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Supplementary Information

An Eleven-Vertex Deltahedron with Hexacapped Trigonal Bipyramidal Geometry

C. W. Liu,*[a] Ping-Kuei Liao,[a] Ching-Shiang Fang,[a] Jean-Yves Saillard,*[b] Samia Kahlal[b], Ju-Chun Wang[c]

[a] *Department of Chemistry, National Dong Hwa University, Hualien, Taiwan 97401, R.O.C.*

Email: chenwei@mail.ndhu.edu.tw

[b] *UMR-CNRS, 6226 "Sciences Chimiques de Rennes", Université de Rennes 1, 35042*

Rennes Cedex, France Email: jean-yves.saillard@univ-rennes1.fr

c *Department of Chemistry, Soochow University, Taipei, Taiwan 111, ROC*

Content

S1 Synthesis

Experimental Details

All of the reactions were carried out under an inert atmosphere using a Schlenk apparatus.

Synthesis.

$[Ag_{11}(H)\{S_2CNPr_2\}_9](NO_3)$, $\mathbf{1_H}$: A solution of $AgNO_3$ (0.208 g, 1.23 mmol), $Na[S_2CNPr_2]$ (0.200 g, 1.00 mmol) and $NaBH_4$ (0.0044 g, 0.11 mmol) in 30mL of CH_3CN were stirred at -20℃ for 3h under nitrogen. The reaction mixture was filtered, and the filtrate was evaporated to dryness under a vacuum to obtain a dark-red solid. The solid was washed with deionized water, then subjected to column chromatography (Al_2O_3) by using ethyl acetate / hexane (1/1) as eluents to afford dark-red powders.

$\mathbf{1_H}$. Yield: 0.164g (53%). Mp: 126℃ (decomp.). Anal calcd for $Ag_{11}H_{127}C_{63}N_{10}O_3S_{18} \cdot 0.5C_6H_6$: C, 27.57; H, 4.56; N, 4.87. Found: C, 27.82; H, 4.75; N, 4.90. ^{1}H NMR (300.13MHz, $CDCl_3$, δ, ppm): 7.50 (bs, 1H, μ_4-H), 3.87 (t, $^3J_{HH}$ = 7 Hz, 36H, CH_2), 1.83 (m, 36H, CH_2), 0.88 (t, $^3J_{HH}$ = 7.4 Hz, 54H, CH_3). IR, cm^{-1}: ν(NO), 1384.2(s), 824.8 (w).

$\mathbf{1_D}$. Yield: 0.173g (56%). Mp:123℃ (decomp.). Anal calcd for $Ag_{11}H_{126}D_1C_{63}N_{10}O_3S_{18} \cdot C_6H_6$: C, 28.41; H, 4.67; N, 4.80. Found: C, 28.46; H, 4.94; N, 4.66. ^{1}H NMR (300.13MHz, $CDCl_3$, δ, ppm): 3.87 (t, $^3J_{HH}$ = 7 Hz, 36H, CH_2), 1.83 (m, 36H, CH_2), 0.88 (t, $^3J_{HH}$ = 7.4 Hz, 54H, CH_3). ^{2}H NMR (300.13MHz, $CDCl_3$, δ, ppm): 7.50 (bs, 1D). IR, cm^{-1}: ν(NO), 1381.4(s), 823.3(w).

Fig. S2. UV-Vis (green curve), normalized emission spectra (blue curve) of compound 1H in DCM glass at 77K, normalized excitation (black curve) and emission spectra (red curve) of $\mathbf{1_H}$ in the solid state at 77K.

