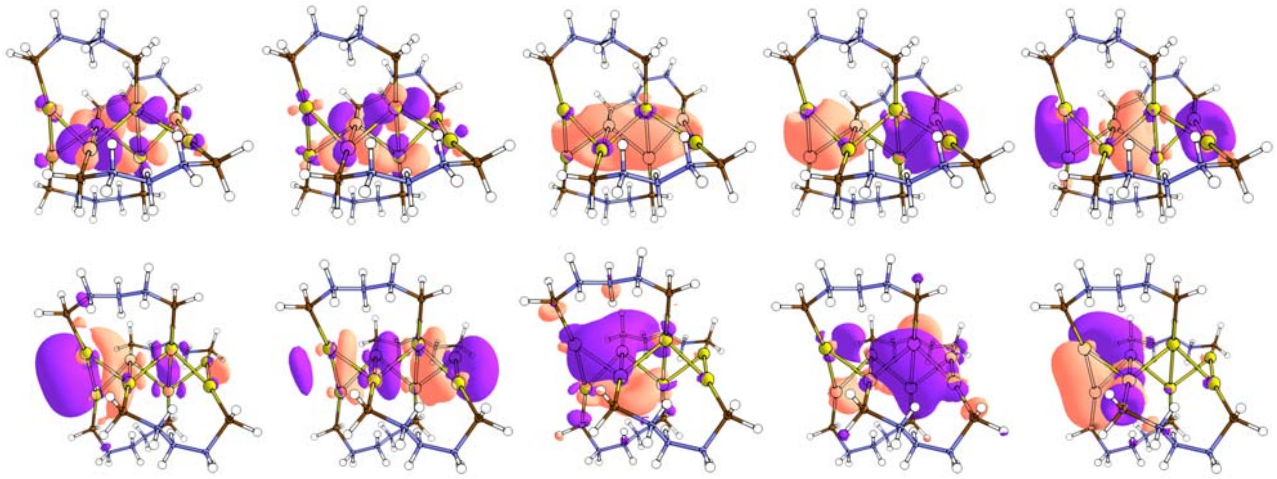


Figure S1.7 Molecular orbitals of 7 used in defining the active space for the CASSCF(10e/10o)/CASPT2 calculation.

Section 2. Schematic structures with selective parameters

Figure S2.1 The schematic models of clusters 1-7.

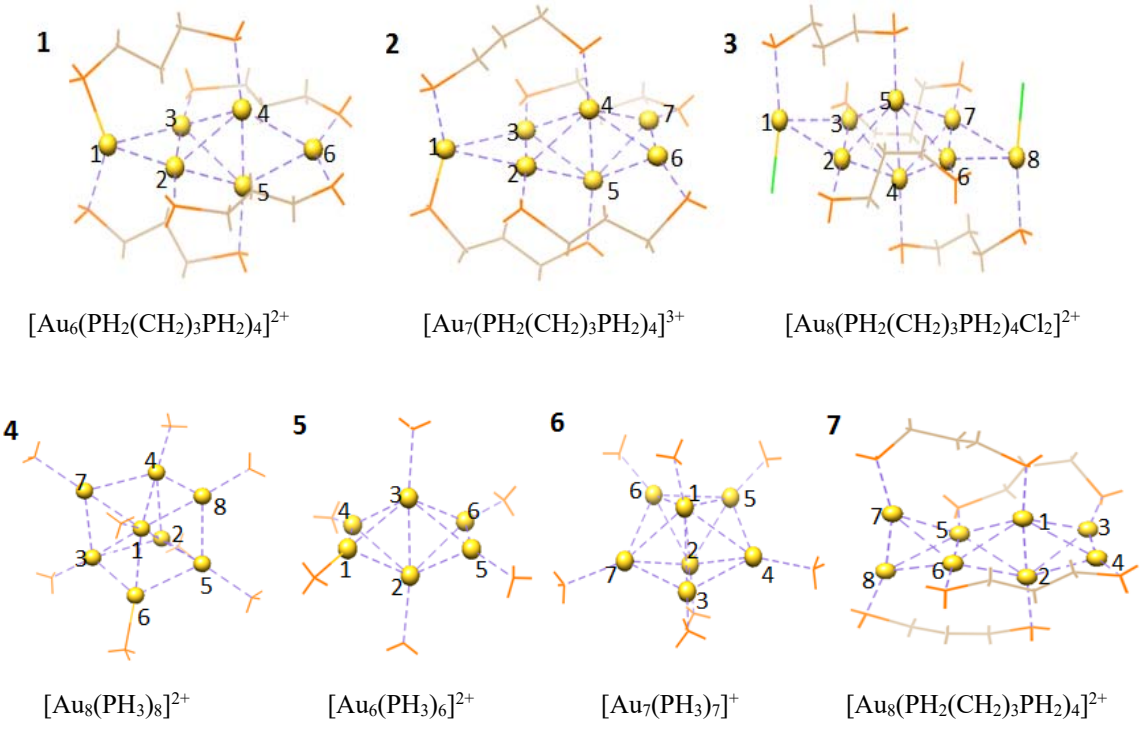


Table S2.2 Summary of average Au-Au bond distances (Å) of clusters 1-7.

	1		2		3		4		5		6		7	
Average of all Au-Au bond distances	**Cal.**	**Exp.**	**Cal.**	**Cal.**	**Cal.**	**Exp.**	**Cal.**	**Exp.**	**Cal.**	**Exp.**	**Cal.**	**Exp.**	**Cal.**	**Exp.**
	2.952	**2.814**	**2.957**	**2.785**	**2.955**	**2.842**	**2.899**	**2.804**	**2.921**	**2.759**	**2.985**	**2.849**	**2.931**	**2.789**

Table S2.3 Key structural parameters (Å) of the critical points for 1 obtained from the CASSCF(8e/8o) calculations.

Au-Au	S_0-min	STC($S_{\Sigma\Sigma}/T_{\Sigma\pi}$)	CI($T_{\Sigma\pi}/T_{\Sigma\Sigma}$)	$T_{\Sigma\Sigma}$-min	crystal structure
1-2	3.017	3.041	3.018	3.037	2.798
1-3	3.017	3.040	3.023	3.036	2.798
2-3	2.773	2.769	2.744	2.760	2.630
2-4	2.980	2.991	3.028	2.950	2.923
2-5	2.979	2.998	3.017	2.950	2.923
3-4	2.976	2.995	3.020	2.948	2.923
3-5	2.977	2.990	3.021	2.949	2.923
4-5	2.774	2.876	3.059	2.762	2.630
4-6	3.015	3.044	3.015	3.036	2.798
5-6	3.013	3.040	3.026	3.036	2.798

Table S2.4 Key structural parameters (Å) of the critical points for 2 obtained from the CASSCF(8e/8o) calculations.

Au-Au	S_0-min	STC($S_{\Sigma\Sigma}/T_{\Sigma\pi}$)	CI($T_{\Sigma\pi}/T_{\Sigma\Sigma}$)	$T_{\Sigma\Sigma}$-min	crystal structure
1-2	3.107	3.181	3.300	3.087	2.948
1-3	3.073	3.101	3.309	3.061	2.899
2-3	2.810	2.862	2.924	2.797	2.651
2-4	2.993	2.999	2.964	2.989	2.825
2-5	2.949	2.955	2.924	2.960	2.778
3-4	3.029	3.038	3.017	3.025	2.878
3-5	2.981	2.992	2.967	2.989	2.839
4-5	2.813	2.806	2.775	2.805	2.653
4-6	2.959	2.961	2.940	2.986	2.804
4-7	3.008	3.013	2.969	3.050	2.798
5-6	2.928	2.929	2.907	2.952	2.737
5-7	2.937	2.941	2.892	2.971	2.721
6-7	2.852	2.904	2.955	2.853	2.670

Table S2.5 Key structural parameters (Å) of the critical points for 3 obtained from the CASSCF(8e/8o) calculations.

Au-Au	S_0-min	STC($S_{\Sigma\Sigma}/T_{\Sigma\pi}$)	CI($T_{\Sigma\pi}/T_{\Sigma\Sigma}$)	$T_{\Sigma\Sigma}$-min	crystal structure
1-2	3.072	3.072	3.043	3.047	2.970
1-3	3.228	3.228	3.219	3.200	3.072

2-3	2.761	2.761	2.822	2.775	2.650
2-4	2.936	2.936	2.922	2.959	2.795
2-5	2.916	2.916	2.915	2.928	2.779
3-4	2.982	2.982	2.977	3.013	2.841
3-5	2.941	2.941	2.939	2.955	2.865
4-5	2.762	2.762	2.758	2.778	2.648
4-6	2.942	2.942	2.939	2.951	2.872
4-7	2.922	2.922	2.925	2.936	2.798
5-6	2.983	2.983	2.973	3.009	2.824
5-7	2.931	2.931	2.924	2.958	2.792
6-7	2.754	2.754	2.806	2.774	2.658
6-8	3.121	3.121	3.109	3.130	3.053
7-8	3.076	3.076	3.064	3.066	3.008

Table S2.6 Key structural parameters (Å) of the critical points for 4 obtained from the CASSCF(10e/10o) calculations.

Au-Au	S_0-min	$T_{\Sigma\Sigma}$-min	crystal structure	Au-Au	S_0-min	$T_{\Sigma\Sigma}$-min	crystal structure
1-2	2.686	2.727	2.634	2-4	3.012	3.044	2.909
1-3	2.800	2.837	2.698	2-5	3.055	3.074	2.960
1-4	2.803	2.847	2.709	3-6	2.961	3.053	2.863
1-5	2.791	2.826	2.682	3-7	2.956	2.920	2.846
1-6	2.814	2.900	2.721	4-7	2.981	3.023	2.902
1-7	2.808	2.834	2.707	4-8	2.961	3.016	2.863
1-8	2.811	2.822	2.723	5-6	2.940	3.007	2.825
2-3	3.026	3.029	2.930	5-8	2.977	2.943	2.897

Table S2.7 Key structural parameters (Å) of the critical points for 5 obtained from the CASSCF(10e/10o) calculations.

Au-Au	S_0-min	$T_{\Sigma\Sigma}$-min	crystal structure	Au-Au	S_0-min	$T_{\Sigma\Sigma}$-min	crystal structure
1-2	3.042	2.956	2.820	2-6	2.974	2.920	2.809
1-3	2.945	2.933	2.777	3-4	2.948	2.938	2.791
1-4	2.792	3.019	2.669	3-5	2.930	2.948	2.839
2-3	2.723	2.736	2.651	3-6	2.924	2.922	2.762
2-4	3.014	2.945	2.796	5-6	2.856	3.073	2.662

2-5	2.986	2.939	2.775				

Table S2.8 Key structural parameters (Å) of the critical points for 6 obtained from the CASSCF(10e/10o) calculations.

Au-Au	S_0-min	$T_{\Sigma\Sigma}$-min	crystal structure	Au-Au	S_0-min	$T_{\Sigma\Sigma}$-min	crystal structure
1-2	2.658	2.701	2.583	2-5	2.912	2.899	2.782
1-3	3.031	3.062	2.895	2-6	2.875	2.900	2.748
1-4	2.986	2.982	2.800	2-7	2.911	2.920	2.794
1-5	3.073	3.113	3.019	3-4	2.975	2.929	2.889
1-6	3.024	3.073	2.950	3-7	3.364	3.459	3.084
1-7	2.985	2.983	2.853	4-5	3.115	3.176	2.909
2-3	2.894	2.923	2.704	5-6	3.024	2.972	2.923
2-4	2.892	2.910	2.707	6-7	3.034	3.024	2.944

Table S2.9 Key structural parameters (Å) of the critical points for 7 obtained from the CASSCF(10e/10o) calculations.

Au-Au	S_0-min	$T_{\Sigma\pi}$-min	crystal structure	Au-Au	S_0-min	$T_{\Sigma\pi}$-min	crystal structure
1-2	2.735	2.723	2.630	2-6	3.055	3.042	2.896
1-3	2.963	2.939	2.831	3-4	2.842	2.884	2.607
1-4	2.960	2.934	2.844	5-6	2.804	2.817	2.630
1-5	2.993	2.986	2.835	5-7	2.990	2.969	2.831
1-6	3.001	2.995	2.860	5-8	2.984	2.959	2.844
2-3	2.921	2.900	2.824	6-7	2.955	2.935	2.824
2-4	2.948	2.930	2.854	6-8	2.970	2.949	2.854
2-5	3.007	2.996	2.860	7-8	2.768	2.780	2.607

Section 3. Wavefuction analyses

Reduced Density Gradient Analyses (RDGA):

Figure S3.1.1 Reduced density gradient isosurface plots (isovalue: 0.5) of $[Au_6]^{2+}$ as the function of dihedral angle Au2-Au1-Au6-Au5 obtained from B3LYP/ECP60MWB calculations. Aurophilicity only extended 4 Bohr in X,Y,Z direction from the centre of $[Au_6]^{2+}$. The intensity of aurophilic interactions are illustrated by the size of green regions.

