Electronic Supplementary Information

Silver mediated duplex-type complexes of pyrimidinophanes and their acyclic counterparts

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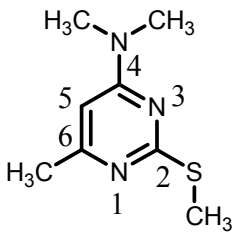
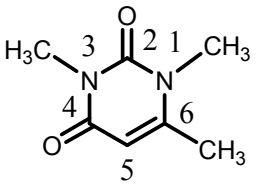
Contents

The structural formulae of the investigated compounds L1-L5

Pyrimidine units

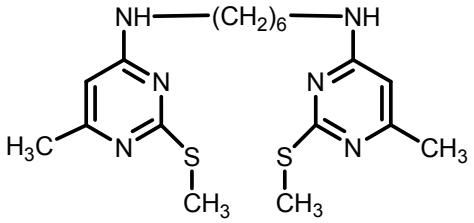


L**1**

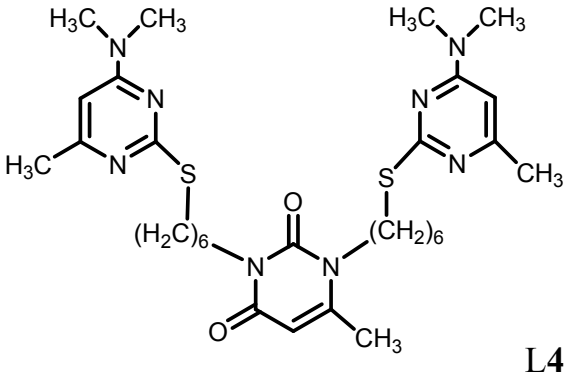


L**2**

Podands

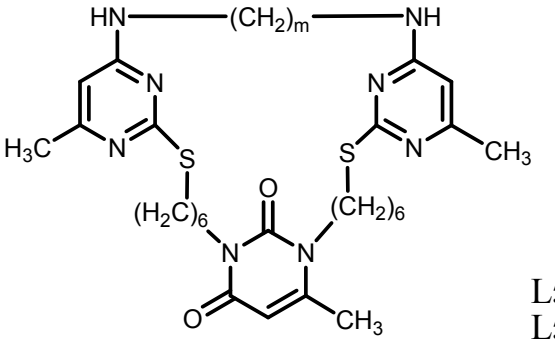


L**3**



L**4**

Pyrimidinophanes



L**5a** m=3
L**5b** m=5

The optimized structures of compound L1, its complexes and coordinates for geometry-optimized structures