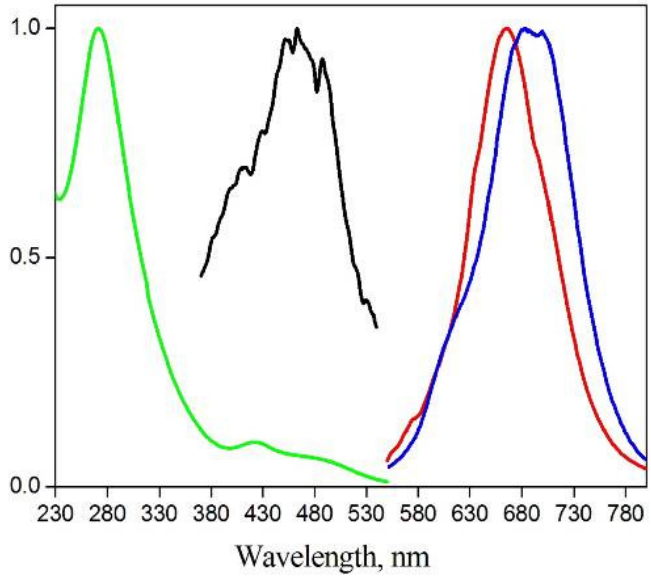


Table S3. Cartesian coordinates of the optimized geometries

$[Ag_{11}(H)\{S_2CNH_2\}_9]^+$ ***(S = 0)*** ***C_3***

Energy = -2632.3886712 a. u.

Atom	**X**	**Y**	**Z**	**(Angstrom)**
Ag	1.657059	.922312	.002502	
Ag	-1.627275	.973899	.002502	
Ag	-.029784	-1.896211	.002502	
Ag	.000000	.000000	-2.279912	
Ag	.000000	.000000	2.286410	
Ag	.022644	3.028146	-1.752221	
Ag	-2.633773	-1.494463	-1.752221	
Ag	2.611130	-1.533683	-1.752221	
Ag	.047214	3.025882	1.747082	
Ag	-2.644098	-1.472053	1.747082	
Ag	2.596884	-1.553829	1.747082	
S	-.899587	-2.047316	3.690176	
S	-1.323234	1.802723	3.690176	
S	2.222821	.244593	3.690176	
S	-2.216833	.281194	-3.688911	
S	.864895	-2.060431	-3.688911	
S	1.351938	1.779237	-3.688911	
S	-1.036459	-3.569701	-1.737857	
S	-2.573222	2.682451	-1.737857	
S	3.609682	.887250	-1.737857	
S	2.626646	2.629508	1.729457	
S	-3.590544	.959988	1.729457	
S	.963898	-3.589496	1.729457	
C	-.039370	-3.437075	3.142833	
C	-2.956910	1.752633	3.142833	
C	2.996279	1.684443	3.142833	
C	-2.960314	1.740564	-3.147468	
C	-.027215	-3.433989	-3.147468	
C	2.987529	1.693425	-3.147468	
N	-.122427	-4.531713	3.904391	
N	-3.863365	2.371882	3.904391	
N	3.985792	2.159831	3.904391	
N	-3.935919	2.234233	-3.915286	
N	.033056	-4.525722	-3.915286	

N	3.902862	2.291489	-3.915286
H	-.701711	-4.531866	4.734358
H	.382107	-5.371553	3.650289
H	-3.573855	2.873632	4.734358
H	-4.842955	2.354862	3.650289
H	4.275566	1.658233	4.734358
H	4.460848	3.016691	3.650289
H	-4.233700	1.735395	-4.744078
H	-4.392037	3.103131	-3.667379
H	.613954	-4.534189	-4.744078
H	-.491372	-5.355181	-3.667379
H	3.619746	2.798795	-4.744078
H	4.883409	2.252050	-3.667379
S	1.305389	4.978167	-.828868
S	-1.281243	4.958554	.851531
C	.000000	5.748667	.002462
N	-.018864	7.088781	-.011241
H	-.719748	7.592566	.515322
H	.670536	7.600651	-.545104
S	-4.963913	-1.358584	-.828868
S	-3.653612	-3.588866	.851531
C	-4.978492	-2.874334	.002462
N	-6.129632	-3.560727	-.011241
H	-6.215481	-4.419603	.515322
H	-6.917624	-3.219624	-.545104
S	3.658525	-3.619583	-.828868
S	4.934855	-1.369688	.851531
C	4.978492	-2.874334	.002462
N	6.148496	-3.528054	-.011241
H	6.935229	-3.172963	.515322
H	6.247089	-4.381026	-.545104
H	.000000	.000000	-.005455

$[Ag_{11}(H)\{S_2CNH_2\}_9]^+$ ***(S = 1)*** ***C_1***

Energy = -2632.3244657 a. u.