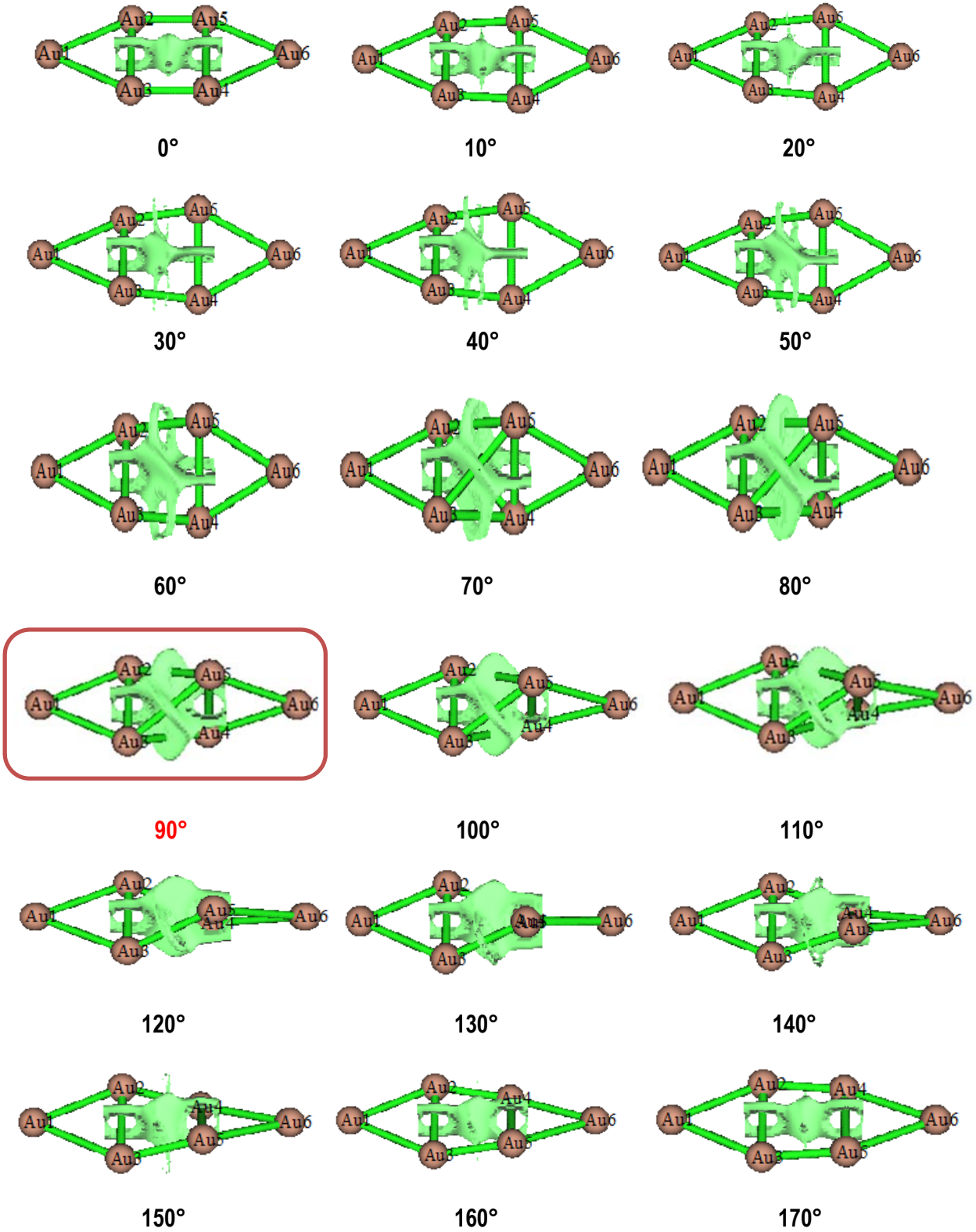
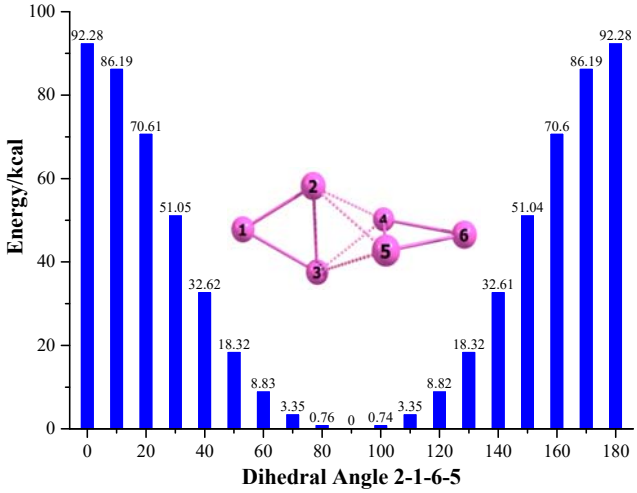


Figure S3.1.2 Energy curve of $[Au_6]^{2+}$ as the function of dihedral angle Au2-Au1-Au6-Au5 obtained from B3LYP/ECP60MWB calculations.



Charge decomposition analyses (CDA):

Table S3.2 Charge Components for molecular orbitals of $[Au_6]^{2+}$ obtained from B3LYP/ECP60MWB calculations.

Orb.	Occ.	d	b	d - b	r	
1	2.000000	-0.000966	-0.000966	0.000000	0.000004	
2	2.000000	0.000407	0.000408	0.000000	0.000499	
…						
25	2.000000	0.024258	0.024258	0.000000	0.269523	
…						
34	2.000000	0.005932	0.005932	0.000000	0.114958	
35	2.000000	0.021100	0.014516	0.006584	-0.023539	
36	2.000000	0.014516	0.021100	-0.006584	-0.023540	
37	2.000000	0.000911	0.000911	0.000000	-0.114555	
…						
53	2.000000	0.002158	0.002158	0.000000	-0.084017	HOMO-3
54	2.000000	0.004825	0.006600	-0.001775	-0.066551	HOMO-2
55	2.000000	0.006600	0.004825	0.001775	-0.066550	HOMO-1
56	2.000000	0.147021	0.147020	0.000000	-0.351242	HOMO
57	0.000000	0.000000	0.000000	0.000000	0.000000	LUMO
58	0.000000	0.000000	0.000000	0.000000	0.000000	LUMO+1
59	0.000000	0.000000	0.000000	0.000000	0.000000	LUMO+2
60	0.000000	0.000000	0.000000	0.000000	0.000000	LUMO+3
…						
216	0.000000	0.000000	0.000000	0.000000	0.000000	

Sum	112.000000	0.272443	0.272443	0.000000	-0.316617

d = The number of electrons donated from fragment 1 (the left $[Au_3]^+$ moiety) to fragment 2 (the right $[Au_3]^+$ moiety)

b = The number of electrons back donated from fragment 2 to fragment 1

r = The number of electrons involved in repulsive polarization

Orbital Composition Analyses(OCA):

Table S3.3 The composition of the frontier orbitals of clusters 1-3 obtained at DFT/B3LYP level of theory. Only the mian contribution made by 6s and 6p shell of Au is presented, whereas the rest originates from the phosphine ligands and 5d shell of Au.

Cluster -Orbital	Orbital Composition(%)															
	Au_1		Au_2		Au_3		Au_4		Au_5		Au_6		Au_7		Au_8	
	6s	6p	6s	6p	6s	6p	6s	6p	6s	6p	6s	6p	6s	6p	6s	6p
1-HOMO	3.5	8.5	7.4	0.5	7.3	0.4	7.3	0.5	7.3	0.5	3.5	8.5				
1-LUMO	11.2	2.6	0	8.6	0	8.8	0	8.7	0	8.7	11.2	2.6				
1-LUMO+1	0	2.1	0.	6.2	0	5.8	1.7	19.1	1.7	19.0	0	9.2				
2-HOMO	0.7	6.7	7.9	2.4	4.4	1.4	0	3.0	0	6.7	4.9	3.3	4.7	2.4		
2-LUMO	5.3	15.4	1.5	11.0	0.6	7.1	3.9	1.7	3.9	2.5	3.6	7.0	5.3	3.4		
2-LUMO+1	0	4.0	1.2	8.3	0.6	8.1	0	6.6	0	18.5	7.9	5.7	4.5	3.4		
3-HOMO	1.1	1.0	6.5	2.3	6.3	0.9	0	6.1	0	6.9	6.3	0.9	6.3	2.1	1.0	1.0
3-LUMO	3.2	8.7	1.6	6.1	0	6.9	4.0	3.0	3.8	1.9	-0.1	7.5	1.9	4.1	2.8	8.6
3-LUMO+1	0	0.7	6.7	5.1	4.3	5.9	-1.6	10.7	-2.0	13.5	5.3	5.5	6.6	7.0	0	0.6

Charge Translocation Calculations

Figure S3.4.1 The scheme of fragment partition for charge translocation of 1 in which the core-Au is defined as part 1, while the rest is defined as part 2.

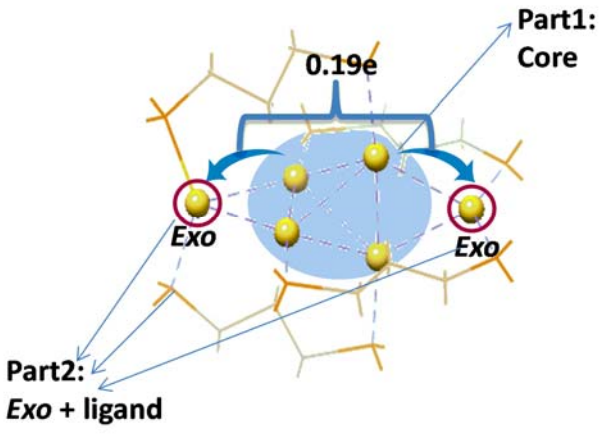


Table S3.4.2 Mulliken charge distribution of part 1 and 2 for 1 in the ground state (S_0) and the $S_{\Sigma\Sigma}(^1\sigma^*\sigma)$ state upon the photo-excitation.

	S_0	$S_{\Sigma\Sigma}(^1\sigma^*\sigma)$	Charge translocation
Part 1	0.2889	0.4795	0.1906
Part 2	1.7111	1.5205	

Section 4. Oscillator strengths

Table S4.1 Summary of the calculated oscillator strengths and the molar extinction coefficients (ε) for clusters 1-7.

Clusters	*oscillator strengths (f)*	*molar extinction coefficients (ε / M^{-1} cm^{-1})*
1 (*N*=6)	1.67	8.9 X 10^4
2 (*N*=7)	1.02	1.9 X 10^4
3 (*N*=8)	1.35	2.7 X 10^4
4 (*N*=8)	0.42	No data given
5 (*N*=6)	0.43	No data given
6 (*N*=7)	0.32	No data given
7 (*N*=8)	1.35	3.0 X 10^4

Section 5. Energy Schematics

Figure S5.1 Radiative relaxtion mechanism for 2 calculated at the CASSCF(8,8)/CASPT2 level of theory. ISC= intersystem crossing, IC= internal conversion and P= phosphorescence.

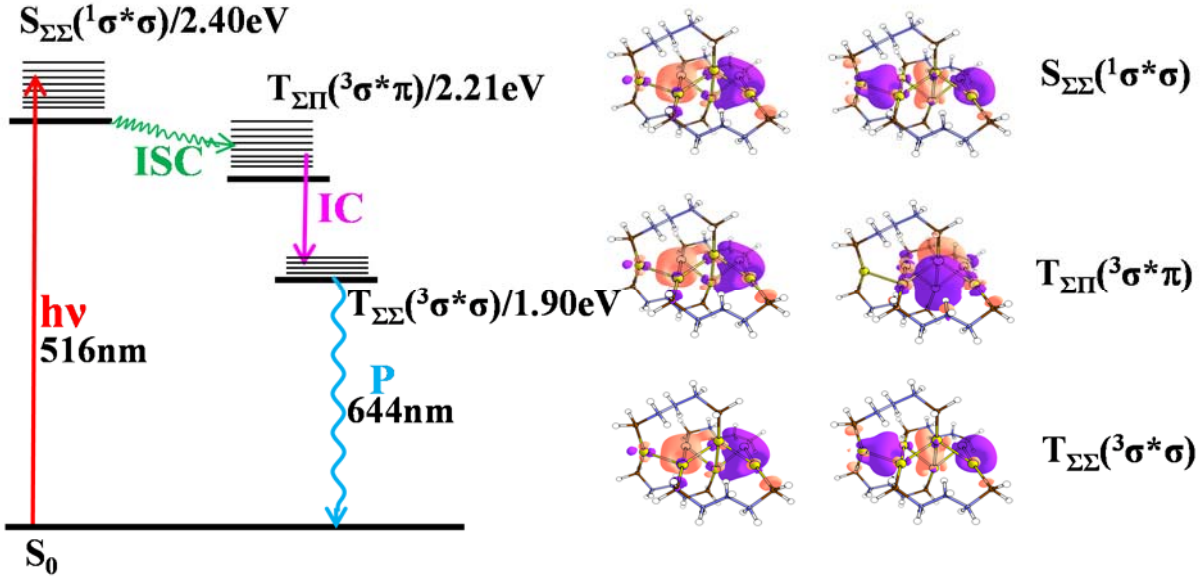


Figure S5.2 Radiative relaxtion mechanism for 3 calculated at the CASSCF(8,8)/CASPT2 level of theory. ISC= intersystem crossing, IC= internal conversion and P= phosphorescence.

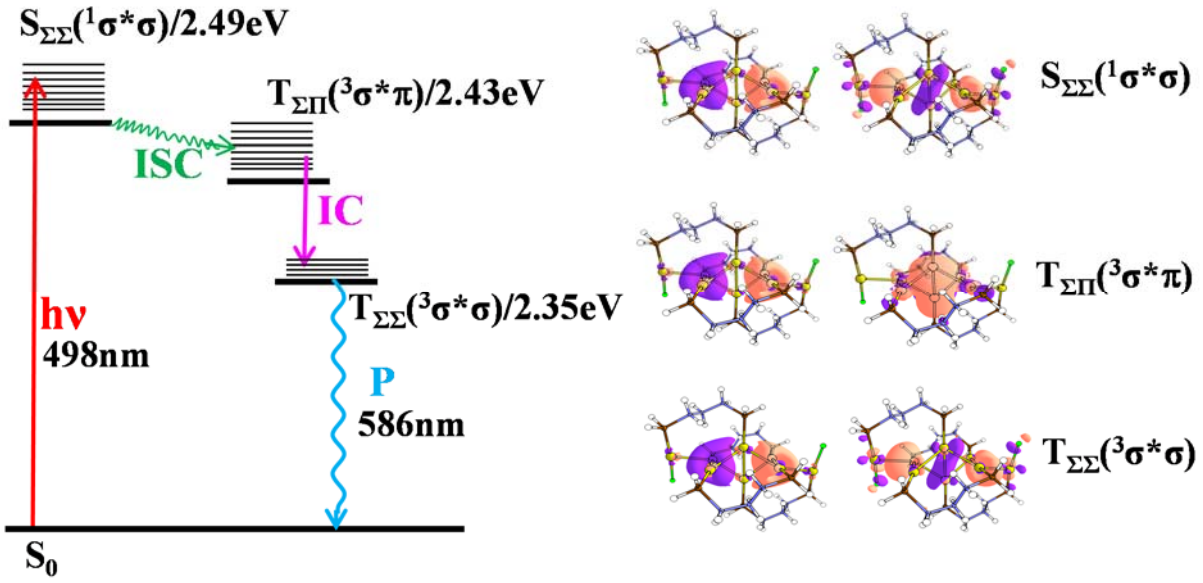


Figure S5.3 Radiative relaxtion mechanism for 4 calculated at the CASSCF(10,10)/CASPT2 level of theory. ISC= intersystem crossing, IC= internal conversion and P= phosphorescence.