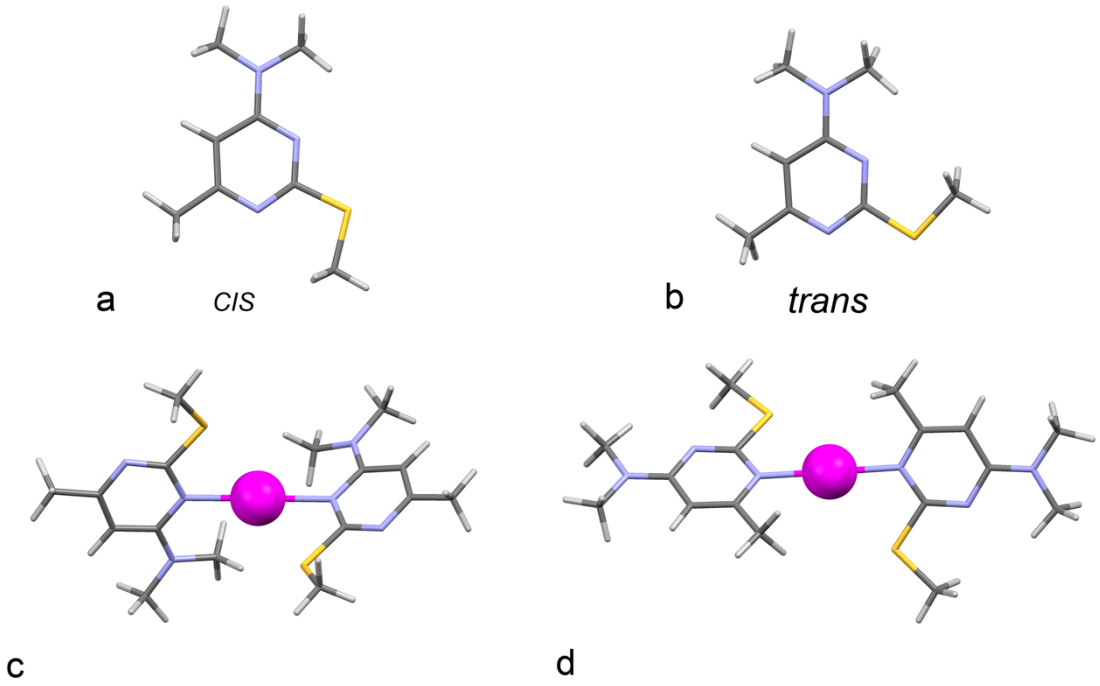


Fig. 1 The optimized structures of (a) *cis* and (b) *trans* conformers of L**1** and $[AgL\mathbf{1}_2]^+$ complex with (c) N3-Ag^+-N3' and (d) N1-Ag^+-N1' coordination modes.

Coordinates of atoms for structure showed in figure 1a

25
C8N3H13S

N	0.000730000	0.011132000	-0.098800000
C	0.036200000	0.210549000	1.246387000
C	1.195564000	-0.035227000	-0.692545000
C	1.228131000	0.347058000	1.942920000
C	-1.294230000	0.279679000	1.939504000
C	2.442329000	0.268103000	1.204016000
H	1.216011000	0.516396000	3.017410000
N	3.662711000	0.360906000	1.804104000
N	2.406367000	0.085383000	-0.138178000
C	4.890371000	0.434021000	1.018969000
C	3.765395000	0.655142000	3.227644000
H	5.672464000	-0.163768000	1.508113000
H	4.700351000	0.039953000	0.016512000
H	5.246005000	1.475344000	0.929787000
H	4.816097000	0.563558000	3.525577000
H	3.424912000	1.677256000	3.468622000
H	3.180512000	-0.060223000	3.824085000
S	1.271486000	-0.283192000	-2.463851000
C	-0.495600000	-0.399305000	-2.911687000
H	-0.512283000	-0.554549000	-3.998055000

H	-0.967997000	-1.247493000	-2.404452000
H	-1.020581000	0.527764000	-2.657100000
H	-1.183764000	0.453064000	3.017570000
H	-1.903798000	1.088252000	1.508422000
H	-1.850094000	-0.657617000	1.784935000

Coordinates of atoms for structure showed in figure 1b

25
C8N3H13S

N	2.477594000	0.092111000	-0.100687000
C	1.287554000	-0.036636000	-0.680619000
N	0.072000000	0.005717000	-0.113925000
C	0.071080000	0.212716000	1.225834000
C	1.247947000	0.362619000	1.951725000
C	2.477710000	0.286156000	1.244733000
C	-1.275327000	0.277054000	1.887703000
S	1.212480000	-0.299786000	-2.449544000
C	2.977802000	-0.308502000	-2.914806000
N	3.683480000	0.392375000	1.871390000
C	3.753483000	0.663515000	3.301098000
C	4.932058000	0.465344000	1.121335000
H	1.207871000	0.540824000	3.024048000
H	5.675884000	-0.208723000	1.571320000
H	4.745129000	0.165253000	0.086281000
H	5.337731000	1.491665000	1.129269000
H	4.795297000	0.554632000	3.623933000
H	3.418416000	1.686168000	3.547320000
H	3.144889000	-0.053309000	3.871234000
H	2.994085000	-0.465358000	-4.000903000
H	3.447971000	0.650220000	-2.669333000
H	3.507154000	-1.125602000	-2.412123000
H	-1.190157000	0.457807000	2.966863000
H	-1.880182000	1.078572000	1.437629000
H	-1.820619000	-0.665140000	1.726331000

Coordinates of atoms for structure showed in figure 1c

51
AgC16N6H26S2

N	-4.048225000	-1.781009000	-4.066035000
C	-2.895388000	-1.212094000	-3.776840000
N	-2.074818000	-0.518254000	-4.601188000
C	-2.511562000	-0.330457000	-5.882052000
C	-3.722345000	-0.954199000	-6.296232000
C	-4.453905000	-1.671309000	-5.367076000
S	-2.256261000	-1.288403000	-2.104741000
C	-3.214111000	-2.665261000	-1.377021000
N	-1.780942000	0.441630000	-6.720529000
C	-2.148998000	0.540885000	-8.134510000
C	-5.740549000	-2.351265000	-5.717227000
C	-0.637724000	1.212123000	-6.246003000
S	2.326963000	-1.954292000	-4.793257000