Atom	**X**	**Y**	**Z**	**(Angstrom)**

Ag	-1.714811	0.588153	0.343635
Ag	0.667250	-0.648255	2.267489
Ag	0.084587	2.288390	2.541151
Ag	-0.502290	0.509837	-2.525022
Ag	2.464866	-0.574238	-2.316182
S	-2.494523	1.228917	2.795667
S	-1.482905	-1.586312	3.615347
S	0.028038	4.693923	1.900646
S	-2.303371	2.296336	-3.211269
S	1.233961	-2.802417	-2.563005
S	4.509593	0.658183	-1.504523
N	-2.789099	0.084706	5.135216
N	-2.252730	5.982841	1.881829
N	0.333416	-3.534831	-4.889168
C	-2.291813	-0.070579	3.902997
H	-3.227989	0.959397	5.394313
H	-2.714330	-0.658491	5.818021
C	-1.633785	4.869644	1.464813
H	-3.200048	6.178397	1.587254
H	-1.763547	6.640722	2.474031
C	0.104365	-2.674915	-3.889259
H	-0.286867	-3.559358	-5.688348
H	1.132956	-4.154744	-4.857218
H	0.353825	0.070000	0.518797
Ag	1.877921	1.129364	0.130219
Ag	3.080039	-1.525790	0.881390
Ag	-2.465137	-1.365426	-1.677988
S	3.822146	1.047529	1.951120
S	1.609515	0.937171	4.146951
S	4.983250	-2.250861	-0.578655
S	1.517131	1.479515	-3.873731
S	-4.072942	0.743308	-1.172443
S	-3.731358	-3.507494	-0.549590
N	4.134186	1.462633	4.508713
N	6.827916	-0.537711	-1.308511
N	-4.877143	2.539410	-2.887275
C	3.232105	1.171308	3.562998
H	5.105727	1.590309	4.256718
H	3.850110	1.561572	5.474696

C	5.510603	-0.708933	-1.127538
H	7.184014	0.326946	-1.692462
H	7.470267	-1.280171	-1.066615
C	-3.795403	1.886306	-2.442516
H	-4.781458	3.249939	-3.601458
H	-5.785611	2.353018	-2.484238
Ag	0.211625	-1.519309	-0.506297
Ag	-2.178188	-2.373098	1.278010
Ag	-0.784226	3.109467	-1.115023
S	-0.120459	-3.912834	0.713507
S	1.938446	-2.934065	2.826933
S	-4.642703	-1.603327	1.491227
S	-1.243608	-1.626742	-4.064611
S	1.738999	3.310217	-1.354505
S	-2.580379	3.768860	0.522287
N	0.932007	-5.335298	2.633172
N	-6.268579	-2.721273	-0.302616
N	2.933555	3.661731	-3.643105
C	0.918919	-4.107881	2.099546
H	0.341603	-6.062648	2.250820
H	1.554798	-5.550262	3.401675
C	-5.028037	-2.609504	0.168390
H	-6.463793	-3.314262	-1.098994
H	-7.026159	-2.195062	0.113935
C	2.104267	2.836839	-2.998809
H	3.211234	3.461969	-4.595750
H	3.305035	4.477662	-3.173241

$[Ag_{11}\{S_2CNH_2\}_9]^{2+}$ ***(S = 0)*** ***C_1***

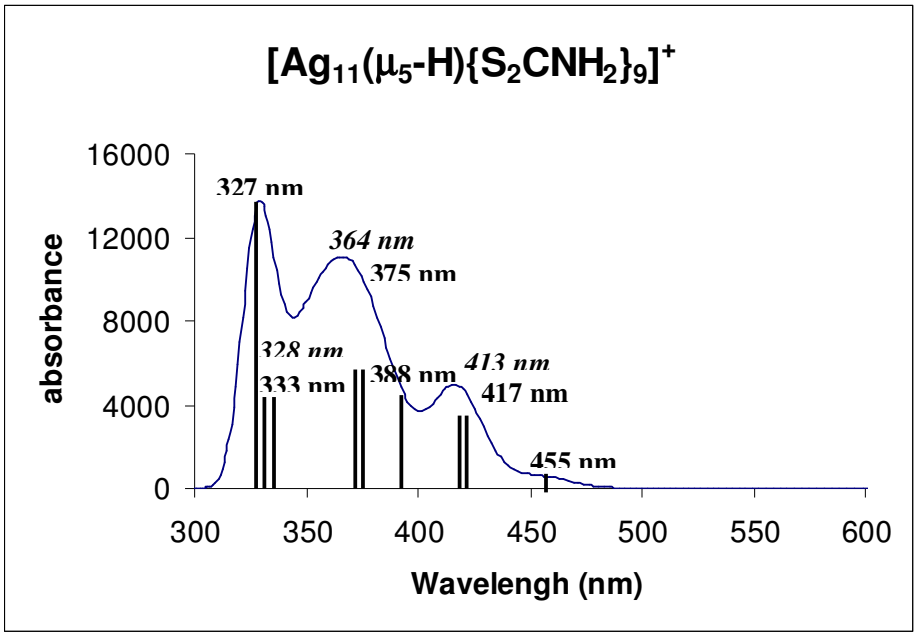
Energy = -2631.5094321 u. a.