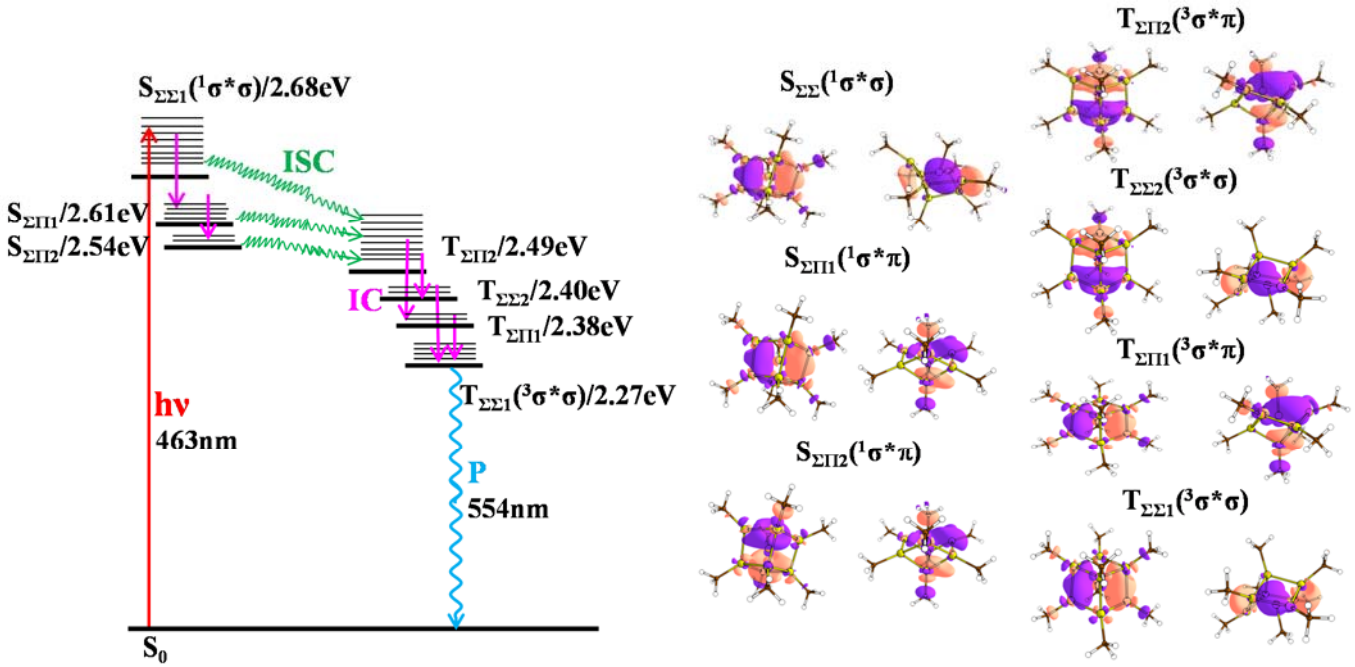


Figure S5.4 Radiative relaxtion mechanism for 5 calculated at the CASSCF(10,10)/CASPT2 level of theory. ISC= intersystem crossing, IC= internal conversion and P= phosphorescence.

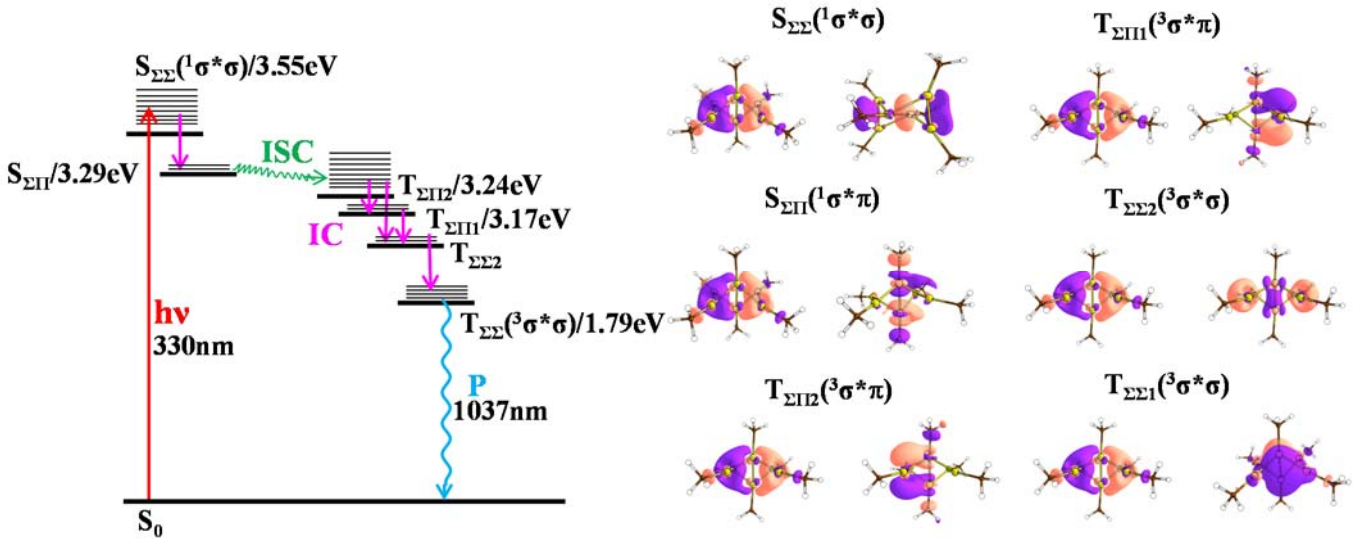


Figure S5.5 Radiative relaxtion mechanism for 6 calculated at the CASSCF(10,10)/CASPT2 level of theory. ISC= intersystem crossing, IC= internal conversion and P= phosphorescence.

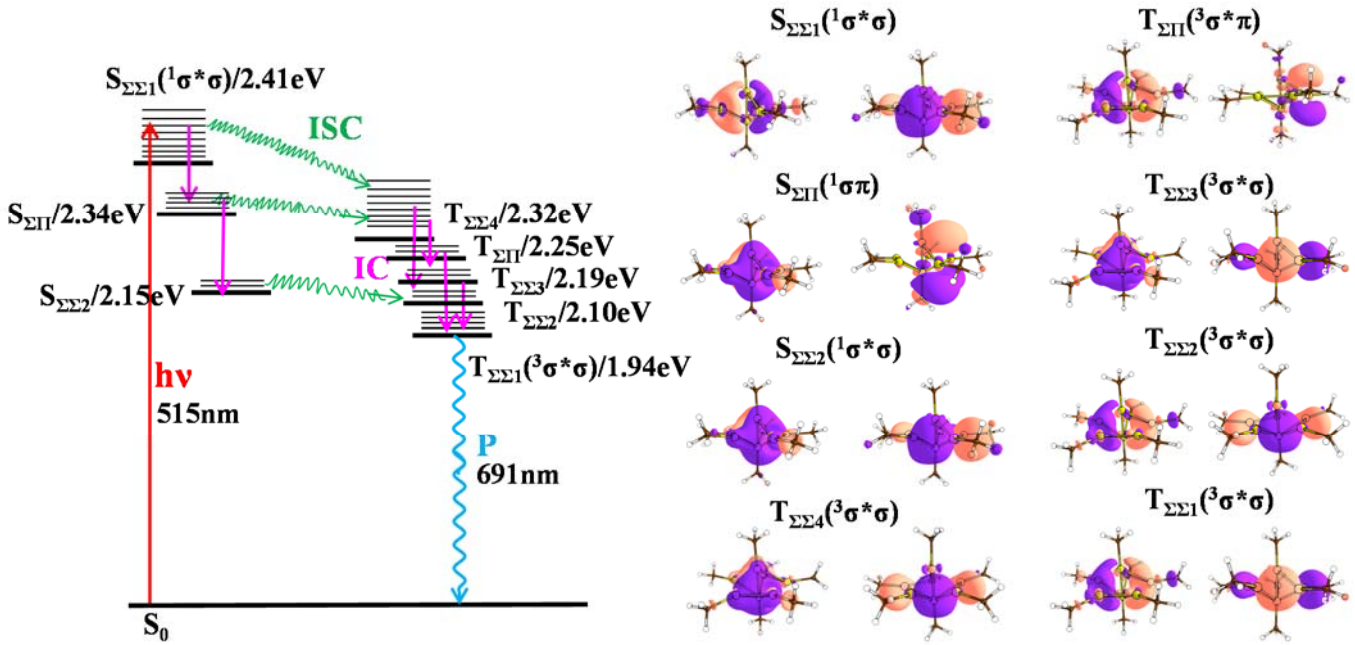
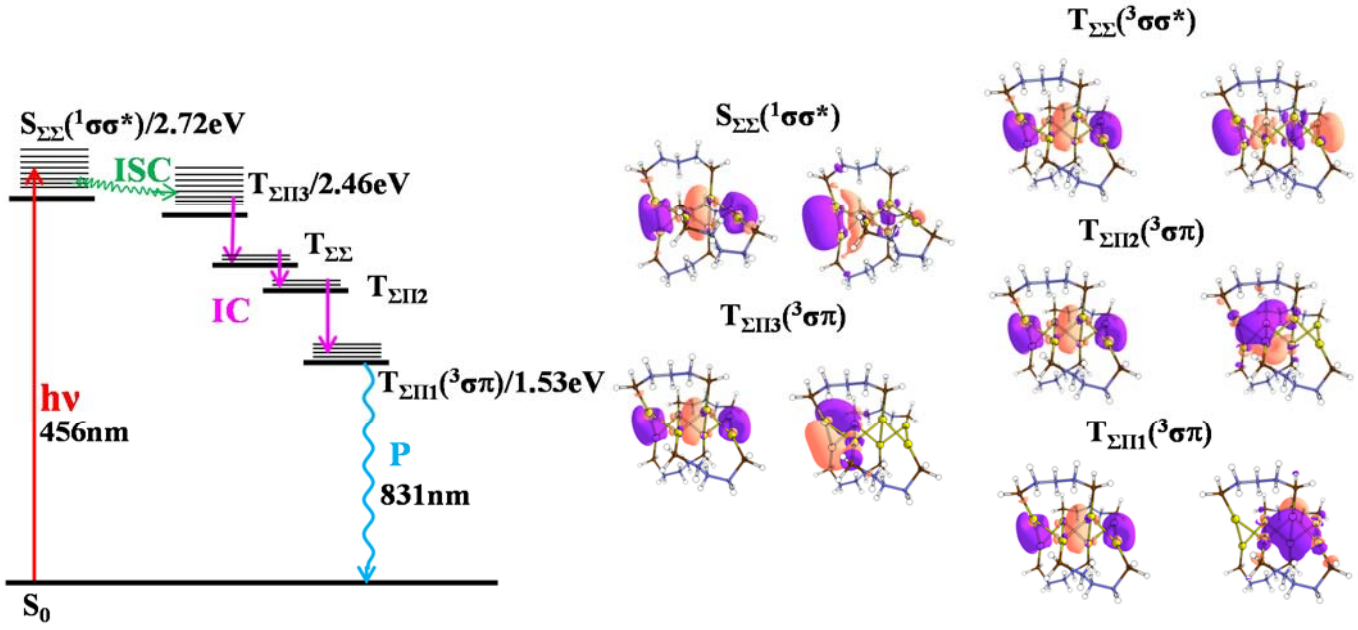


Figure S5.6 Radiative relaxtion mechanism for 7 calculated at the CASSCF(10,10)/CASPT2 level of theory. ISC= intersystem crossing, IC= internal conversion and P= phosphorescence.



Section 6. Tables

Table S6.1 The absolute energies (A.E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of cluster 1 at the CAS(8,8)/CASPT2 level of theory.The corresponding energy profiles are plotted in Figure 3 of the main article.