C	3.213861000	-3.550838000	-4.878809000
C	2.972607000	-1.232623000	-3.285600000
N	2.186137000	-0.229757000	-2.827524000
C	2.633848000	0.443637000	-1.726190000
C	3.815650000	-0.009095000	-1.074345000
C	4.511636000	-1.072405000	-1.619984000
N	4.098905000	-1.683522000	-2.771344000
N	1.941009000	1.520038000	-1.285464000
C	2.315660000	2.168817000	-0.027119000
C	5.766039000	-1.606160000	-1.001950000
C	0.832816000	2.079198000	-2.050424000
H	-4.082186000	-0.859512000	-7.317589000
H	-0.424515000	2.004528000	-6.971634000
H	-0.865493000	1.683796000	-5.280532000
H	0.271599000	0.590601000	-6.147576000
H	-1.347230000	1.062497000	-8.666223000
H	-2.262922000	-0.455933000	-8.583573000
H	-3.084785000	1.105895000	-8.270879000
H	-2.908144000	-2.711319000	-0.324949000
H	-4.282937000	-2.441101000	-1.452616000
H	-2.977091000	-3.606524000	-1.884014000
H	-6.001333000	-2.212210000	-6.773364000
H	-5.665620000	-3.428604000	-5.504948000
H	-6.556091000	-1.958578000	-5.091296000
H	4.181416000	0.476678000	-0.173306000
H	0.659507000	3.107302000	-1.714399000
H	1.078441000	2.105216000	-3.120643000
H	-0.104700000	1.512163000	-1.900777000
H	1.539921000	2.895478000	0.233307000
H	2.383897000	1.436295000	0.789616000
H	3.276905000	2.699577000	-0.115480000
H	2.905235000	-4.007437000	-5.826877000
H	4.292603000	-3.364659000	-4.879852000
H	2.930376000	-4.191842000	-4.037401000
H	6.035277000	-1.060846000	-0.089307000
H	5.640544000	-2.672276000	-0.759038000
H	6.597618000	-1.538034000	-1.719525000
Ag	0.054753000	-0.514591000	-3.689390000

Coordinates of atoms for structure showed in figure 1d

51
AgC16N6H26S2

C	2.557389000	0.005723000	1.305240000
N	1.458513000	-0.541557000	1.898693000
C	0.369633000	-0.661764000	1.166753000
N	0.212674000	-0.294518000	-0.130183000
C	1.303776000	0.257535000	-0.739562000
C	2.493352000	0.423079000	-0.055536000
S	-1.104009000	-1.373154000	1.872149000
C	-0.577439000	-1.741787000	3.581261000
C	1.142719000	0.672104000	-2.169076000
N	3.681785000	0.132382000	2.042465000

C	3.748933000	-0.281306000	3.441941000
C	4.889884000	0.714055000	1.461011000
H	3.346875000	0.866004000	-0.562508000
H	3.986843000	0.584161000	4.079068000
H	2.784631000	-0.699405000	3.742107000
H	4.533978000	-1.041649000	3.570824000
H	5.679224000	0.699827000	2.219592000
H	5.235436000	0.133469000	0.592175000
H	4.724806000	1.757964000	1.152302000
H	-1.456342000	-2.186320000	4.064158000
H	0.251589000	-2.457264000	3.576671000
H	-0.290389000	-0.819526000	4.097292000
H	2.074647000	1.082804000	-2.575678000
H	0.841045000	-0.188471000	-2.786801000
H	0.355529000	1.437309000	-2.258971000
Ag	-1.718709000	-0.610718000	-1.145921000
N	-3.653781000	-0.873594000	-2.169399000
C	-4.828678000	-0.349892000	-1.709173000
C	-3.724543000	-1.590351000	-3.319616000
C	-6.013827000	-0.552013000	-2.390984000
N	-4.802209000	-1.833422000	-4.037575000
C	-5.983939000	-1.320209000	-3.590538000
N	-7.097623000	-1.564632000	-4.314148000
C	-7.069581000	-2.336979000	-5.553930000
C	-8.392116000	-1.038247000	-3.886407000
H	-7.420898000	-1.715593000	-6.391812000
H	-6.046636000	-2.668048000	-5.750669000
H	-7.727830000	-3.214238000	-5.463916000
H	-9.154220000	-1.378873000	-4.594846000
H	-8.662418000	-1.406243000	-2.885067000
H	-8.395054000	0.062803000	-3.876862000
S	-2.145248000	-2.233332000	-3.837159000
C	-2.572349000	-3.121500000	-5.374131000
H	-1.627159000	-3.546414000	-5.733810000
H	-3.288007000	-3.922799000	-5.161966000
H	-2.978599000	-2.425626000	-6.115731000
H	-6.934937000	-0.123094000	-2.004582000
C	-4.763307000	0.449380000	-0.444934000
H	-5.755845000	0.802963000	-0.141095000
H	-4.343172000	-0.158133000	0.372099000
H	-4.107139000	1.323890000	-0.579241000

