Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary information:

Electronic and Optical Properties of $[Au(CH_3CSS)]_4$ Cluster. A Quantum Chemistry Study

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Tables.

Table S1. Cartesian coordinates (in Angstroms) for the optimized geometries of the systems studied in this work. Ground State (S_o).

MP2 (gas)

Au	-0.0649404	-2.1458380	-1.0284203
Au	-0.0374936	0.6167545	-1.3114784
Au	0.0087404	-0.5839635	1.2676846
Au	0.0254375	2.1787233	0.9850744
S	2.0646294	-2.2658367	-1.8882250
S	2.2351337	0.7854444	-1.6030317
S	-2.3171011	0.7060878	-1.5764043
S	-2.2115767	-2.8013993	-0.5265828
S	-2.2591370	-0.6172148	1.6297199
S	2.2868678	-0.8032677	1.4633426
S	2.1921294	2.2510852	1.7534390
S	-2.1241196	2.8873174	0.5745052
C	-2.9323452	-1.8481102	0.6769909
C	-4.3774634	-2.1545095	0.9548230
C	2.8493862	-0.7628845	-1.9215832
C	4.3235584	-0.8188432	-2.2076830
C	2.9461149	0.7318454	1.7532816
C	4.4318639	0.7589128	1.9765365
C	-2.9188114	1.9528050	-0.5969583
C	-4.3679312	2.2916996	-0.8090937
H	-4.4518453	-3.0328333	1.6049950
H	-4.8685558	-1.3192481	1.4594568
H	-4.9145132	-2.3747288	0.0290590
H	4.5627509	-1.6548506	-2.8693471
H	4.6756159	0.1065805	-2.6691942
H	4.8701123	-0.9668560	-1.2694473
H	4.9376235	0.9689390	1.0274889
H	4.7061099	1.5474193	2.6817966
H	4.7965644	-0.1968994	2.3594098
H	-4.4517102	3.2116057	-1.3975278
H	-4.8852654	1.4963509	-1.3502657
H	-4.8729142	2.4572206	0.1460021

SCS-MP2 (gas)

Au	-0.0702402	-2.2257229	-1.0680397
Au	-0.0348469	0.6455001	-1.3710559
Au	0.0108390	-0.6088745	1.3246979
Au	0.0257170	2.2624845	1.0227016
S	2.1166041	-2.3404387	-1.8187255
S	2.2526200	0.7119646	-1.7130534
S	-2.3296746	0.8353536	-1.5941408
S	-2.2728298	-2.7865584	-0.6296774
S	-2.2760836	-0.7458193	1.6470806
S	2.3088700	-0.7270087	1.5665450
S	2.2442106	2.3273568	1.6809000
S	-2.1800087	2.8747047	0.6788156
C	-2.9523313	-1.9044497	0.6326140
C	-4.4021412	-2.2183165	0.9114311
C	2.8654168	-0.8375366	-1.9394272
C	4.3444560	-0.8967930	-2.2340982
C	2.9645605	0.8081442	1.7681587
C	4.4551850	0.8356760	2.0031229
C	-2.9343686	2.0082122	-0.5518307
C	-4.3884435	2.3535211	-0.7633599
H	-4.4636386	-3.0897710	1.5731590
H	-4.8987419	-1.3813300	1.4076917
H	-4.9373665	-2.4567689	-0.0108152
H	4.5767740	-1.7317680	-2.8997667
H	4.6974614	0.0298089	-2.6921586
H	4.8918659	-1.0522327	-1.2971856
H	4.9661689	1.0370123	1.0546766
H	4.7237483	1.6318587	2.7023851
H	4.8155118	-0.1169803	2.3972980
H	-4.4608788	3.2647376	-1.3678096
H	-4.9126336	1.5537311	-1.2914575

PBE(gas)

Au	-0.0874916	-2.2769043	-1.1201182
Au	-0.0371742	0.7082141	-1.5033558
Au	0.0153418	-0.6600871	1.4217854
Au	0.0322896	2.3242983	1.0403869
S	2.1338659	-2.3897913	-1.8252222
S	2.2776503	0.6907327	-1.8081872
S	-2.3562867	0.9258307	-1.6414332
S	-2.3182042	-2.8072250	-0.6886848
S	-2.2999559	-0.8236669	1.6723615
S	2.3402982	-0.7021312	1.6342643
S	2.2800150	2.3805075	1.6645374
S	-2.2037231	2.9080463	0.7155838
C	-2.9939756	-1.9432946	0.6049369
C	-4.4430926	-2.2280446	0.8608222
C	2.9003358	-0.8807883	-1.9368685
C	4.3846474	-0.9481526	-2.1306310
C	3.0089283	0.8509805	1.7520510
C	4.4983521	0.8795367	1.9165480
C	-2.9686980	2.0539823	-0.5349310
C	-4.4277521	2.3564906	-0.6985256
H	-4.5396429	-3.1174292	1.5063412
H	-4.9376628	-1.3951590	1.3797155
H	-4.9885805	-2.4400284	-0.0695135