1	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0			
Root1	-4011.927751	-4008.300858	0
Root2		-4008.209058	2.50
Root3		-4008.208836	2.50
Root4		-4008.219704	2.21
Root5		-4008.179044	3.31
Path-$S_{\Sigma\Sigma}$			
Root1		-4008.303835	-0.08
Root2		-4008.225361	2.05
Root3		-4008.213949	2.36
Root4	-4011.827488	-4008.223454	2.11
Root5		-4008.178998	3.31
STC($S_{\Sigma\Sigma}$/$T_{\Sigma\Pi}$):$S_{\Sigma\Sigma}$			
Root1		-4008.304787	-0.11
Root2		-4008.225093	2.06
Root3		-4008.214809	2.34
Root4	-4011.800135	-4008.225677	2.04
Root5		-4008.181452	3.25

STC($S_{\Sigma\Sigma}$/$T_{\Sigma\Pi}$):$T_{\Sigma\Pi}$			
Root1		-4008.253671	1.28
Root2	-4011.83737	-4008.228525	1.97
Root3		-4008.218029	2.25
Root4		-4008.181307	3.25
Root5		-4008.17063	3.54
Path-$T_{\Sigma\Pi}$-1			
Root1		-4008.247236	1.46
Root2	-4011.837584	-4008.227964	1.98
Root3		-4008.2123	2.41
Root4		-4008.175103	3.42
Root5		-4008.170865	3.54
Path-$T_{\Sigma\Pi}$-2			
Root1		-4008.238675	1.69
Root2	-4011.832281	-4008.2283	1.97
Root3		-4008.205851	2.58
Root4		-4008.209524	2.48
Root5		-4008.177159	3.36
Path-$T_{\Sigma\Pi}$-3			
Root1		-4008.233626	1.83
Root2	-4011.839574	-4008.226712	2.02
Root3		-4008.201047	2.71
Root4		-4008.205452	2.60
Root5		-4008.175558	3.41
Path-$T_{\Sigma\Pi}$-4			
Root1		-4008.230939	1.90
Root2	-4011.840289	-4008.22584	2.04
Root3		-4008.198504	2.78
Root4		-4008.203273	2.65
Root5		-4008.174552	3.44
CI($T_{\Sigma\Pi}$/$T_{\Sigma\Sigma}$)			
Root1		-4008.228674	1.96
Root2	-4011.835161	-4008.225207	2.06
Root3		-4008.196276	2.84
Root4		-4008.201437	2.70
Root5		-4008.173972	3.45
Path-$T_{\Sigma\Sigma}$-1			
Root1	-4011.847607	-4008.235407	1.78
Root2		-4008.225576	2.05
Root3		-4008.203244	2.66
Root4		-4008.207076	2.55
Root5		-4008.173355	3.47
Path-$T_{\Sigma\Sigma}$-2			

Root1	-4011.865039	-4008.238658	1.69
Root2		-4008.201162	2.71
Root3		-4008.199067	2.77
Root4		-4008.179147	3.31
Root5		-4008.151456	4.06
Path-$T_{\Sigma\Sigma}$-3			
Root1	-4011.865772	-4008.241719	1.61
Root2		-4008.204292	2.63
Root3		-4008.202325	2.68
Root4		-4008.17995	3.29
Root5		-4008.15298	4.02
Path-$T_{\Sigma\Sigma}$-4			
Root1	-4011.866284	-4008.243758	1.55
Root2		-4008.207591	2.54
Root3		-4008.205523	2.59
Root4		-4008.180576	3.27
Root5		-4008.154413	3.98
Path-$T_{\Sigma\Sigma}$-5			
Root1	-4011.852739	-4008.247236	1.46
Root2		-4008.227964	1.98
Root3		-4008.2123	2.41
Root4		-4008.175103	3.42
Root5		-4008.170865	3.54
Path-$T_{\Sigma\Sigma}$-6			
Root1	-4011.854397	-4008.251118	1.35
Root2		-4008.229363	1.94
Root3		-4008.217199	2.28
Root4		-4008.175038	3.42
Root5		-4008.175811	3.40
$T_{\Sigma\Sigma}$-min			
Root1	-4011.866454	-4008.251943	1.33
Root2		-4008.21431	2.35
Root3		-4008.204779	2.61
Root4		-4008.173574	3.46
Root5		-4008.15414	3.99

Table S6.2 The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of 2 at the CAS(8,8)/CASPT2 level of theory.

2	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0			
Root1	-4146.505307	-4143.022691	0
Root2		-4142.923661	2.69
Root3		-4142.934388	2.40

Root4		-4142.895918	3.45
Root5		-4142.895409	3.46
STC($S_{\Sigma\Sigma}/T_{\Sigma\Pi}$):$S_{\Sigma\Sigma}$			
Root1		-4143.033187	-0.29
Root2		-4142.935354	2.38
Root3	-4146.354751	-4142.941321	2.21
Root4		-4142.901776	3.29
Root5		-4142.897493	3.41
STC($S_{\Sigma\Sigma}/T_{\Sigma\Pi}$):$T_{\Sigma\Pi}$			
Root1		-4142.961328	1.67
Root2	-4146.379693	-4142.94154	2.21
Root3		-4142.909539	3.08
Root4		-4142.899798	3.34
Root5		-4142.909959	3.07
CI($T_{\Sigma\Pi}/T_{\Sigma\Sigma}$)			
Root1		-4142.951083	1.95
Root2	-4146.37307	-4142.950125	1.97
Root3		-4142.912602	2.99
Root4		-4142.90785	3.12
Root5		-4142.899011	3.36
$T_{\Sigma\Sigma}$-min			
Root1	-4146.415062	-4142.952912	1.90
Root2		-4142.927006	2.60
Root3		-4142.897374	3.41
Root4		-4142.898827	3.37
Root5		-4142.886606	3.70

Table S6.3 The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of 3 at the CAS(8,8)/CASPT2 level of theory.

3	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0			
Root1	-5200.668473	-5197.482238	0
Root2		-5197.386601	2.60
Root3		-5197.39067	2.49
Root4		-5197.36327	3.24
Root5		-5197.346996	3.68
$T_{\Sigma\Pi}$			
Root1		-5197.40202	2.18
Root2	-5200.548607	-5197.389521	2.52
Root3		-5197.366014	3.16
Root4		-5197.338941	3.90
Root5		-5197.346743	3.69

CI($T_{\Sigma\Pi}/T_{\Sigma\Sigma}$)			
Root1		-5197.394855	2.38
Root2	-5200.554339	-5197.392725	2.43
Root3		-5197.361493	3.28
Root4		-5197.362371	3.26
Root5		-5197.33601	3.98
$T_{\Sigma\Sigma}$-min			
Root1	-5200.568594	-5197.395931	2.35
Root2		-5197.380435	2.77
Root3		-5197.358867	3.36
Root4		-5197.331518	4.10
Root5		-5197.341745	3.82

Table S6.4 The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of 4 at the CAS(10,10)/CASPT2 level of theory.

4	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0			
Root1	-3817.843075	-3819.212847	0
Root2		-3819.119495	2.54
Root3		-3819.11676	2.61
Root4		-3819.114191	2.68
Root5		-3819.114481	2.68
$T_{\perp}$			
Root1	-3817.728811	-3819.126337	2.35
Root2		-3819.12553	2.38
Root3		-3819.124431	2.40
Root4		-3819.12115	2.49
Root5		-3819.026245	5.08
$T_{\Sigma\Sigma}$-min			
Root1	-3817.735732	-3819.129225	2.27
Root2		-3819.112614	2.73
Root3		-3819.111501	2.76
Root4		-3819.107908	2.85
Root5		-3819.024224	5.13

Table S6.5 The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of 5 at the CAS(10,10)/CASPT2 level of theory.

5	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0			
Root1	-2863.285807	-2864.263655	0
Root2		-2864.18866	2.04
Root3		-2864.14264	3.29

Root4		-2864.133306	3.55
Root5		-2864.153581	2.99
$T_{\perp}$			
Root1	-2863.197527	-2864.196484	1.83
Root2		-2864.163916	2.71
Root3		-2864.147048	3.17
Root4		-2864.144365	3.24
Root5		-2864.129196	3.66
$T_{\Sigma\Sigma}$-min			
Root1	-2863.216485	-2864.197728	1.79
Root2		-2864.138805	3.40
Root3		-2864.133679	3.54
Root4		-2864.111329	4.14
Root5		-2864.143079	3.28

Table S6.6 The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of 6 at the CAS(10,10)/CASPT2 level of theory.

6	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0			
Root1	-3340.780592	-3341.970059	0
Root2		-3341.88396	2.34
Root3		-3341.890881	2.15
Root4		-3341.875443	2.57
Root5		-3341.881587	2.41
$T_{\perp}$			
Root1	-3340.700417	-3341.899833	1.91
Root2		-3341.892731	2.10
Root3		-3341.88733	2.25
Root4		-3341.889454	2.19
Root5		-3341.884748	2.32
$T_{\Sigma\Sigma}$-min			
Root1	-3340.702182	-3341.898561	1.94
Root2		-3341.888732	2.21
Root3		-3341.882188	2.39
Root4		-3341.873615	2.62
Root5		-3341.807078	4.43

Table S6.7 The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of 7 at the CAS(10,10)/CASPT2 level of theory.

7	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0			
Root1	-4281.649315	-4278.362589	0

Root2		-4278.296717	1.79
Root3		-4278.28857	2.01
Root4		-4278.27046	2.51
Root5		-4278.262638	2.72
$T_{\perp}$			
Root1	-4281.575983	-4278.302551	1.63
Root2		-4278.294067	1.86
Root3		-4278.289225	2.00
Root4		-4278.272462	2.46
Root5		-4278.236012	3.44
$T_{\Sigma\Pi}$-min			
Root1	-4281.576479	-4278.30645	1.53
Root2		-4278.295294	1.83
Root3		-4278.287454	2.04
Root4		-4278.274258	2.40
Root5		-4278.238171	3.38

Section 7. Cartesian Coordinates

Cluster **1** S_0-min

79	3.799354850	-0.000625662	-0.004176394
79	1.121471850	0.297375224	1.354061073
15	4.649261588	2.331393650	-0.515030579
15	0.805551323	0.827108411	3.769844640
6	3.459546871	3.753151368	-0.818253043
6	1.994618216	3.314434372	-0.735033570
6	-0.954721717	0.972106586	4.419794849
79	1.117758264	-0.297186657	-1.354231839
15	4.649103210	-2.332949394	0.506410319
79	-1.121104601	-1.355272915	0.296864642
79	-1.121791690	1.354265992	-0.296913882
6	0.961983272	4.423519505	-0.960113546
6	-1.987369207	0.728225446	3.314580589
15	0.792288654	-0.827867188	-3.770495984
6	3.459446406	-3.749130817	0.834810618
79	-3.797080192	0.001066345	0.001145108
15	-0.798562410	-3.771560858	0.828544016
15	-0.798620424	3.772201167	-0.825082832
6	-3.452347022	0.825348743	3.750138461

6	-0.968710390	-0.971589755	-4.418838070
6	1.994599192	-3.318230981	0.717523931
15	-4.642463861	0.513261677	2.330721685
15	-4.651928170	-0.512489232	-2.322893608
6	0.962063628	-4.417542538	0.986463456
6	-1.999709949	-0.728210422	-3.312170409
6	-3.465435100	-0.824538430	-3.745208899
1	5.479828061	-2.868080374	-0.473277753
1	5.515507996	-2.423432004	1.591368711
1	-5.499886736	-1.612756912	-2.401034434
1	-5.502410806	0.450916956	-2.856027727
1	-5.490486114	1.613283803	2.412224792
1	-5.491167165	-0.450310614	2.866481407
1	5.506837532	2.867552049	0.440554363
1	1.396845212	2.003829334	4.220621888
1	-1.374131322	-4.666092853	-0.069455906
1	-1.392941498	4.677630981	0.049287368
1	-1.381120446	4.215732751	-2.009028522
1	5.489179417	2.410454583	-1.621598649
1	-1.399240904	-4.235041270	1.995488506
1	1.379518912	0.054161090	-4.673180966
1	1.381002884	-2.006301566	-4.220358374
1	1.392805780	-0.057711526	4.669720501
1	-1.071269026	1.960105265	4.850458329
1	-1.072488843	0.258503790	5.227310980
1	-1.816542621	1.434766578	2.514443839
1	-1.817410249	-0.249863675	2.886617337
1	-3.669887974	1.806679619	4.156484997
1	-3.671140912	0.106381931	4.531586511
1	-3.685461137	-0.105005409	-4.525790978
1	-3.684199176	-1.805557938	-4.151647206
1	-1.828832847	0.249492902	-2.883725901
1	-1.827921577	-1.435174119	-2.512593598
1	-1.086986168	-0.257119880	-5.225516503
1	-1.086122159	-1.959122853	-4.850324484

1	1.078818788	-4.824846388	1.984330650
1	1.079927377	-5.241644418	0.292125109
1	1.819344165	-2.499628072	1.400939954
1	1.829237535	-2.916683124	-0.272951509
1	3.669434713	-4.135361749	1.825904010
1	3.685611582	-4.544389627	0.133531931
1	3.682405419	4.171812547	-1.793172719
1	3.672839677	4.526054884	-0.088450898
1	1.826820587	2.527723124	-1.457713894
1	1.821782978	2.867256958	0.233637952
1	1.080008690	5.218406748	-0.232477387
1	1.078586399	4.871482387	-1.940370711

Cluster **1** STC($S_{\Sigma\Sigma}/T_{\Sigma\Pi}$)

79	-3.806257512	-0.001394112	0.000034931
79	-1.099545311	0.161185025	1.376925039
15	-4.687506471	-2.382079337	0.252499951
15	-0.800421304	0.451472063	3.868879231
6	-3.516242312	-3.878101394	0.426077968
6	-2.039642220	-3.444554295	0.369072963
6	0.985630833	0.520605149	4.534634281
79	-1.098698294	-0.160595997	-1.373110173
15	-4.690740686	2.375605033	-0.273661088
79	1.130751804	1.429718222	-0.159691078
79	1.133008935	-1.428142993	0.160275946
6	-1.042067089	-4.608656341	0.518903971
6	1.998600915	0.388161186	3.381187193
15	-0.799125259	-0.450215007	-3.866009365
6	-3.521299665	3.876280198	-0.414513096
79	3.812550075	-0.000783764	-0.002461066
15	0.744680657	3.949638400	-0.435328098
15	0.749434018	-3.947454205	0.442409966
6	3.466511028	0.431982253	3.839519229
6	0.985980878	-0.520391933	-4.534395416
6	-2.044379536	3.440800232	-0.388850095