The optimized structures of compound L3, its complexes and coordinates for geometry-optimized structures

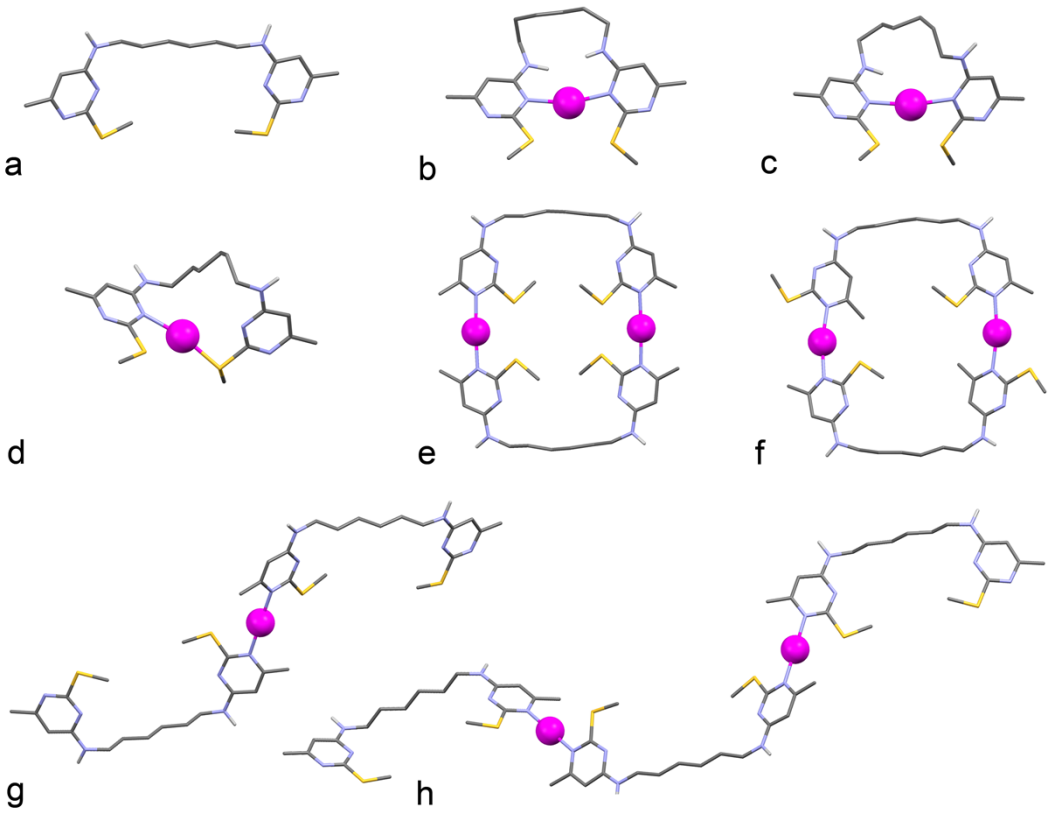


Fig. 2 The optimized structures of (a) compound L**3** and its complexes: $[AgL\mathbf{3}]^{+}$ with the (b) N3-Ag^{+}-N3 (*cis/cis* oriented NH groups), (c) N3-Ag^{+}-N3 (*trans/cis* oriented NH groups), (d) S-Ag^{+}-N3 (*trans/trans* oriented NH groups) coordination modes; $[Ag_2L\mathbf{3}_2]^{2+}$ with the (e) N1-Ag^{+}-N1 (*cis/cis* oriented SCH_3 groups) and (f) *trans/trans* oriented SCH_3 groups; (g) $[AgL\mathbf{3}_2]^{+}$ and (h) $[Ag_2L\mathbf{3}_3]^{2+}$. Only hydrogen atoms of NH groups are shown.