H	4.6825923	-1.8377228	-2.7036587
H	4.7775810	-0.0543763	-2.6347711
H	4.8767650	-1.0188901	-1.1453809
H	4.9731093	1.0854173	0.9419864
H	4.8142723	1.6808126	2.6005776
H	4.8933124	-0.0754806	2.2885890
H	-4.5553131	3.3207402	-1.2187301
H	-4.9409587	1.5907336	-1.2958185
H	-4.9339294	2.4443566	0.2737062

TPSS (gas)

Au	-0.0741369	-2.2594819	-1.0902099
Au	-0.0336424	0.6812206	-1.4437733
Au	0.0200173	-0.6500446	1.3962396
Au	0.0234754	2.2904466	1.0441132
S	2.1581729	-2.3812252	-1.7817488
S	2.2881875	0.6965248	-1.7464280
S	-2.3603656	0.8744367	-1.6069397
S	-2.3188134	-2.7819674	-0.6874361
S	-2.3031345	-0.7792544	1.6534403
S	2.3511158	-0.7170158	1.6013532
S	2.2833176	2.3628540	1.6468668
S	-2.2226042	2.8713838	0.7342809
C	-3.0050771	-1.8940140	0.5854728
C	-4.4692788	-2.1463964	0.8168536
C	2.9227580	-0.8695916	-1.8857130
C	4.4119788	-0.9312233	-2.0817888
C	3.0217072	0.8361113	1.7149833
C	4.5187471	0.8677922	1.8488666
C	-2.9869684	2.0024626	-0.5075777
C	-4.4553700	2.2862191	-0.6674067
H	-4.5931384	-3.0214644	1.4704528
H	-4.9498053	-1.2950780	1.3099560
H	-4.9930743	-2.3572950	-0.1213671
H	4.7011838	-1.7945600	-2.6908170
H	4.7997098	-0.0202859	-2.5486858
H	4.8984077	-1.0434825	-1.1022776
H	4.9646788	1.0464828	0.8599825
H	4.8444411	1.6829706	2.5045321
H	4.9139949	-0.0773970	2.2338514
H	-4.5931046	3.2421796	-1.1918233
H	-4.9547383	1.5091985	-1.2544885
H	-4.9517265	2.3710022	0.3055993

MP2 (CS_2)

Au	-0.0681708	-2.1766471	-1.0494302
Au	-0.0319646	0.6326935	-1.3322083
Au	0.0097778	-0.5935222	1.2883119
Au	0.0259292	2.2160545	1.0063499
S	2.0933032	-2.2981294	-1.8144235
S	2.2366438	0.7406715	-1.6505657
S	-2.3084706	0.7750982	-1.5691777
S	-2.2458408	-2.7564657	-0.6107986
S	-2.2567702	-0.6867792	1.6246608
S	2.2870226	-0.7527570	1.5081392

S	2.2200661	2.2882144	1.6789458
S	-2.1549686	2.8448759	0.6608581
C	-2.9379773	-1.8548263	0.6283626
C	-4.3875449	-2.1472653	0.8951732
C	2.8543665	-0.8006189	-1.8998039
C	4.3306264	-0.8582279	-2.1726467
C	2.9497800	0.7736848	1.7315679
C	4.4372152	0.7974941	1.9414948
C	-2.9201548	1.9576981	-0.5454480
C	-4.3734348	2.2812065	-0.7485775
H	-4.4676071	-2.9810393	1.6006347
H	-4.8886067	-1.2844618	1.3385939
H	-4.9087953	-2.4297773	-0.0213346
H	4.5714886	-1.6806773	-2.8495501
H	4.6952632	0.0744997	-2.6063273
H	4.8638750	-1.0340346	-1.2321140
H	4.9336616	0.9663307	0.9797863
H	4.7246786	1.6111501	2.6108428
H	4.7993878	-0.1450551	2.3555282
H	-4.4655381	3.1293262	-1.4352251
H	-4.9083639	1.4361373	-1.1863970
H	-4.8519620	2.5566571	0.1931412

SCS-MP2 (CS_2)