15	4.648493127	0.261861293	2.356565114
15	4.650645148	-0.258751747	-2.360342249
6	-1.047697509	4.611221369	-0.486629107
6	2.000094952	-0.387574878	-3.382454329
6	3.467598064	-0.429604813	-3.842349364
1	-5.536223751	2.515297005	-1.388690173
1	-5.581600753	2.757090018	0.745313992
1	5.508831155	0.780834374	-2.755555277
1	5.519305266	-1.351298789	-2.518919261
1	5.508780248	-0.775776747	2.752457145
1	5.515366123	1.355958417	2.513790126
1	-5.567525537	-2.534115384	1.338662036
1	-1.417741305	-0.534703045	4.660024291
1	1.333836681	4.495335467	-1.589857190
1	1.360186088	-4.509650220	1.577690056
1	1.351203098	-4.736095240	-0.554696107
1	-5.543473532	-2.760054400	-0.797373127
1	1.365691669	4.751667487	0.539000975
1	-1.411914254	-1.594034124	-4.409822408
1	-1.416010351	0.538095039	-4.654966425
1	-1.410796399	1.597215119	4.411155274
1	1.102282877	-0.286945908	5.253730340
1	1.108365802	1.465850227	5.058214322
1	1.823328943	-0.549123897	2.854743155
1	1.830717866	1.189145238	2.661891137
1	3.681405083	-0.378076798	4.531564281
1	3.689732999	1.371949339	4.337388267
1	3.691484126	-1.369094877	-4.340790400
1	3.680994045	0.381052261	-4.534179416
1	1.833645974	-1.189136946	-2.663456274
1	1.824477898	0.549293187	-2.855294287
1	1.107894934	-1.465948998	-5.057652457
1	1.101840850	0.286795135	-5.254047470
1	-1.176836554	5.303566422	0.341631958
1	-1.182141545	5.161734404	-1.414417173

1	-1.852615496	2.887554203	0.529700976
1	-1.862063490	2.749177188	-1.211504162
1	-3.743558713	4.544911242	0.413137965
1	-3.757813711	4.394858228	-1.340004167
1	-3.748183299	-4.574780461	-0.375363097
1	-3.741847306	-4.364428446	1.371591038
1	-1.853308226	-2.936167250	-0.576862109
1	-1.852634240	-2.714426230	1.155738024
1	-1.175828080	-5.116625383	1.470753044
1	-1.170639068	-5.337968394	-0.277069090

Cluster **1** CI($T_{\Sigma\Pi}/T_{\Sigma\Sigma}$)

79	3.749892145	0.010789051	0.005045033
79	1.063025937	-0.057866993	-1.367933074
15	4.730200253	-2.363833120	0.073357037
15	0.806370918	-0.158931005	-3.911523266
6	3.625365186	-3.925668253	0.113323043
6	2.132542069	-3.542198245	0.121523042
6	-0.982205220	-0.172982031	-4.596718319
79	1.055481933	0.054265015	1.374153139
15	4.709897183	2.393518244	-0.066530974
79	-1.161467257	1.523592096	-0.056860974
79	-1.150339210	-1.533703139	0.054312038
6	1.194048012	-4.765689351	0.145799043
6	-1.986919296	-0.120669040	-3.429012232
15	0.791588912	0.154351018	3.917821332
6	3.593953076	3.946026347	-0.142941978
79	-3.760618435	-0.003673056	-0.001832969
15	-0.659071250	4.151250307	-0.151763982
15	-0.626690138	-4.162163333	0.140074043
6	-3.457799411	-0.133103059	-3.885690266
6	-0.998797223	0.164710996	4.598508388
6	2.103996968	3.553264299	-0.109238975
15	-4.618900498	-0.077765073	-2.369039150
15	-4.629101501	0.082159938	2.360806216

6	1.156739878	4.767876377	-0.183023979
6	-2.000553299	0.119166980	3.428056294
6	-3.472646415	0.133069959	3.880913330
1	5.565436240	2.647724279	1.022087113
1	5.611878264	2.577449270	-1.131501055
1	-5.499598599	1.167202014	2.569342232
1	-5.500628537	-0.985569152	2.641915235
1	-5.491571563	-1.160557167	-2.580910163
1	-5.486524588	0.992139999	-2.653455173
1	5.616833321	-2.607735127	-0.992449044
1	1.425214982	-1.265201079	-4.524534314
1	-1.243265306	4.868608357	0.910265102
1	-1.224248174	-4.899602395	-0.900690037
1	-1.204020172	-4.814421390	1.246875126
1	5.604632346	-2.542768120	1.161821123
1	-1.261154307	4.814981349	-1.238353065
1	1.427555977	-0.889548051	4.616883386
1	1.404972946	1.263665116	4.530844383
1	1.440863954	0.888184086	-4.607137322
1	-1.103113215	-1.081273101	-5.182190365
1	-1.091063240	0.687998037	-5.251925369
1	-1.816178272	-0.971738104	-2.771498181
1	-1.808459296	0.779695035	-2.842562188
1	-3.686867415	-1.036762135	-4.444366311
1	-3.682792438	0.729948002	-4.506712313
1	-3.700915420	-0.730791109	4.499586380
1	-3.701765442	1.036069029	4.440624377
1	-1.822386272	-0.779191088	2.838630252
1	-1.826432298	0.972458045	2.774239245
1	-1.109539220	-0.699831070	5.248665436
1	-1.121266243	1.069741064	5.188687434
1	1.308433881	5.326953411	-1.102521055
1	1.306786881	5.434597430	0.661911085
1	1.891009962	2.884854245	-0.943074039
1	1.899820959	2.996306255	0.805632097

1	3.836722088	4.477033396	-1.059576051
1	3.850947092	4.577546402	0.703387088
1	3.888535213	-4.490874297	1.003499111
1	3.870429213	-4.521314297	-0.762062028
1	1.927022046	-2.917191203	0.990934110
1	1.912371043	-2.942222202	-0.761225023
1	1.346189032	-5.392821426	-0.728599024
1	1.353346033	-5.364212410	1.038736114

Cluster **1** $T_{\Sigma\Sigma}$-min

79	-3.809609443	-0.000932437	-0.001819385
79	-1.105845267	0.422837742	1.314018331
15	-4.678023911	-2.306262202	0.738569998
15	-0.810954492	1.184934738	3.679592371
6	-3.452644859	-3.665571184	1.183454540
6	-1.991992428	-3.214083283	1.026065203
6	0.964271593	1.381313887	4.296944705
79	-1.104064120	-0.422192791	-1.313795823
15	-4.678252108	2.304142387	-0.742000575
79	1.105497021	1.314544418	-0.422570253
79	1.105663066	-1.314707701	0.423011386
6	-0.963970772	-4.295801952	1.391057977
6	1.991530070	1.032201722	3.209344326
15	-0.810010938	-1.183598619	-3.679959530
6	-3.453243073	3.670349168	-1.166186835
79	3.809002672	0.000256656	-0.000498157
15	0.810282215	3.681917840	-1.182097073
15	0.810776535	-3.680464878	1.185540673
6	3.452310298	1.177169808	3.664390040
6	0.964772121	-1.382320387	-4.297944167
6	-1.992563415	3.209323837	-1.039773577
15	4.676587756	0.739348095	2.302257426
15	4.677091787	-0.740382166	-2.302923099
6	-0.964689887	4.303412642	-1.366265308
6	1.992256810	-1.032641823	-3.210614733

6	3.453076954	-1.178830314	-3.665144583
1	-5.506088323	2.283169061	-1.863913674
1	-5.537424665	2.940394424	0.153172715
1	5.520482474	0.170339823	-2.938108278
1	5.520932592	-1.850295049	-2.288117873
1	5.519854234	-0.171575499	2.937317719
1	5.520314248	1.849353579	2.288111878
1	-5.529538178	-2.297705321	1.842759210
1	-1.395173208	0.391650882	4.665407114
1	1.378864182	4.001218481	-2.413989381
1	1.399295308	-4.023733555	2.401384205
1	1.386674352	-4.661537960	0.380237524
1	-5.513549405	-2.943289796	-0.178217817
1	1.405046782	4.673655235	-0.404226843
1	-1.392645688	-2.404736675	-4.014465777
1	-1.393012858	-0.387244169	-4.664055748
1	-1.390746307	2.408032618	4.011811895
1	1.081964408	0.739752159	5.162781355
1	1.083223140	2.406292197	4.629128716
1	1.824943251	0.014368131	2.879381838
1	1.825947323	1.668753660	2.349078976
1	3.655345702	0.531301049	4.511002898
1	3.656505351	2.194718570	3.977447019
1	3.656842162	-2.196788802	-3.977152050
1	3.656734438	-0.533885048	-4.512304838
1	1.826160708	-1.668145911	-2.349679243
1	1.826155411	-0.014430267	-2.881534626
1	1.082921864	-2.407802177	-4.628831684
1	1.082916117	-0.741929739	-5.164563979
1	-1.082053378	5.155560557	-0.706501338
1	-1.083928184	4.657278279	-2.383900495
1	-1.821910336	2.853278837	-0.031796943
1	-1.831506409	2.364464815	-1.698345109
1	-3.649391542	4.505744564	-0.503751034
1	-3.663848464	4.002350481	-2.176355305

1	-3.659889107	-4.518741051	0.547675391
1	-3.651921920	-3.967792106	2.205259056
1	-1.828478563	-2.901840268	0.001878341
1	-1.823877044	-2.342730151	1.646237872
1	-1.082585503	-4.612532242	2.420994894
1	-1.081559106	-5.171267215	0.762732909

Cluster **2** S_0-min

79	4.085531213	-0.232345844	0.039070077
79	1.231518026	-1.440060017	-0.188599941
79	1.448635964	1.343335201	0.128142086
79	-0.944576188	0.243842045	-1.367346031
79	-0.828028169	-0.078575974	1.424542186
79	-3.036509301	-1.353054133	-0.014514930
79	-3.079888389	1.474867080	0.356216099
15	4.722267257	-0.140742818	-2.331127103
15	4.406928243	-0.360940842	2.478029264
15	0.968286080	-3.879563214	-0.345197951
15	1.751374919	3.778412396	0.184631085
15	-0.548912168	0.627905086	-3.765855216
15	-0.507993146	-0.059647965	3.864141370
15	-4.121210327	-3.398121325	-0.776010987
15	-3.654785499	3.842997246	0.233155094
6	3.636370147	0.806385222	-3.501963195
1	3.569312112	1.812680299	-3.102122162
1	4.138865183	0.879227242	-4.459314271
6	2.236271060	0.185291133	-3.653787206
1	1.922091045	-0.214305906	-2.698674136
1	2.281137083	-0.648076926	-4.347521260
6	1.178488947	1.199497183	-4.133857246
1	1.286752950	1.405363199	-5.192248326
1	1.302523929	2.140231258	-3.608155204
6	2.965918125	-0.138641867	3.629939352
1	3.360355146	0.118473160	4.607098427
1	2.416531057	0.724432181	3.268139327

6	2.064846091	-1.377122988	3.736734359
1	1.783917076	-1.723022025	2.748126285
1	2.630061157	-2.179960034	4.199619399
6	0.793770985	-1.179504009	4.579839428
1	1.040711998	-0.833755978	5.577509525
1	0.313874976	-2.145301099	4.700930433
6	-0.749518035	-4.539289316	-0.111311937
1	-0.679067001	-5.539086388	0.301612098
1	-1.220248091	-3.915671280	0.641168126
6	-1.583538099	-4.576791340	-1.401198034
1	-1.187335044	-5.350413373	-2.049033084
1	-1.493769116	-3.642719268	-1.950270077
6	-3.068203202	-4.890474410	-1.126532012
1	-3.163910189	-5.569071476	-0.286375947
1	-3.504814222	-5.396148469	-1.978817079
6	0.338134779	4.750436431	-0.521475968
1	0.594168772	5.802544531	-0.552734971
1	0.220577784	4.416923401	-1.547465044
6	-0.945755311	4.490553372	0.281015096
1	-0.932584327	5.077423419	1.193738168
1	-0.955791279	3.448761296	0.583584121
6	-2.239517420	4.780953358	-0.504053966
1	-2.146152402	4.430012335	-1.526528046
1	-2.459508467	5.840725410	-0.542915966
1	4.838754304	-1.394644909	-2.920131153
1	5.987212362	0.377429259	-2.572205124
1	-1.354778256	1.538416134	-4.438850268
1	-4.772147599	4.226770245	-0.495942965
1	-4.776009382	-3.173557323	-1.980639078
1	-0.703282147	-0.488354002	-4.581474278
1	1.413014128	-4.506871251	-1.504723043
1	5.309061293	0.593587254	2.930180298
1	5.017924322	-1.523778917	2.931400300
1	1.912380912	4.319439442	1.456537184
1	2.875721990	4.298289471	-0.447788963

1	-0.166978156	1.201436141	4.343162405
1	-1.609537223	-0.327905016	4.666505432
1	-3.890499535	4.482073291	1.444855184
1	1.706416157	-4.578032245	0.604121120
1	-5.165861394	-3.888458393	-0.004186924

Cluster **2** STC($S_{\Sigma\Sigma}/T_{\Sigma\Pi}$)

79	4.119157919	-0.246665518	0.042007921
79	1.199244612	-1.487777142	-0.182547974
79	1.460285505	1.347213493	0.113503244
79	-0.950736033	0.236888466	-1.363321596
79	-0.831076590	-0.062351426	1.423655025
79	-3.041718918	-1.354563188	0.000782627
79	-3.062189156	1.528028152	0.355041738
15	4.741644701	-0.184328401	-2.341500491
15	4.422345869	-0.345814279	2.490971235
15	0.917175242	-3.954971448	-0.328039210
15	1.799203911	3.810107377	0.144717113
15	-0.560583882	0.593955556	-3.781676456
15	-0.499926405	-0.023941175	3.875655970
15	-4.188695339	-3.398676469	-0.755514688
15	-3.642105629	3.922831678	0.214978273
6	3.642579687	0.767277197	-3.532276679
1	3.578576582	1.781423799	-3.141012600
1	4.142077342	0.825466485	-4.497809133
6	2.239058247	0.140232034	-3.669424664
1	1.923567127	-0.245653313	-2.701010988
1	2.278162954	-0.706624938	-4.356611233
6	1.189764735	1.160464789	-4.161502989
1	1.295474690	1.350986929	-5.228622165
1	1.317010321	2.110647112	-3.644737518
6	2.961677933	-0.116174271	3.653271158
1	3.355003587	0.146550374	4.634281485
1	2.402778798	0.744067229	3.285361099
6	2.070679751	-1.369925987	3.756327681