Coordinates of atoms for structure showed in figure 2a

54
C18N6H28S2

N	2.121502000	0.201631000	1.408735000
C	2.643846000	1.426706000	1.137869000
C	1.854366000	2.567655000	1.111312000
C	0.469123000	2.416469000	1.375262000
N	-0.058635000	1.198404000	1.641968000
C	0.803540000	0.179514000	1.644856000
N	-0.367053000	3.488680000	1.388642000
H	0.026179000	4.380416000	1.104256000
C	4.120106000	1.474999000	0.869249000
S	0.187609000	-1.463851000	1.993461000
C	-1.594220000	-1.161751000	2.254692000
C	-1.814142000	3.398022000	1.541526000
C	-2.561115000	3.142605000	0.225547000

C	-4.073073000	3.014568000	0.430239000
C	-4.841022000	2.759368000	-0.870705000
C	-6.347373000	2.584357000	-0.659587000
C	-7.095025000	2.328767000	-1.975132000
N	-8.527467000	2.116193000	-1.806011000
H	-9.125707000	2.933917000	-1.742098000
C	-9.091369000	0.916879000	-1.501778000
N	-8.286465000	-0.171464000	-1.471231000
C	-8.887010000	-1.330956000	-1.195043000
N	-10.180606000	-1.558764000	-0.934370000
C	-10.982088000	-0.461522000	-0.962898000
C	-10.481277000	0.801698000	-1.244348000
S	-7.894344000	-2.818690000	-1.141021000
C	-6.226796000	-2.185025000	-1.531192000
C	-12.436648000	-0.693439000	-0.672502000
H	-11.131895000	1.677240000	-1.268233000
H	-6.965219000	3.182118000	-2.658428000
H	-6.681493000	1.438413000	-2.469233000
H	-5.564518000	-3.059284000	-1.493291000
H	-6.204538000	-1.742227000	-2.533001000
H	-5.912342000	-1.443842000	-0.788120000
H	-13.012589000	0.240078000	-0.709561000
H	-12.859278000	-1.402222000	-1.400529000
H	-12.555672000	-1.147120000	0.322973000
H	-6.764642000	3.482525000	-0.172394000
H	-6.532095000	1.735861000	0.019614000
H	-4.435520000	1.855626000	-1.359643000
H	-4.660242000	3.594765000	-1.570742000
H	-4.460452000	3.932225000	0.908208000
H	-4.275203000	2.190826000	1.137939000
H	-2.166967000	2.218458000	-0.228346000
H	-2.346519000	3.963823000	-0.479969000
H	-2.158672000	4.338858000	1.997740000
H	-2.024521000	2.585353000	2.250838000
H	2.281829000	3.548110000	0.895833000
H	-2.032536000	-2.147640000	2.455393000
H	-1.753913000	-0.499867000	3.112945000
H	-2.047025000	-0.725702000	1.357359000
H	4.460730000	2.495425000	0.651908000
H	4.675316000	1.091519000	1.738579000
H	4.370648000	0.825663000	0.016891000

Coordinates of atoms for structure showed in figure 2b

55
AgC18N6H28S2

C	1.719067000	0.551392000	0.225087000
N	0.490303000	0.653411000	0.702184000
C	0.297096000	0.204028000	1.974998000
C	1.338202000	-0.306988000	2.736806000
C	2.626425000	-0.365525000	2.155595000
N	2.801648000	0.049848000	0.867359000
C	-1.097453000	0.308744000	2.507748000