Atom	**X**	**Y**	**Z** (Angstrom)
Ag	0.136079	-0.071158	4.377787
Ag	-0.104422	0.056075	-3.691145
Ag	1.493199	3.389241	1.563045
Ag	-3.651471	-0.486099	1.637456
Ag	2.287410	-2.985703	1.450277

Ag	0.518684	3.093114	-1.842236
Ag	-2.991095	-0.998486	-1.813045
Ag	2.309146	-1.990553	-1.966411
Ag	-1.852575	-3.041931	0.125145
Ag	-1.724861	3.116546	0.189371
Ag	3.567785	-0.078230	0.025083
S	1.105998	-2.405485	4.018256
S	0.030238	-4.070569	1.757722
C	-0.181627	-3.307678	3.307485
N	-1.330807	-3.488687	3.956612
H	-1.443520	-3.129757	4.896633
H	-2.055427	-4.083819	3.573319
S	4.456308	-3.347422	-1.779271
S	-4.059152	-2.901170	1.283793
C	-5.290911	-2.936225	0.004229
N	-6.362349	-3.662842	0.327830
H	-6.429361	-4.123972	1.226306
H	-7.131479	-3.751187	-0.325800
S	2.401545	-0.402798	-4.091558
S	-0.085567	-3.082080	-1.688883
C	3.007923	1.028071	-3.342246
N	3.797325	1.819680	-4.058738
H	4.203624	2.649382	-3.641286
H	4.023439	1.586451	-5.019835
S	1.653866	1.958263	4.066813
S	3.576956	1.983024	1.755893
C	3.062365	1.336769	3.288281
N	3.812789	0.402762	3.870684
H	3.583535	0.076229	4.801279
H	4.681349	0.097050	3.448328
S	-2.385784	0.244913	4.129958
S	-3.450754	2.007632	1.940220
C	-2.572104	1.810498	3.430343
N	-2.104416	2.896970	4.043414
H	-1.670165	2.817060	4.954610
H	-2.283496	3.821455	3.669908
S	-5.229041	-2.173068	-1.503185
S	-0.424824	4.932176	1.304987
C	0.092606	6.035199	0.011362

N	0.022137	7.321382	0.359395
H	-0.293647	7.596929	1.280663
H	0.297007	8.040919	-0.298894
S	-1.769901	-1.890072	-3.995184
S	-2.752253	1.630911	-1.581634
C	-0.793270	-3.126745	-3.292927
N	-0.542067	-4.209207	-4.019651
H	-0.003228	-4.973588	-3.628348
H	-0.909452	-4.292507	-4.961630
S	0.634857	5.618655	-1.534594
S	4.571400	-2.112008	1.070846
C	5.184794	-3.096794	-0.274164
N	6.356042	-3.678110	-0.007816
H	6.810688	-3.551295	0.887479
H	6.799810	-4.266650	-0.703008
S	-0.955978	2.474175	-3.959159
S	2.667337	1.545010	-1.701311
C	-2.489794	2.252547	-3.200080
N	-3.577310	2.570516	-3.892360
H	-4.494641	2.489206	-3.468427
H	-3.498607	2.923253	-4.840312

Figure S4. TDDFT-simulated absorption spectrum of $[Ag_{11}(\mu_5\text{-H})\{S_2CNH_2\}_9]^+$. Solid lines represent the calculated electronic transitions and their lengths are proportional to their oscillator strengths. Values in italics indicate the theoretical λ_{max} values on the simulated curves.



S5. Full reference for Gaussian 03.

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr. T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, *Gaussian 03, Revision B.04, Gaussian, Inc., Pittsburgh PA*, **2003**.