1	1.784112432	-1.715570680	2.761373607
1	2.641873076	-2.175503049	4.220509708
6	0.800950016	-1.171087159	4.609269276
1	1.057456146	-0.816614006	5.606320051
1	0.312291027	-2.134959997	4.731490896
6	-0.830413065	-4.596118497	-0.086409374
1	-0.771768864	-5.598164741	0.336482048
1	-1.294607808	-3.952301151	0.659043701
6	-1.656894756	-4.631764263	-1.386421886
1	-1.268107723	-5.421877278	-2.030321376
1	-1.553292947	-3.694893245	-1.938480072
6	-3.149321587	-4.928517153	-1.108447200
1	-3.251505942	-5.598985654	-0.258696559
1	-3.593451914	-5.430403541	-1.963815454
6	0.370980076	4.797199051	-0.572689864
1	0.636949858	5.851877080	-0.612039162
1	0.243626988	4.450363921	-1.597530371
6	-0.911185707	4.557655174	0.247579603
1	-0.887262238	5.160858611	1.157318634
1	-0.929322405	3.514877818	0.559575026
6	-2.201923403	4.851759163	-0.544526517
1	-2.114055691	4.488028482	-1.566769769
1	-2.414494650	5.917420233	-0.588870506
1	4.857534434	-1.460970255	-2.908166376
1	6.023937792	0.329931145	-2.572382890
1	-1.376338181	1.514671877	-4.454512586
1	-4.771834686	4.305585719	-0.519017459
1	-4.852638973	-3.157795901	-1.965578059
1	-0.737153401	-0.539221425	-4.589960673
1	1.365565503	-4.595770399	-1.493067586
1	5.339563281	0.622664872	2.921058732
1	5.044925819	-1.517432711	2.943407633
1	1.978568503	4.355067152	1.424915219
1	2.937539275	4.313320021	-0.503363342
1	-0.146632597	1.248870669	4.346545727

1	-1.624496191	-0.276804665	4.673310466
1	-3.877096560	4.568624802	1.436411838
1	1.658405424	-4.653237217	0.636953351
1	-5.246949055	-3.863017138	0.035091310

Cluster **2** CI($T_{\Sigma\Pi}/T_{\Sigma\Sigma}$)

79	4.231344236	-0.253847919	0.046891005
79	1.170918029	-1.464816077	-0.188878013
79	1.387370982	1.435812153	0.107924012
79	-0.967031173	0.232303007	-1.345017101
79	-0.824843157	-0.049685008	1.411740113
79	-2.968213293	-1.434188161	0.020009007
79	-3.033161360	1.499633062	0.369613031
15	4.733935276	-0.210005907	-2.374501180
15	4.447773254	-0.318728918	2.512153195
15	0.960131062	-4.000555274	-0.339307023
15	1.714036955	3.969721354	0.095817008
15	-0.621706156	0.573977040	-3.791588290
15	-0.508366131	-0.013847002	3.886390299
15	-4.187005342	-3.482617342	-0.743577052
15	-3.775393466	3.889964230	0.220799022
6	3.602027168	0.763007144	-3.554278271
1	3.563107144	1.776074225	-3.154412241
1	4.085502203	0.803639157	-4.530250344
6	2.189947069	0.140641067	-3.654170277
1	1.881043057	-0.210967967	-2.669250204
1	2.215106092	-0.723331995	-4.322185332
6	1.147220969	1.160148124	-4.170961318
1	1.253973975	1.330304142	-5.242826399
1	1.252458957	2.116799200	-3.659153280
6	2.941225132	-0.085284936	3.650414283
1	3.313994155	0.196691098	4.635472361
1	2.385075073	0.758619122	3.240474252
6	2.071240092	-1.356894050	3.741337291
1	1.775818076	-1.686814083	2.742179216

1	2.659602154	-2.161119101	4.189828323
6	0.806952992	-1.187454061	4.615392360
1	1.067485007	-0.837497028	5.613973435
1	0.309840974	-2.150496148	4.712293366
6	-0.819785058	-4.618743359	-0.074995005
1	-0.773671034	-5.606357411	0.384872031
1	-1.263572108	-3.925419317	0.639087051
6	-1.629062123	-4.677999384	-1.386132104
1	-1.214204072	-5.462755427	-2.022961151
1	-1.545163134	-3.734623307	-1.932292148
6	-3.119556230	-5.015231440	-1.128048084
1	-3.221984222	-5.695315493	-0.285133021
1	-3.551718255	-5.493098504	-2.004019150
6	0.214260820	4.876738393	-0.649952050
1	0.432805817	5.942004485	-0.716877054
1	0.106107817	4.479842359	-1.659627125
6	-1.044345271	4.592813340	0.195332018
1	-1.027291280	5.200044392	1.103947087
1	-1.022886245	3.546766262	0.499621043
6	-2.350110374	4.849516335	-0.588112042
1	-2.278066363	4.457291306	-1.601873123
1	-2.591473420	5.909730388	-0.642603048
1	4.829004308	-1.499157003	-2.928205223
1	6.024835383	0.296256163	-2.612348197
1	-1.466724238	1.487333093	-4.450446340
1	-4.936006562	4.221004235	-0.500699036
1	-4.866662403	-3.223910338	-1.947229150
1	-0.793366144	-0.569248048	-4.596019350
1	1.400791113	-4.658845316	-1.503737112
1	5.359573325	0.667264174	2.932984228
1	5.076776325	-1.490724998	2.971674229
1	1.867210956	4.548402399	1.370235106
1	2.835475028	4.506852417	-0.566621043
1	-0.174110131	1.258577103	4.385531342
1	-1.657592217	-0.293740047	4.650301363

1	-4.007520495	4.542904279	1.444926114
1	1.706369135	-4.686992312	0.638305049
1	-5.235473412	-3.953825404	0.065031010

Cluster **2** $T_{\Sigma\Sigma}$-min

79	4.065640313	-0.265274020	0.024133001
79	1.220002092	-1.433476110	-0.240425021
79	1.454519114	1.327696103	0.142812012
79	-0.945420072	0.285154024	-1.375687108
79	-0.850326063	-0.099575008	1.400693109
79	-3.090571239	-1.333312102	-0.073255007
79	-3.141677241	1.484984112	0.366977030
15	4.750131365	-0.122590011	-2.360403184
15	4.402716341	-0.450170033	2.487848190
15	0.927677071	-3.879164299	-0.452256034
15	1.769696136	3.781855292	0.271872019
15	-0.554414040	0.725760056	-3.801905294
15	-0.551501041	-0.139229011	3.871279299
15	-4.172036320	-3.368573258	-0.905498067
15	-3.673953283	3.884064301	0.301661026
6	3.647683279	0.863137068	-3.502127271
1	3.604644277	1.862057145	-3.079746236
1	4.130607319	0.939415074	-4.469946342
6	2.234183170	0.262967019	-3.630673278
1	1.921730146	-0.116088010	-2.663712205
1	2.259226171	-0.581449044	-4.313639331
6	1.197050093	1.292396101	-4.125600318
1	1.322247101	1.502355118	-5.182264397
1	1.309234103	2.228682172	-3.587931277
6	2.934782224	-0.235256017	3.627701281
1	3.312704253	-0.009553999	4.619490356
1	2.405391182	0.643053050	3.269837250
6	2.018735157	-1.468456113	3.676902282
1	1.729446131	-1.762152137	2.671762208

1	2.577981199	-2.299712179	4.097608313
6	0.754002056	-1.303145099	4.542810350
1	1.009399078	-0.989756076	5.549384442
1	0.260764022	-2.266320173	4.624138358
6	-0.808613063	-4.533120347	-0.236984019
1	-0.750699058	-5.542024433	0.158231014
1	-1.270498096	-3.908701301	0.520357039
6	-1.623762127	-4.531457350	-1.539839118
1	-1.214981095	-5.283861407	-2.207120167
1	-1.531614116	-3.576485274	-2.053017159
6	-3.112327240	-4.861852372	-1.299942100
1	-3.223071248	-5.565906414	-0.482672036
1	-3.538348274	-5.326575419	-2.181079170
6	0.346098029	4.780758366	-0.411890033
1	0.598879047	5.835004475	-0.398665031
1	0.240629019	4.477502342	-1.448882111
6	-0.939738074	4.482838343	0.376606029
1	-0.924467071	5.020289384	1.320746100
1	-0.955000075	3.424213261	0.615528049
6	-2.224776171	4.827626373	-0.399091029
1	-2.142614164	4.509754346	-1.433717108
1	-2.428403185	5.892371469	-0.393438030
1	4.847289372	-1.365020106	-2.983334232
1	6.018208443	0.395520030	-2.611908202
1	-1.350227105	1.657790129	-4.464568345
1	-4.782141366	4.292519328	-0.431940035
1	-4.825962370	-3.097506239	-2.103486164
1	-0.707614055	-0.377216027	-4.640149357
1	1.372078103	-4.474137346	-1.630757125
1	5.305529405	0.489993039	2.979625228
1	4.993675383	-1.630723125	2.933978224
1	1.929031146	4.281105329	1.563169120
1	2.901568224	4.308390332	-0.344534024
1	-0.203094016	1.107026083	4.388207338
1	-1.666210127	-0.427186034	4.654204357

1	-3.920918300	4.482222344	1.534153119
1	1.665344129	-4.598686356	0.484404038
1	-5.219438400	-3.864619296	-0.137528013

Cluster **3** S_0-min

79	4.972048301	0.030638003	0.261276001
79	2.168183083	-1.049337074	0.899371052
79	2.135813083	1.535260126	-0.072188027
79	-0.311840105	0.478527049	1.263384080
79	0.312399937	-0.439268024	-1.266208114
79	-2.143359251	-1.486388099	0.063518987
79	-2.163128250	1.088934101	-0.913053088
79	-4.924905460	-0.116526984	-0.293148040
6	4.082755228	-0.755821055	-3.240273266
1	3.361812177	0.055465010	-3.152783264
1	4.463632257	-0.775349061	-4.262042348
6	3.461211175	-2.113202160	-2.856510236
1	4.213551233	-2.897669219	-2.973782249
1	3.164006155	-2.096961154	-1.807110158
6	2.245783085	-2.518759185	-3.720108303
1	1.893903053	-3.496732262	-3.397185279
1	2.517831103	-2.588393195	-4.772695388
6	0.639004955	-4.313143323	1.725667112
1	0.744956961	-5.287491398	2.201853150
1	-0.132096104	-3.754370275	2.254530152
6	0.306628931	-4.471074331	0.227791999
1	1.035108985	-5.149543388	-0.226671037
1	0.398692940	-3.506812257	-0.276154042
6	-1.094945179	-5.054238375	-0.061126021
1	-1.215060191	-6.034770474	0.398322013
1	-1.221653189	-5.166953383	-1.136316108
6	1.019450006	5.090226402	0.171905997
1	1.155695018	5.174294405	1.248442078
1	1.119721019	6.084073495	-0.262647041
6	-0.373191100	4.489073358	-0.124890027

1	-0.433625110	3.497747282	0.327919007
1	-1.112731159	5.123674410	0.372904011
6	-0.717476131	4.400586355	-1.625737143
1	0.059059928	3.883280309	-2.187351185
1	-0.845255137	5.395395450	-2.051379175
6	-2.317129254	2.408653206	3.792561273
1	-2.598714279	2.407892206	4.844869354
1	-2.000570227	3.415599282	3.527825251
6	-3.509891349	2.001222173	2.898718202
1	-3.200435326	2.028715175	1.853031123
1	-4.286825407	2.758213234	3.033462213
6	-4.090188396	0.612171070	3.231188229
1	-4.479212426	0.584252070	4.249695310
1	-3.340860341	-0.170736991	3.123274224
17	4.757436281	0.296650024	2.650080186
17	-4.662430444	-0.316726003	-2.684895223
15	5.499849324	-0.293526026	-2.074152181
15	2.237635078	-3.317426250	1.971941135
15	2.460076116	4.002330314	-0.433529054
15	-0.775142142	1.312277116	3.568663256
15	0.744302972	-1.358654094	-3.546679291
15	-2.527488286	-3.930993284	0.494169020
15	-2.294417252	3.381913277	-1.920328165
15	-5.484442487	0.141811036	2.039844138
1	-6.497590589	1.089725110	2.267854158
1	-3.352263333	4.234747343	-1.550461140
1	-6.054352572	-1.014097050	2.599928180
1	-2.432251262	3.385478280	-3.320852276
1	-2.779656306	-4.306846315	1.827170119
1	-3.649529377	-4.490313327	-0.146408030
1	2.421541095	-3.305222248	3.366808240
1	3.265235160	-4.196730319	1.577785101
1	0.245939942	2.054834168	4.192944304
1	-0.936356155	0.277980037	4.509776328
1	-0.298473114	-2.089356147	-4.148011340

1	0.946092990	-0.366475020	-4.524568367
1	3.586145204	4.549322353	0.211042999
1	2.693392132	4.424175346	-1.756156152
1	6.080736397	0.846014062	-2.656171223
1	6.495991416	-1.260199100	-2.296170194

Cluster **3** STC($S_{\Sigma\Sigma}/T_{\Sigma\Pi}$)

79	4.972048301	0.030638003	0.261276001
79	2.168183083	-1.049337074	0.899371052
79	2.135813083	1.535260126	-0.072188027
79	-0.311840105	0.478527049	1.263384080
79	0.312399937	-0.439268024	-1.266208114
79	-2.143359251	-1.486388099	0.063518987
79	-2.163128250	1.088934101	-0.913053088
79	-4.924905460	-0.116526984	-0.293148040
6	4.082755228	-0.755821055	-3.240273266
1	3.361812177	0.055465010	-3.152783264
1	4.463632257	-0.775349061	-4.262042348
6	3.461211175	-2.113202160	-2.856510236
1	4.213551233	-2.897669219	-2.973782249
1	3.164006155	-2.096961154	-1.807110158
6	2.245783085	-2.518759185	-3.720108303
1	1.893903053	-3.496732262	-3.397185279
1	2.517831103	-2.588393195	-4.772695388
6	0.639004955	-4.313143323	1.725667112
1	0.744956961	-5.287491398	2.201853150
1	-0.132096104	-3.754370275	2.254530152
6	0.306628931	-4.471074331	0.227791999
1	1.035108985	-5.149543388	-0.226671037
1	0.398692940	-3.506812257	-0.276154042
6	-1.094945179	-5.054238375	-0.061126021
1	-1.215060191	-6.034770474	0.398322013
1	-1.221653189	-5.166953383	-1.136316108
6	1.019450006	5.090226402	0.171905997