N	3.712823000	-0.837883000	2.803113000
C	3.745015000	-1.369733000	4.167275000
S	2.100561000	1.105022000	-1.422177000
H	1.173063000	-0.636291000	3.760671000
H	4.613801000	-0.629990000	2.372983000
H	-1.171917000	-0.070675000	3.533898000
H	-1.429542000	1.357668000	2.486991000
H	-1.787704000	-0.256872000	1.863756000
C	5.104173000	-2.023034000	4.423518000
H	2.936426000	-2.110043000	4.276399000
H	5.163324000	-2.283076000	5.490104000
C	5.385525000	-3.260062000	3.542382000
H	5.885724000	-1.260085000	4.257985000
C	6.830426000	-3.298482000	3.029486000
H	5.158359000	-4.181573000	4.102509000
H	4.689402000	-3.252794000	2.686291000
C	7.180531000	-4.470083000	2.103629000
H	7.039746000	-2.351266000	2.501053000
H	7.521953000	-3.315806000	3.888025000
H	8.230723000	-4.362958000	1.788688000
H	7.119858000	-5.424645000	2.652151000
C	6.281299000	-4.611522000	0.860300000
H	6.718491000	-5.337001000	0.157674000
H	5.298895000	-5.011871000	1.143389000
N	6.010009000	-3.358651000	0.154791000
H	5.125835000	-2.895273000	0.358545000
C	6.852426000	-2.679568000	-0.651073000
N	6.445574000	-1.448798000	-1.079600000
C	7.271107000	-0.779655000	-1.921227000
N	8.447023000	-1.184950000	-2.367641000
C	8.870660000	-2.406106000	-1.931104000
C	8.106589000	-3.181988000	-1.073008000
S	6.609169000	0.795228000	-2.416237000
C	10.205063000	-2.860148000	-2.434263000
H	8.458507000	-4.155546000	-0.738056000
H	10.477162000	-3.845625000	-2.037567000
H	10.195462000	-2.905545000	-3.533749000
H	10.980087000	-2.131681000	-2.151980000
C	7.954422000	1.481301000	-3.443121000
H	7.586272000	2.456833000	-3.783420000
H	8.862228000	1.606273000	-2.844045000
H	8.141598000	0.826552000	-4.300236000
C	0.451998000	1.522277000	-2.087878000
H	0.637540000	1.886987000	-3.105485000
H	-0.184638000	0.631885000	-2.114221000
H	-0.005973000	2.309659000	-1.480767000
Ag	4.608315000	-0.426787000	-0.345125000
H	3.565859000	-0.563787000	4.899193000

Coordinates of atoms for structure showed in figure 2c

55
AgC18N6H28S2

C	1.679697000	0.378344000	0.437284000
N	0.476530000	0.037714000	0.864123000
C	0.387109000	-0.354581000	2.167639000
C	1.490922000	-0.357142000	3.006527000
C	2.740374000	0.041117000	2.474864000
N	2.830965000	0.371634000	1.154645000
C	-0.973275000	-0.757431000	2.644242000
N	3.872828000	0.126151000	3.212399000
C	4.203559000	-0.686658000	4.387770000
S	1.922444000	0.907923000	-1.245203000
H	1.390069000	-0.623007000	4.056956000
H	4.674154000	0.523887000	2.720187000
H	-0.963724000	-1.057746000	3.698900000
H	-1.679824000	0.076064000	2.514060000
H	-1.350515000	-1.593238000	2.035695000
C	5.432257000	-1.561379000	4.098237000
H	3.335402000	-1.313715000	4.630665000
H	5.678234000	-2.126789000	5.011178000
C	5.233940000	-2.502256000	2.905158000
H	6.295040000	-0.898588000	3.906147000
C	6.523522000	-3.149418000	2.384423000
H	4.501587000	-3.286112000	3.162738000
H	4.773139000	-1.925361000	2.085193000
C	6.381182000	-3.698128000	0.955512000
H	7.342149000	-2.408868000	2.404975000
H	6.832987000	-3.964061000	3.057710000
H	7.221172000	-4.375005000	0.724101000
H	5.468309000	-4.309848000	0.874873000
C	6.317127000	-2.616200000	-0.128522000
H	6.040668000	-3.062329000	-1.099005000
H	5.534185000	-1.877842000	0.109634000
N	7.598550000	-1.926407000	-0.244682000
H	8.416791000	-2.528160000	-0.174277000
C	7.858905000	-0.678269000	-0.694506000
N	6.864456000	0.230416000	-0.886429000
C	7.244007000	1.434959000	-1.398228000
N	8.459892000	1.849421000	-1.680357000
C	9.473498000	0.966205000	-1.418256000
C	9.208990000	-0.300546000	-0.941897000
S	5.841895000	2.493415000	-1.729395000
C	10.861583000	1.449502000	-1.697567000
H	10.013268000	-1.013253000	-0.755899000
H	11.612846000	0.682345000	-1.474329000
H	10.951814000	1.744607000	-2.753848000
H	11.074756000	2.346287000	-1.096147000
C	6.619765000	4.138678000	-1.898982000
H	5.803326000	4.820567000	-2.165367000
H	7.078774000	4.444847000	-0.953076000
H	7.364516000	4.104608000	-2.700521000