Au	-0.0692950	-2.2240273	-1.0685496
Au	-0.0325040	0.6487497	-1.3696384
Au	0.0105751	-0.6100354	1.3267371
Au	0.0259987	2.2629285	1.0259828
S	2.1201965	-2.3396644	-1.8100274
S	2.2548147	0.7110255	-1.7098616
S	-2.3273059	0.8394043	-1.5891824
S	-2.2749852	-2.7787259	-0.6396909
S	-2.2765504	-0.7493524	1.6440440
S	2.3084370	-0.7239199	1.5680523
S	2.2474346	2.3289714	1.6723310
S	-2.1834230	2.8659876	0.6925423
C	-2.9583834	-1.8986313	0.6227062
C	-4.4110162	-2.2005817	0.8926507
C	2.8727746	-0.8372250	-1.9276045
C	4.3524379	-0.8972012	-2.2110649
C	2.9701438	0.8098049	1.7582804
C	4.4615133	0.8359935	1.9785575
C	-2.9394518	2.0019428	-0.5393256
C	-4.3956743	2.3353745	-0.7453533
H	-4.4814212	-3.0406174	1.5931011
H	-4.9146179	-1.3426127	1.3445517
H	-4.9343847	-2.4792441	-0.0248544
H	4.5873039	-1.7234893	-2.8868346
H	4.7143979	0.0343933	-2.6513774
H	4.8906101	-1.0691717	-1.2716825
H	4.9631215	1.0010978	1.0179458
H	4.7428037	1.6535433	2.6472223
H	4.8212533	-0.1054584	2.3992891
H	-4.4780132	3.1916907	-1.4244410
H	-4.9331569	1.4966768	-1.1941993
H	-4.8767187	2.6038813	0.1980563

PBE(CS_2)

Au	-0.0865486	-2.2765098	-1.1178573
Au	-0.0371616	0.7080856	-1.5028229
Au	0.0154595	-0.6609238	1.4232097
Au	0.0316603	2.3232742	1.0400428
S	2.1354158	-2.3876207	-1.8245755
S	2.2779514	0.6895164	-1.8095743
S	-2.3571907	0.9262449	-1.6390859
S	-2.3182627	-2.8064278	-0.6865656
S	-2.3006234	-0.8248192	1.6713066
S	2.3407195	-0.7010308	1.6362866
S	2.2797436	2.3781474	1.6659860
S	-2.2046734	2.9078599	0.7134654
C	-3.0021958	-1.9441052	0.6071591
C	-4.4482612	-2.2255829	0.8595833
C	2.9094917	-0.8793996	-1.9366328
C	4.3895081	-0.9469015	-2.1322658
C	3.0171164	0.8496131	1.7526872
C	4.5024476	0.8780381	1.9169079
C	-2.9777325	2.0548237	-0.5363326
C	-4.4332867	2.3546701	-0.6980052
H	-4.5445682	-3.1153708	1.5059338
H	-4.9455077	-1.3945681	1.3792924
H	-4.9955428	-2.4401987	-0.0693968
H	4.6891381	-1.8362385	-2.7053730
H	4.7858261	-0.0531596	-2.6339562
H	4.8846302	-1.0191727	-1.1478053
H	4.9785033	1.0813843	0.9416413
H	4.8215904	1.6815350	2.5974641
H	4.9003636	-0.0756933	2.2892452
H	-4.5599834	3.3188670	-1.2202263
H	-4.9497489	1.5903472	-1.2945751
H	-4.9413629	2.4468241	0.2732021

TPSS (CS_2)

Au	-0.0712603	-2.2546467	-1.0856766
Au	-0.0364049	0.6831941	-1.4488346
Au	0.0154398	-0.6488874	1.4000846
Au	0.0287103	2.2886627	1.0373889
S	2.1613325	-2.3704810	-1.7827634
S	2.2848050	0.7042564	-1.7496904
S	-2.3643290	0.8662422	-1.6021587
S	-2.3152445	-2.7833360	-0.6779203
S	-2.3082673	-0.7759574	1.6536335
S	2.3465894	-0.7210923	1.6027392
S	2.2892508	2.3551883	1.6444922
S	-2.2178654	2.8720018	0.7261520
C	-3.0142402	-1.8926204	0.5895907
C	-4.4765027	-2.1407762	0.8134732
C	2.9306666	-0.8580988	-1.8859122
C	4.4166877	-0.9141582	-2.0792223
C	3.0305909	0.8269204	1.7140115
C	4.5241316	0.8523007	1.8477921
C	-2.9947785	1.9980388	-0.5078099
C	-4.4601379	2.2785814	-0.6632496
H	-4.6025172	-3.0144061	1.4694654

H	-4.9604765	-1.2896045	1.3035612
H	-4.9984269	-2.3551119	-0.1250556
H	4.7111820	-1.7688139	-2.6981461
H	4.8062359	0.0037370	-2.5305206
H	4.9016994	-1.0391191	-1.0999970
H	4.9722939	0.9996568	0.8541671
H	4.8578356	1.6834521	2.4789543
H	4.9155086	-0.0844908	2.2564432
H	-4.5967753	3.1982925	-1.2503147
H	-4.9734870	1.4697916	-1.1929366
H	-4.9453313	2.4327919	0.3066226

Wavelengths (λ) and oscillator strengths (f) for the UV/Vis spectra of the $Au(S_2CCH_3)]_4$ CC2, SCS-CC2, ADC(2) and TDDFT (PBE and TPSS). All spectra were calculated in the gas phase and with the COSMO solvation model (epsilon = 2.6, CS_2). Wavelengths (λ) are given in nm.