1	1.155695018	5.174294405	1.248442078
1	1.119721019	6.084073495	-0.262647041
6	-0.373191100	4.489073358	-0.124890027
1	-0.433625110	3.497747282	0.327919007
1	-1.112731159	5.123674410	0.372904011
6	-0.717476131	4.400586355	-1.625737143
1	0.059059928	3.883280309	-2.187351185
1	-0.845255137	5.395395450	-2.051379175
6	-2.317129254	2.408653206	3.792561273
1	-2.598714279	2.407892206	4.844869354
1	-2.000570227	3.415599282	3.527825251
6	-3.509891349	2.001222173	2.898718202
1	-3.200435326	2.028715175	1.853031123
1	-4.286825407	2.758213234	3.033462213
6	-4.090188396	0.612171070	3.231188229
1	-4.479212426	0.584252070	4.249695310
1	-3.340860341	-0.170736991	3.123274224
17	4.757436281	0.296650024	2.650080186
17	-4.662430444	-0.316726003	-2.684895223
15	5.499849324	-0.293526026	-2.074152181
15	2.237635078	-3.317426250	1.971941135
15	2.460076116	4.002330314	-0.433529054
15	-0.775142142	1.312277116	3.568663256
15	0.744302972	-1.358654094	-3.546679291
15	-2.527488286	-3.930993284	0.494169020
15	-2.294417252	3.381913277	-1.920328165
15	-5.484442487	0.141811036	2.039844138
1	-6.497590589	1.089725110	2.267854158
1	-3.352263333	4.234747343	-1.550461140
1	-6.054352572	-1.014097050	2.599928180
1	-2.432251262	3.385478280	-3.320852276
1	-2.779656306	-4.306846315	1.827170119
1	-3.649529377	-4.490313327	-0.146408030
1	2.421541095	-3.305222248	3.366808240
1	3.265235160	-4.196730319	1.577785101

1	0.245939942	2.054834168	4.192944304
1	-0.936356155	0.277980037	4.509776328
1	-0.298473114	-2.089356147	-4.148011340
1	0.946092990	-0.366475020	-4.524568367
1	3.586145204	4.549322353	0.211042999
1	2.693392132	4.424175346	-1.756156152
1	6.080736397	0.846014062	-2.656171223
1	6.495991416	-1.260199100	-2.296170194

Cluster **3** CI($T_{\Sigma\Pi}/T_{\Sigma\Sigma}$)

79	4.916933458	0.027919799	0.277065079
79	2.149726211	-1.082795195	0.886451126
79	2.112617292	1.568638008	-0.078084950
79	-0.301102929	0.462025000	1.267329155
79	0.307995092	-0.420010089	-1.273445042
79	-2.115467128	-1.510331094	0.060472064
79	-2.146555048	1.125633109	-0.902419012
79	-4.876557298	-0.125928903	-0.294840963
6	4.054858369	-0.719342232	-3.239896190
1	3.323653338	0.082861855	-3.148105183
1	4.440840397	-0.723004244	-4.259878267
6	3.446560279	-2.087838318	-2.874250163
1	4.205285310	-2.864692401	-3.000763171
1	3.146894257	-2.089786304	-1.824937081
6	2.233662174	-2.490341308	-3.740898232
1	1.880148112	-3.467937373	-3.418957203
1	2.506090194	-2.558329324	-4.793548311
6	0.651820993	-4.379656405	1.667370184
1	0.761125967	-5.357570495	2.135072224
1	-0.123141049	-3.828372337	2.197940228
6	0.328172959	-4.524684405	0.167041069
1	1.051609996	-5.208656482	-0.287143963
1	0.434051003	-3.558463333	-0.327202967
6	-1.077887166	-5.089089401	-0.136440950

1	-1.207677205	-6.077182496	0.303867081
1	-1.202076176	-5.180954408	-1.213942034
6	1.000329318	5.131832318	0.235439076
1	1.135936333	5.198691318	1.313289157
1	1.106845359	6.131610387	-0.183835954
6	-0.395534805	4.544261317	-0.072572945
1	-0.464789840	3.551074241	0.371252089
1	-1.132582842	5.181708390	0.425186088
6	-0.731832836	4.465816320	-1.575056065
1	0.047848207	3.954011256	-2.136812106
1	-0.862164811	5.462832422	-1.994312098
6	-2.298499019	2.377373210	3.815717349
1	-2.579570043	2.371562220	4.868205431
1	-1.981538965	3.385084276	3.554725331
6	-3.489545124	1.972848218	2.919930283
1	-3.178820102	2.015240211	1.874618205
1	-4.271441161	2.723353302	3.062107292
6	-4.057954215	0.575387128	3.238950307
1	-4.449573245	0.535361135	4.256009384
1	-3.300373180	-0.199732957	3.127944298
17	4.656927445	0.260939826	2.656590262
17	-4.582930283	-0.302339923	-2.676530148
15	5.460162512	-0.254294238	-2.061790103
15	2.242002145	-3.377338375	1.930325207
15	2.438596399	4.049085188	-0.387333970
15	-0.760324935	1.278761077	3.579448333
15	0.736030096	-1.326747171	-3.559018218
15	-2.507263237	-3.969493273	0.436723094
15	-2.300458985	3.441232289	-1.884865087
15	-5.444443354	0.102024135	2.040642217
1	-6.468463404	1.037601241	2.274046235
1	-3.362453043	4.292506389	-1.519310057
1	-6.003012431	-1.066709937	2.586231258
1	-2.426334997	3.454340296	-3.286231193
1	-2.756105272	-4.363945291	1.764384191

1	-3.629405343	-4.524754277	-0.209360956
1	2.417782159	-3.379542383	3.326173312
1	3.273703197	-4.252307477	1.533976178
1	0.263859164	2.015302104	4.206373383
1	-0.922596985	0.239756003	4.513805404
1	-0.308722007	-2.053535192	-4.162195264
1	0.939529144	-0.331605102	-4.532197293
1	3.566065499	4.594242193	0.258344079
1	2.664720425	4.486767215	-1.705357073
1	6.024782571	0.904414831	-2.622451144
1	6.473122545	-1.202181345	-2.291675119

Cluster **3** $T_{\Sigma\Sigma}$-min

79	4.959489427	0.049704979	0.275303982
79	2.187935217	-1.050049125	0.904307032
79	2.152995199	1.546686079	-0.074497044
79	-0.321356987	0.475349980	1.269143058
79	0.325984071	-0.442804086	-1.271701138
79	-2.149996113	-1.504456184	0.067811964
79	-2.181053129	1.087698011	-0.918747110
79	-4.931847335	-0.120513096	-0.308772062
6	4.153044366	-0.780094087	-3.234263288
1	3.444816306	0.044140971	-3.163946284
1	4.546984400	-0.814757086	-4.250258365
6	3.504004327	-2.124017198	-2.847445261
1	4.245707387	-2.920292250	-2.950537265
1	3.198938305	-2.095726197	-1.800021178
6	2.291449235	-2.522408232	-3.720531327
1	1.934242214	-3.500165310	-3.402720299
1	2.569910256	-2.590032237	-4.771646405
6	0.661712120	-4.317743381	1.745976094
1	0.773723137	-5.287714457	2.230177134
1	-0.110621943	-3.757941343	2.271494135
6	0.327796095	-4.490467396	0.250306983

1	1.056838156	-5.171958447	-0.199029056
1	0.416473100	-3.531016322	-0.262851060
6	-1.073716006	-5.077254453	-0.030072042
1	-1.195010009	-6.050922551	0.443988994
1	-1.200785015	-5.205635462	-1.103517125
6	1.011023086	5.106315343	0.142295974
1	1.146002099	5.205395353	1.217779056
1	1.114299090	6.093955404	-0.306100061
6	-0.382155013	4.503966290	-0.147744050
1	-0.442090015	3.517526213	0.315274984
1	-1.121360077	5.143985334	0.343882988
6	-0.726587039	4.400263276	-1.647347165
1	0.050552022	3.879870243	-2.204910207
1	-0.857797056	5.391080380	-2.081739201
6	-2.359535153	2.407076114	3.791745255
1	-2.647000174	2.405358114	4.842533333
1	-2.036948136	3.413287196	3.531343232
6	-3.550914244	2.009026077	2.889721183
1	-3.234876219	2.025531079	1.845272104
1	-4.316151304	2.779554132	3.012848193
6	-4.161484283	0.633305965	3.224421211
1	-4.560307310	0.618936961	4.239044289
1	-3.427123217	-0.165319090	3.128339201
17	4.699388400	0.359220005	2.674203165
17	-4.630566311	-0.355067112	-2.712769249
15	5.559885488	-0.326302043	-2.050805198
15	2.255610240	-3.310463294	1.982211116
15	2.453046208	4.007147267	-0.444608073
15	-0.815073026	1.308705037	3.577749235
15	0.787149115	-1.361708155	-3.556460313
15	-2.507298126	-3.943721373	0.508123001
15	-2.301287158	3.373947191	-1.932143190
15	-5.551660380	0.179698920	2.020568116
1	-6.550158475	1.146516989	2.241557133
1	-3.362689241	4.222375248	-1.563450160

1	-6.142641404	-0.961345169	2.590572162
1	-2.443560166	3.365004185	-3.332206298
1	-2.765836143	-4.297314404	1.845526103
1	-3.629100209	-4.504970425	-0.130169052
1	2.442325251	-3.284663294	3.376558220
1	3.289573323	-4.183163357	1.591065085
1	0.204955048	2.050610101	4.204626283
1	-0.979067035	0.271591957	4.515160310
1	-0.254682961	-2.091781218	-4.160405359
1	0.991487121	-0.366159075	-4.530295388
1	3.577674288	4.556637318	0.199246977
1	2.694754224	4.406471303	-1.772214173
1	6.160879498	0.797373047	-2.644213241
1	6.544407536	-1.309994113	-2.257384211

Cluster **4** S_0-min

79	-0.005956631	-0.014830843	-0.715332291
79	0.035256551	0.160570539	1.964844159
79	2.546333791	0.504389137	0.312514128
79	-1.792289692	1.888262156	0.307366403
79	-0.754696479	-2.407673799	0.511578285
79	1.843345544	-2.132261309	-0.836288425
79	0.859957110	2.654070516	-0.816825783
79	-2.737224519	-0.662524735	-0.862339932
15	0.005171109	-0.008905566	-3.204006087
15	0.071236963	0.293133774	4.347172653
15	4.759904936	1.104842746	1.175464572
15	-3.444914966	3.428712030	1.245440458
15	-1.365191851	-4.494840983	1.623517620
15	3.404471621	-3.867467593	-1.496790681
15	1.567977198	4.869174053	-1.537641048
15	-4.976519060	-1.282194490	-1.593890235
1	-3.072285874	4.753402580	1.449145160
1	-4.626899642	3.608659341	0.535060419

1	-3.951952582	3.116449134	2.502466997
1	1.254103894	0.718468385	4.939223415
1	-0.842660169	1.150205455	4.947966486
1	-0.167284226	-0.878117939	5.055850572
1	2.680565262	4.945387769	-2.367699570
1	0.653282326	5.623377603	-2.263531314
1	1.922515180	5.776995377	-0.546160785
1	5.840714139	0.982853928	0.308720308
1	4.936610665	2.412714419	1.614928401
1	5.241753037	0.405150760	2.277096355
1	4.640690721	-3.877305638	-0.861098096
1	3.010588712	-5.188084944	-1.313552989
1	3.797882430	-3.897855459	-2.829466670
1	0.919526709	-0.822634890	-3.865137705
1	-1.153305237	-0.390468546	-3.872882304
1	0.257083097	1.189440968	-3.863936224
1	-0.404139439	-5.102600228	2.424943715
1	-2.442953813	-4.471797436	2.502990941
1	-1.727437290	-5.564439640	0.811776813
1	-5.185569754	-2.613765318	-1.933693029
1	-6.017392293	-1.077918774	-0.695302365
1	-5.478803891	-0.645057716	-2.722524187

Cluster **4** $T_{\Sigma\Sigma}$-min

79	0.016843733	0.007168955	-0.753550757
79	-0.093678576	-0.146295707	1.966961667
79	-2.579200609	0.397495115	0.322739791
79	0.997194139	-2.448747690	0.301751991
79	1.626308792	1.950359466	0.518830177
79	-0.963354979	2.735999431	-0.791812432
79	-1.794741868	-2.170727140	-0.824179018
79	2.813242842	-0.350453221	-0.880687449
15	-0.017230112	0.031653081	-3.289827185
15	-0.184146655	-0.227558838	4.369902457