Table S2. Gas phase

CC2		**SCS-CC2**		**ADC(2)**	
λ\nm	***F***	**λ\nm**	***f***	**λ\nm**	***F***
579	$0.45E^{-5}$	580	$0.38E^{-5}$	618	$0.70E^{-6}$
546	0.00076	58	0.00093	576	0.00015
522	0.00027	525	0.00004	551	0.00014
468	0.03061	470	0.04212	494	0.00347
446	0.03988	449	0.02841	471	0.02197
431	0.00077	433	0.00045	444	0.00049
424	0.00005	421	0.00003	443	0.01623
414	0.08239	415	0.08022	442	0.00017
410	0.00022	411	0.00433	429	0.08373
400	0.05934	404	0.05211	419	0.05369
380	$0.45E^{-5}$	399	0.00001	409	0.00003

PBE λ\nm	*f*		TPSS λ\nm	*f*	
650	0.00002		646	$0.461E^{-5}$	
632	0.00048		623	0.000497	
604	0.00131		597	0.001145	
526	0.00001		525	$0.987\ E^{-5}$	
509	0.00898		504	0.012916	
504	0.00435		499	0.006059	
492	0.01253		483	0.000011	
489	0.00008		478	0.011299	
484	0.00461		467	0.000715	
481	0.00125		466	0.003433	
479	0.00043		464	0.000818	
467	0.02046		454	0.001695	
455	0.00029		445	0.001568	
454	0.00118		441	0.000586	
451	0.00207		440	0.000813	
443	0.00117		436	0.002595	
437	0.01775		432	0.014449	
436	0.02242		424	0.018933	
435	0.01222		424	0.018378	
427	0.00170		417	0.002393	
417	0.00170		408	0.002552	
415	0.00002		405	0.000011	
413	0.00016		403	0.000475	
400	0.00167		387	0.001584	
394	0.00012		384	$0.287E^{-5}$	

Table S3. CS_2 phase

CC2 λ\nm	*f*	SCS-CC2 λ\nm	*f*	ADC(2) λ\nm	*f*
568	$0.45E^{-5}$	576	$0.40E^{-5}$	618	$0.40E^{-5}$
537	0.000760	544	0.00083	575	0.00015
503	0.000274	513	0.00005	551	0.00019
453	0.000361	464	0.03612	494	0.00509
441	0.039884	446	0.03955	472	0.02924
419	0.000772	430	0.00055	445	0.00016
411	0.000051	420	0.00014	444	0.02525
410	0.082390	409	0.08291	443	0.00018
408	0.000219	405	0.00450	431	0.11637
400	0.059335	403	0.04833	422	0.06600
380	$0.20E^{-5}$	395	0.00002	411	0.00003

PBE			TPSS		
λ\nm	*f*		λ\nm	*f*	
634	0.00003		633	0.000010	
616	0.00059		610	0.000581	
589	0.00182		585	0.001579	
515	0.00002		516	0.000019	
500	0.01394		497	0.019034	
495	0.00445		490	0.008037	
485	0.01987		474	0.000037	
479	0.00032		472	0.017513	
477	0.00714		463	0.000935	
474	0.00197		460	0.005654	
473	0.00022		458	0.000727	
462	0.02805		449	0.024583	
449	0.00019		439	0.022841	
447	0.00173		435	0.000047	
445	0.04483		435	0.002744	
438	0.01471		431	0.000379	
432	0.02460		426	0.019369	
430	0.02955		420	0.025336	
427	0.01435		419	0.026465	
421	0.00276		411	0.003888	
412	0.02277		403	0.002953	
409	0.00004		400	0.000014	
408	0.00031		398	0.000919	
398	0.00232		386	0.002155	
391	0.00017		379	0.000001	

Table S4. Cartesian coordinates (in Angstroms) for the optimized geometries of the systems studied in this work at first triplet excited state (T_1) in the ethanol phase.

MP2

Au	-0.168190	-2.289460	0.003963
Au	0.023368	-0.018209	1.463335
Au	-0.027089	-0.013625	-1.454017
Au	0.175928	2.272730	-0.019998
S	-2.332573	-2.578332	0.722489
S	-2.221416	0.290084	1.850869
S	2.292210	-0.251944	1.749702
S	1.926812	-2.867641	-0.745007
S	2.243956	-0.015171	-1.809875
S	-2.302835	0.067577	-1.768129
S	-1.942513	2.880441	-0.673587
S	2.340115	2.583346	0.689997
C	2.840720	-1.546609	-1.430061
C	4.263675	-1.839586	-1.791110
C	-3.025085	-1.216408	1.437527
C	-4.502119	-1.242380	1.679783
C	-2.828701	1.637380	-1.444291
C	-4.281154	1.933378	-1.653472
C	3.023481	1.236265	1.439590
C	4.477135	1.303699	1.790780
H	4.315495	-2.402700	-2.730368
H	4.827131	-0.908846	-1.926125
H	4.742368	-2.445763	-1.013041
H	-4.840742	-2.263524	1.890939
H	-4.767022	-0.589643	2.519872
H	-5.044889	-0.894438	0.793033
H	-4.837639	1.817390	-0.715997
H	-4.419925	2.968186	-1.987991
H	-4.711309	1.250425	-2.395449
H	4.622064	1.847075	2.731910
H	4.891164	0.296260	1.915822
H	5.038129	1.833940	1.012243

SCS-MP2

Au	-0.058887	-2.326663	-0.017163
Au	0.020064	-0.030839	1.456178
Au	-0.023543	0.005701	-1.433710
Au	0.066075	2.333505	-0.012065
S	-2.211945	-2.718646	0.700092
S	-2.250393	0.121082	1.810737
S	2.301080	-0.149710	1.750465
S	2.069857	-2.791489	-0.762918
S	2.253920	0.063114	-1.770806
S	-2.306021	0.000154	-1.740354
S	-2.082492	2.828214	-0.677413
S	2.243695	2.675519	0.654841
C	2.902809	-1.456760	-1.421343
C	4.343951	-1.683421	-1.786948
C	-2.962731	-1.382052	1.409345
C	-4.444226	-1.479746	1.649265

C	-2.915496	1.534240	-1.382137
C	-4.389616	1.747983	-1.590022
C	2.977328	1.368084	1.446837
C	4.431810	1.482085	1.812101
H	4.433663	-2.222073	-2.740795
H	4.881163	-0.731366	-1.901024
H	4.857863	-2.288982	-1.027205
H	-4.746065	-2.514233	1.865480
H	-4.755902	-0.839655	2.486618
H	-5.013532	-1.163753	0.763794
H	-4.951909	1.581812	-0.660381
H	-4.602789	2.779226	-1.904847
H	-4.789756	1.059325	-2.347424
H	4.564288	2.026699	2.757545
H	4.889791	0.491250	1.940618
H	4.993927	2.032825	1.044814

PBE

Au	-0.1681680	-1.9450166	-1.2064992
Au	0.1073954	0.8662539	-1.5772256
Au	0.1472297	-0.8278679	1.5419541
Au	-0.0784617	1.9889727	1.1811011
S	2.0914030	-2.3573422	-1.6386149
S	2.4375361	0.7010136	-1.8336383
S	-2.1684621	1.2434116	-1.8636972
S	-2.4791897	-1.9607004	-1.0555250
S	-2.1233961	-1.1545889	1.9200702
S	2.4899381	-0.7175618	1.6898810
S	2.2068197	2.3485104	1.5141523
S	-2.3926901	2.0544149	1.1224852
C	-3.0341541	-1.5100035	0.5077783
C	-4.5152447	-1.5616578	0.7053726
C	2.9631010	-0.9100465	-1.8225007
C	4.4443324	-1.0898316	-1.9483362
C	3.0523353	0.8804985	1.6526315
C	4.5417548	1.0251519	1.7044739
C	-3.0167366	1.6160110	-0.4178125
C	-4.5029543	1.6970591	-0.5581020
H	-4.8344771	-2.5482646	1.0869057
H	-4.8530832	-0.8098284	1.4347535
H	-5.0585054	-1.3921224	-0.2359899
H	4.6976425	-1.9999830	-2.5112891
H	4.9269216	-0.2295332	-2.4321393
H	4.8848150	-1.2007693	-0.9425276
H	4.9282366	1.1868543	0.6835021
H	4.8443748	1.8979148	2.3015916
H	5.0321184	0.1309577	2.1128830
H	-4.8180200	2.6915308	-0.9218054
H	-4.8825714	0.9561083	-1.2778361
H	-5.0129249	1.5319626	0.4023660