15	-4.855256982	0.691892644	1.183097842
15	1.961673450	-4.424326204	1.310815967
15	2.906737269	3.698356631	1.668255112
15	-1.776862418	4.906005980	-1.507244604
15	-3.246851394	-3.983477036	-1.557425557
15	5.116585292	-0.580542389	-1.597244515
1	1.117720068	-5.514643849	1.489635083
1	2.987388491	-5.009226463	0.580721277
1	2.554851597	-4.354556772	2.568653640
1	-1.441305082	-0.198592051	4.961649227
1	0.355806923	-1.360013666	4.966279279
1	0.462303993	0.773000720	5.086367287
1	-4.301329679	-3.608616530	-2.381801217
1	-2.719502733	-5.043335911	-2.286702472
1	-3.932826973	-4.673262829	-0.564410532
1	-5.817105213	1.187656593	0.309274188
1	-5.485370399	-0.469533755	1.614492492
1	-5.073013483	1.512887004	2.285188597
1	-2.924192218	5.338165195	-0.855121716
1	-0.930744108	5.988463602	-1.296736053
1	-2.136168537	5.104230803	-2.836240917
1	-0.577215483	1.123808294	-3.951414218
1	1.202895554	-0.031880331	-3.954032360
1	-0.690313309	-0.994968414	-3.942224664
1	2.267799372	4.620884230	2.491707273
1	3.896090092	3.242510759	2.532286130
1	3.650757000	4.556651166	0.866119035
1	5.774807653	0.598015224	-1.927197129
1	6.011034334	-1.126826404	-0.684205619
1	5.391440432	-1.350012883	-2.721493037

Cluster **5** S_0-min

79	2.329897571	-1.339401657	-0.150557934
79	0.021558163	-0.091783984	1.388370269

79	-0.023147144	-0.021120808	-1.333058531
79	2.183147559	1.446572036	-0.041243482
79	-2.245782757	-1.418620438	-0.031314185
79	-2.150146981	1.434945742	0.046606868
15	3.707194044	-3.469061991	-0.053919685
15	0.276279595	-0.274142486	3.893252183
15	-0.205393402	0.037723316	-3.845613133
15	3.306947255	3.694765205	0.274157070
15	-3.790699294	-3.407074083	0.209404613
15	-3.775621176	3.375351960	0.028357540
1	3.010896624	-4.673996634	0.159452646
1	4.457049885	-3.771231159	-1.205355091
1	4.689244866	-3.523445267	0.951998930
1	-0.680222497	-1.048495021	4.577491087
1	1.479578249	-0.831660262	4.364956221
1	0.223969974	0.932861362	4.615007320
1	-5.146207698	-3.105269074	0.433727104
1	-3.867319455	-4.289357425	-0.884414042
1	-3.510198410	-4.286083934	1.271748976
1	-4.557129289	3.537700408	1.186937113
1	-3.249882944	4.669127717	-0.149277753
1	-4.755845384	3.320994143	-0.978886421
1	-1.414754211	0.519707575	-4.380720851
1	0.740935775	0.810984105	-4.545548700
1	-0.085710146	-1.204709759	-4.495975147
1	3.171961288	4.279790429	1.546774536
1	4.701694316	3.723009623	0.090872974
1	2.884747510	4.739964166	-0.568804968

Cluster **5** $T_{\Sigma\Sigma}$-min

79	-2.209849648	-1.448800798	0.159439354
79	-0.049419890	-0.105586594	-1.346279924
79	0.027456536	-0.004264862	1.387212647
79	-2.050345158	1.563492934	0.025192827

79	2.139082213	-1.527447062	0.005490246
79	2.012777542	1.541442573	-0.097958318
15	-3.549738910	-3.501718127	0.059615590
15	-0.357758492	-0.333710265	-3.735680666
15	0.264221465	0.085195849	3.829955668
15	-3.121862379	3.736887455	-0.353246748
15	3.654750536	-3.426205963	-0.294769164
15	3.649210580	3.362000601	-0.054935139
1	-2.800191510	-4.655453962	-0.129617247
1	-4.312516338	-3.853812190	1.165869493
1	-4.483896888	-3.617999377	-0.962125362
1	0.568240553	-1.109151339	-4.422868675
1	-1.545812677	-0.907414086	-4.172393467
1	-0.339279173	0.828049971	-4.497122001
1	4.999101868	-3.206835894	-0.569432837
1	3.737355507	-4.310115074	0.773432730
1	3.306114949	-4.286308348	-1.328192201
1	4.414236985	3.553704299	-1.198633344
1	3.102190913	4.627070476	0.116394848
1	4.630883156	3.359974286	0.928476854
1	1.469269316	0.574787195	4.320891303
1	-0.635988099	0.864278562	4.547933146
1	0.175408891	-1.112637781	4.528986404
1	-2.927116102	4.271270718	-1.620643775
1	-4.495524553	3.885400912	-0.206186110
1	-2.651244905	4.770389069	0.446487472

Cluster **6** S_0-min

79	-0.027642643	0.046513828	1.405074808
15	-0.181507844	0.074023541	3.808032441
79	-0.005728487	0.043461433	-1.253211865
15	-0.009028907	0.033941185	-3.590582863
79	-2.382063525	1.224222545	-0.097590598
15	-4.554793352	2.549062890	-0.266108982

79	-1.952726576	-1.719384567	-0.042016748
15	-3.693124422	-3.451457957	0.345682805
79	1.088047475	-2.393412028	-0.093104048
15	2.120492799	-4.667023200	0.025899919
79	2.607884730	0.220548070	-0.068085236
15	5.090232228	0.442182097	0.083493592
79	0.697334538	2.576385439	-0.003678459
15	1.121898171	5.037244980	0.231536711
1	1.548451901	5.734341151	-0.897808391
1	0.118499291	5.907357452	0.656149070
1	2.128138489	5.421745355	1.116764241
1	-5.249301047	2.438019992	-1.469558770
1	-5.583570244	2.201117614	0.608650808
1	-4.607160696	3.934748151	-0.116429367
1	0.949378593	0.343122148	4.576733284
1	-1.055533459	0.993047876	4.384118206
1	-0.616860660	-1.075695763	4.464409703
1	-3.398876249	-4.786936871	0.073372743
1	-4.157108643	-3.596357472	1.652184115
1	-4.920379222	-3.364608202	-0.309921768
1	3.409461488	-4.860063197	-0.470695733
1	2.297170434	-5.218595103	1.294660133
1	1.492963354	-5.748973537	-0.590917237
1	0.818246534	-0.866421666	-4.260293269
1	-1.196515079	-0.237964272	-4.268291307
1	0.355126888	1.192499063	-4.275694185
1	5.783033713	0.715167203	-1.094715283
1	5.672432016	1.405880395	0.905053907
1	5.816537618	-0.669476965	0.509284360

Cluster **6** $T_{\Sigma\Sigma}$-min

79	-0.054683701	0.067584253	1.432832028
15	-0.260040949	0.153340099	3.828318774
79	-0.000628975	0.034914490	-1.267265347

15	0.008492252	0.004729770	-3.622508523
79	-2.426873000	1.206091324	-0.132494003
15	-4.605823650	2.491571661	-0.371635663
79	-1.983719842	-1.686843817	-0.013970375
15	-3.703071579	-3.352403713	0.412163861
79	1.115561369	-2.373836004	-0.103360154
15	2.114315025	-4.568768780	0.004580003
79	2.630464126	0.183235825	-0.057497987
15	5.080237377	0.394372843	0.111430129
79	0.755403952	2.555239188	-0.000582592
15	1.211385695	4.955503362	0.230465857
1	1.668593838	5.617601157	-0.905290751
1	0.231210828	5.853713643	0.650599895
1	2.228089133	5.282040693	1.122231341
1	-5.279982998	2.328154260	-1.580087287
1	-5.626515307	2.125549040	0.502816930
1	-4.700959427	3.879652328	-0.252139042
1	0.856627987	0.430466679	4.613028636
1	-1.146988560	1.085864793	4.358563548
1	-0.715674023	-0.991203371	4.476972953
1	-3.404682541	-4.690136995	0.171904013
1	-4.163617327	-3.461634205	1.723346125
1	-4.930044481	-3.282847528	-0.248637185
1	3.397819281	-4.756308023	-0.502695510
1	2.298124271	-5.088999912	1.283013799
1	1.485533737	-5.656364184	-0.597704136
1	0.842719484	-0.906134688	-4.265012737
1	-1.174636690	-0.257790538	-4.309098118
1	0.393186893	1.166649542	-4.287886270
1	5.780684748	0.637979796	-1.069233599
1	5.713608039	1.329716967	0.933821994
1	5.758100733	-0.745584005	0.534004547

Cluster **7** S_0-min

79	-1.144642939	0.636141185	-1.053637036
79	-1.158839045	-0.987744938	1.146729136
79	-3.128581057	1.168451354	1.081710127
79	-3.519243229	-1.076371793	-0.616653000
6	-0.252259668	3.825588373	2.707403254
1	-0.840199759	3.113800358	3.278353300
1	-0.027478598	4.653791424	3.370538305
6	-1.022866697	4.324172462	1.475855159
1	-0.518060600	5.199674497	1.078777126
1	-1.008547743	3.569462404	0.697470098
6	-2.482418784	4.717208587	1.757591180
1	-2.907211788	5.141753645	0.853800112
1	-2.541960739	5.484417668	2.521440240
6	0.315970979	-2.371312141	4.233592372
1	0.363375052	-1.351755062	4.602891399
1	0.176404930	-3.021724178	5.089279434
6	1.617011058	-2.724135251	3.454342312
1	1.535520079	-2.317957210	2.453665234
1	1.696406997	-3.802112334	3.349290304
6	2.895673194	-2.173669286	4.109930359
1	3.199048178	-2.775355354	4.958664429
1	2.726280244	-1.165092200	4.472766391
15	1.318249394	2.927228203	2.298469221
15	-1.178371141	-2.454424048	3.107430286
15	-3.586309958	3.297451545	2.224610216
15	4.270232308	-2.042481367	2.874098268
79	1.136546252	0.933284064	0.860990112
79	1.141426113	-1.296715108	-0.839342021
79	3.161998404	0.801845923	-1.334868058
79	3.534561328	-0.842627227	0.859948109
6	0.225085310	2.907048272	-3.635874233
1	0.817169304	2.079947174	-4.015779264
1	-0.020640670	3.533698335	-4.486188300
6	1.004110422	3.713840283	-2.586468154
1	0.500668444	4.663130392	-2.430371143

1	0.997393390	3.192847247	-1.635627080
6	2.460966552	4.012617213	-2.974774186
1	2.897195627	4.661672239	-2.222678127
1	2.514882591	4.544790251	-3.917918256
6	-0.330108139	-3.480984185	-3.422407216
1	-0.375480088	-2.597098114	-4.050338264
1	-0.191815185	-4.334121259	-4.076172269
6	-1.616293245	-3.611874114	-2.589109156
1	-1.535141199	-2.963455069	-1.725284089
1	-1.701484315	-4.626682182	-2.212608127
6	-2.891537320	-3.244778003	-3.370429215
1	-3.193752394	-4.044891046	-4.035773263
1	-2.714538251	-2.366040943	-3.982023259
15	-1.320459858	2.119113313	-2.982946186
15	1.161657988	-3.266142259	-2.339429132
15	3.546129540	2.507988030	-3.047871191
15	-4.281087400	-2.791413878	-2.226776128
1	-4.851938019	3.862547668	2.120069208
1	-3.477246955	3.244508536	3.611708322
1	-5.332901469	-2.509672788	-3.092038192
1	-4.703594512	-4.017687948	-1.721142086
1	-2.214179857	3.184120447	-2.892544180
1	-1.807209934	1.521135295	-4.142663274
1	1.253214918	-4.500997362	-1.700330085
1	2.212935063	-3.398505338	-3.241982206
1	4.822959675	3.055704994	-3.088671191
1	3.435446503	2.086018007	-4.369734289
1	2.194003530	3.952627230	1.948133196
1	1.798163417	2.655613153	3.577682321
1	-1.297178234	-3.823264147	2.873591268
1	-2.234198209	-2.287537969	3.999301351
1	4.697883256	-3.357348493	2.713786253
1	5.330352422	-1.526901391	3.611651325

Cluster **7** $T_{\Sigma\Pi}$-min

79	-1.147134883	0.563041307	-1.081032167
79	-1.146350621	-0.907270499	1.210374850
79	-3.068014138	1.257715190	1.032084716
79	-3.485362941	-1.123981182	-0.540179516
6	-0.203052714	4.022613678	2.426802101
1	-0.794104039	3.363215143	3.052739093
1	0.034877390	4.897013147	3.022299780
6	-0.976566286	4.434485704	1.164707298
1	-0.474297790	5.281862096	0.708068227
1	-0.965302997	3.627201457	0.443231450
6	-2.436980789	4.843123366	1.425992031
1	-2.870454268	5.196280476	0.496496268
1	-2.491619017	5.665304264	2.130423953
6	0.317259732	-2.072085489	4.360439624
1	0.359887145	-1.029615231	4.655732484
1	0.180610090	-2.661729939	5.259280213
6	1.601404372	-2.472085836	3.616264565
1	1.517033823	-2.142358445	2.588598876
1	1.686152183	-3.554005110	3.591178949
6	2.881592550	-1.870328398	4.225697518
1	3.190376381	-2.409467572	5.113222980
1	2.712249443	-0.838530993	4.513825889
15	1.354492310	3.076604690	2.089257371
15	-1.159708097	-2.237469657	3.251936713
15	-3.533769817	3.462513242	2.010966110
15	4.250012572	-1.836914617	2.978999397
79	1.137011150	0.987650380	0.794110013
79	1.125181187	-1.361342166	-0.760848540
79	3.111933183	0.701066550	-1.403928747
79	3.492931817	-0.799079136	0.904775444
6	0.199940569	2.685088611	-3.785641137
1	0.791446765	1.842712293	-4.130089472
1	-0.050752453	3.270277721	-4.663462218
6	0.986082888	3.543802488	-2.782712982

1	0.489349919	4.502640368	-2.676963359
1	0.980203623	3.075389885	-1.805574465
6	2.443932151	3.810891205	-3.193580512
1	2.892394507	4.490967099	-2.477562900
1	2.497148840	4.292615622	-4.163233245
6	-0.347448087	-3.704599144	-3.201686057
1	-0.387166623	-2.859180396	-3.880251642
1	-0.210440023	-4.595869926	-3.802205607
6	-1.635402476	-3.782679020	-2.363584761
1	-1.549581070	-3.092743956	-1.536276866
1	-1.730352993	-4.776764999	-1.937322385
6	-2.907521981	-3.441848887	-3.163392929
1	-3.222359557	-4.273929050	-3.781557148
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