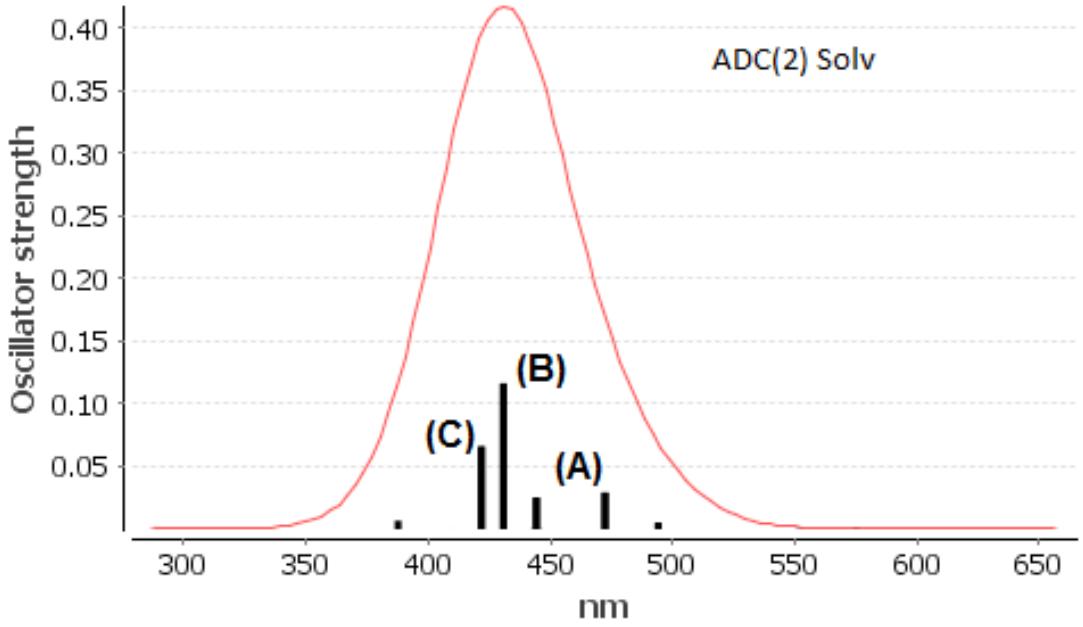
TPSS

Au	0.0788403	-2.2498667	-0.6373154
Au	-0.1739943	0.5015820	-1.5547727
Au	-0.1205913	-0.4584735	1.5144806

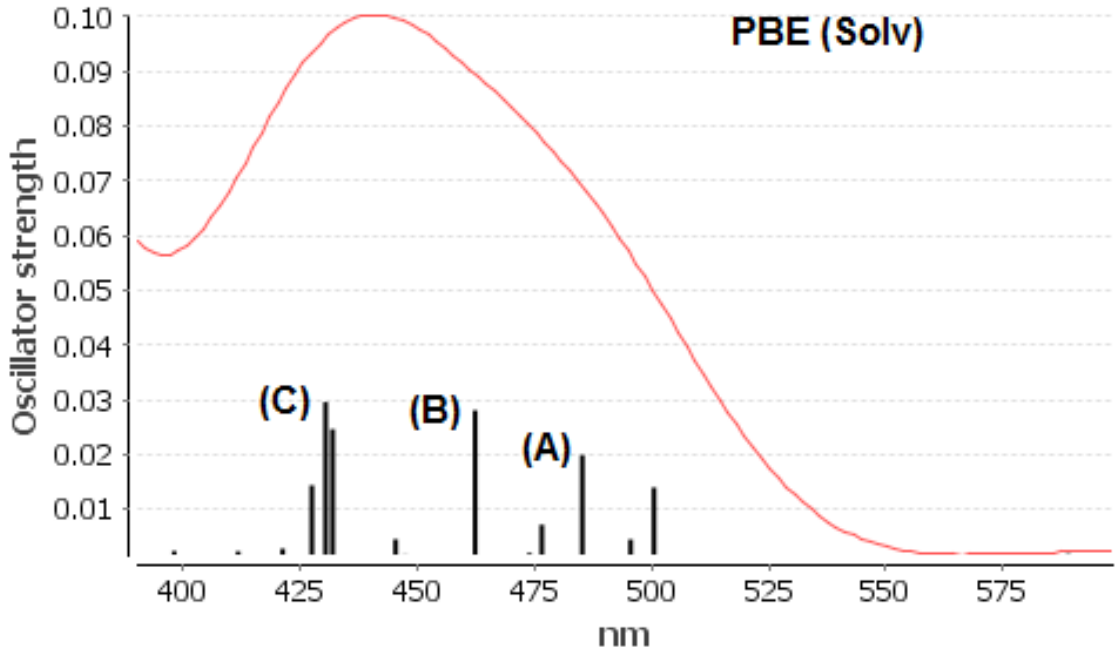
Au	0.1578556	2.2867665	0.5867532
S	2.4021911	-2.2212745	-0.6513556
S	2.0765657	0.4453064	-2.1795136
S	-2.5087204	0.8310990	-1.5794924
S	-2.2177199	-2.6991766	-0.7200218
S	-2.4585108	-0.7375012	1.6421254
S	2.1556253	-0.4536276	2.0418873
S	2.4779843	2.2049657	0.5008585
S	-2.1223488	2.7860406	0.7689971
C	-3.0431481	-1.8309727	0.4906995
C	-4.5191041	-2.0784608	0.5451670
C	2.9890609	-0.8067460	-1.4362448
C	4.4691960	-0.7488261	-1.6514357
C	3.0648588	0.7775814	1.2614737
C	4.5507334	0.6860301	1.4162564
C	-3.0184359	1.9360104	-0.4037141
C	-4.4898371	2.2144249	-0.3927943
H	-4.7139029	-3.0308727	1.0585495
H	-5.0414355	-1.2893576	1.0937731
H	-4.9456442	-2.1578891	-0.4608467
H	4.7429818	-1.2158446	-2.6098344
H	4.8303092	0.2855326	-1.6777128
H	5.0095778	-1.2859607	-0.8643983
H	5.0706648	1.2159302	0.6109192
H	4.8729707	1.1410604	2.3652377
H	4.8895768	-0.3560560	1.4227791
H	-4.6866942	3.1750462	-0.8898478
H	-5.0517176	1.4405849	-0.9238672
H	-4.8702723	2.2944528	0.6315733

Figures.

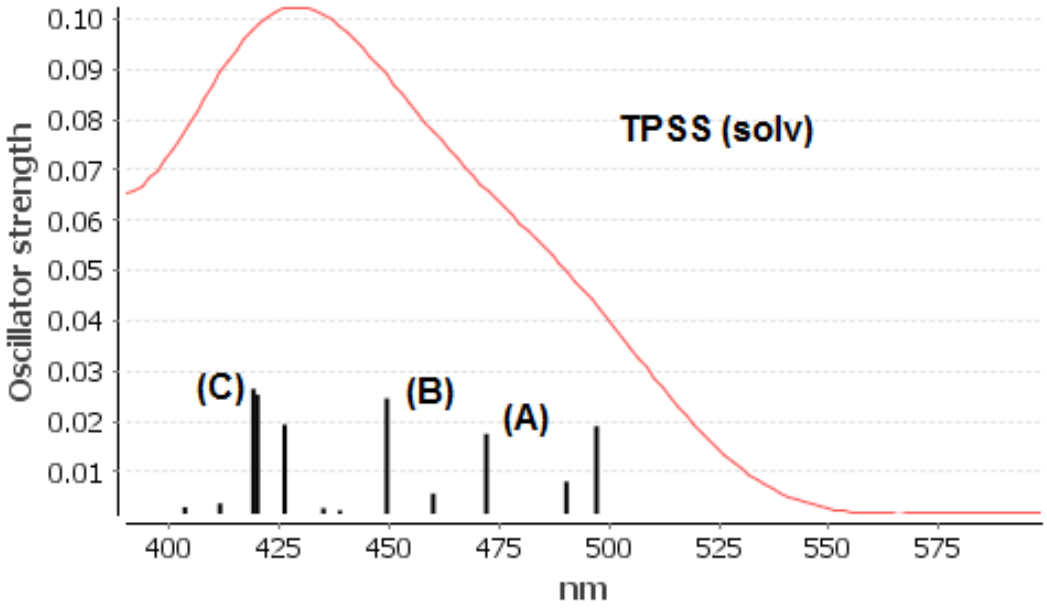
F1. Calculated ADC(2) electronic spectra of $[Au(S_2CCH_3)]_4$ in the CS_2 phase.



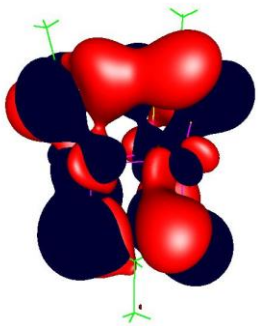
F2. Calculated PBE electronic spectra of $[Au(S_2CCH_3)]_4$ in the CS_2 phase.



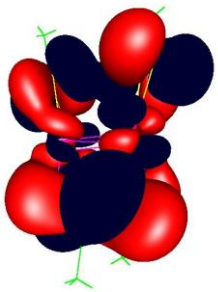
F3. Calculated TPSS electronic spectra of $[Au(S_2CCH_3)]_4$ in the CS_2 phase.



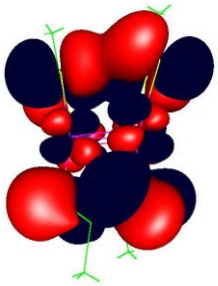
F4. Most important active molecular orbitals in the electronic transitions of $[Au(S_2CCH_3)]_4$ in the CS_2 phase at the ADC(2) level.



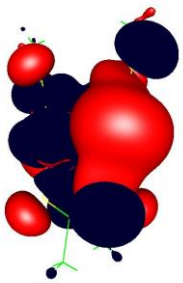
78a



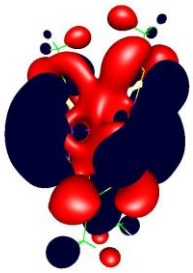
81a



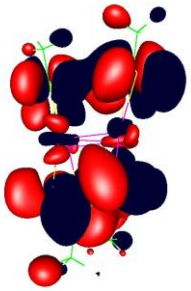
82a



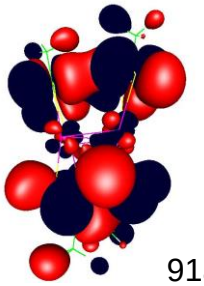
84a (HOMO)



85a (LUMO)

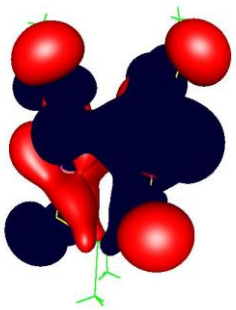


86a

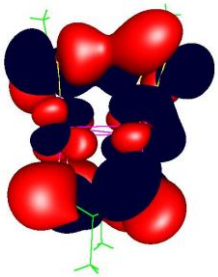


91a

F5. Most important active molecular orbitals in the electronic transitions of $[Au(S_2CCH_3)]_4$ in the CS_2 phase at the PBE level.



79a



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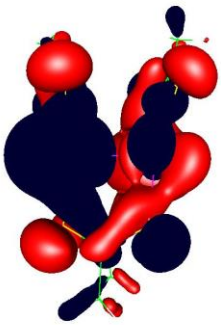
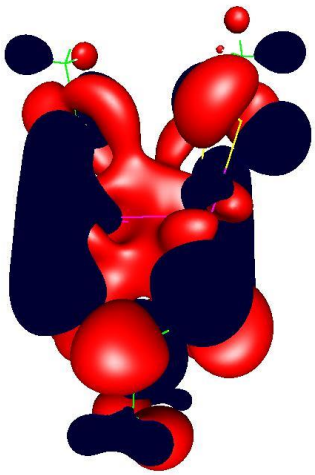
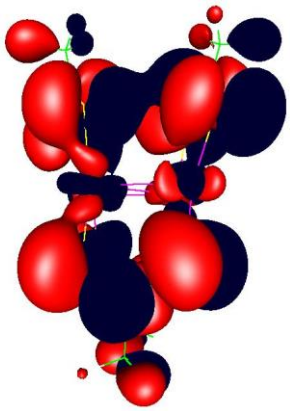


83a (HOMO-1)

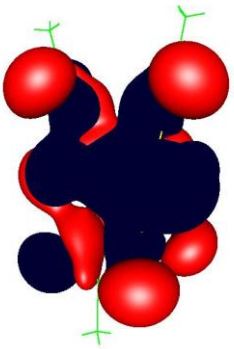


85a (LUMO)



87a

F6. Most important active molecular orbitals in the electronic transitions of $[Au(S_2CCH_3)]_4$ in the CS_2 phase at the TPSS level.



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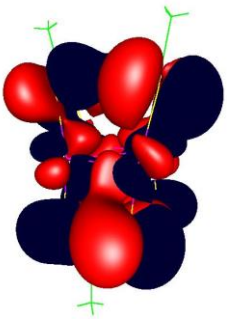
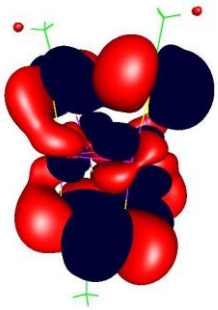


80a



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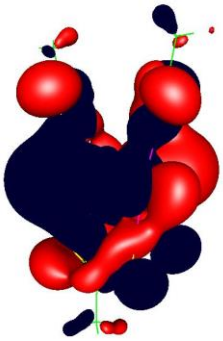
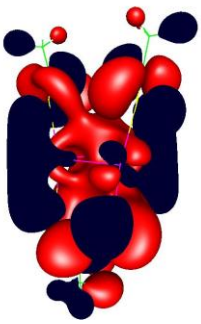


83a (HOMO-1)



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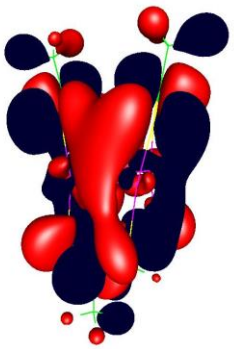

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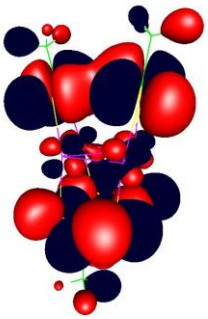

88a