C	0.297116000	0.555563000	-2.000117000
H	0.390294000	0.875582000	-3.045084000
H	0.076754000	-0.515843000	-1.949779000
H	-0.481577000	1.135275000	-1.494330000
Ag	4.747343000	0.433859000	-0.027436000
H	4.393918000	-0.032958000	5.252492000

Coordinates of atoms for structure showed in figure 2d

55
AgC18N6H28S2

C	-0.232094000	-0.829560000	2.242598000
N	-1.166410000	-1.588351000	2.776894000
C	-0.878313000	-2.128947000	4.000507000
C	0.329375000	-1.888282000	4.620840000
C	1.289865000	-1.066550000	3.966430000
N	0.994178000	-0.526605000	2.755421000
C	-1.941861000	-2.985404000	4.612727000
N	2.474593000	-0.839409000	4.580434000
C	3.628626000	-0.064428000	4.140718000
S	-0.513167000	-0.072416000	0.653415000
H	0.558546000	-2.316931000	5.597046000
H	2.579368000	-1.304679000	5.478463000
H	-1.636238000	-3.379154000	5.589652000
H	-2.868754000	-2.404621000	4.733595000
H	-2.177427000	-3.827123000	3.943989000
C	4.745477000	-0.900500000	3.503884000
H	4.017566000	0.462311000	5.024580000
H	5.081272000	-1.655762000	4.234740000
C	4.362815000	-1.583286000	2.189748000
H	5.604327000	-0.227835000	3.337889000
C	5.522440000	-2.359452000	1.557220000
H	3.509884000	-2.264181000	2.351192000
H	4.019241000	-0.808814000	1.475358000
C	5.169547000	-3.072114000	0.245482000
H	6.369809000	-1.672914000	1.386978000
H	5.883164000	-3.113695000	2.276630000
H	6.030954000	-3.680701000	-0.076950000
H	4.340175000	-3.779974000	0.413530000
C	4.755140000	-2.149122000	-0.911201000
H	4.514739000	-2.759883000	-1.795793000
H	3.858427000	-1.569659000	-0.662130000
N	5.797297000	-1.193976000	-1.275349000
H	6.676118000	-1.573710000	-1.618893000
C	5.737724000	0.148375000	-1.133051000
N	4.592685000	0.712411000	-0.665243000
C	4.610369000	2.042558000	-0.579957000
N	5.573801000	2.901892000	-0.848862000
C	6.741822000	2.335172000	-1.290851000
C	6.855411000	0.967981000	-1.456911000
S	2.993600000	2.732491000	-0.099790000
C	7.865635000	3.279193000	-1.586745000
H	7.782999000	0.521393000	-1.817845000

H	8.758532000	2.749423000	-1.940616000
H	7.554928000	4.007245000	-2.351180000
H	8.124351000	3.853300000	-0.684125000
C	3.451879000	4.286594000	0.750602000
H	2.507010000	4.778398000	1.009727000
H	4.041366000	4.082736000	1.649863000
H	4.019640000	4.899254000	0.042981000
C	-2.203367000	-0.628732000	0.238967000
H	-2.419104000	-0.185826000	-0.741032000
H	-2.233063000	-1.721427000	0.178309000
H	-2.913289000	-0.262026000	0.987418000
Ag	2.157071000	0.911432000	1.411521000
H	3.287323000	0.727696000	3.449651000

Coordinates of atoms for structure showed in figure 2e

110
Ag2C36N12H56S4

C	-0.124768000	-6.757707000	13.350600000
N	-0.743069000	-6.114493000	12.310914000
C	0.063968000	-5.606574000	11.348725000
N	1.381725000	-5.684308000	11.294980000
C	2.003647000	-6.329821000	12.315755000
C	1.249984000	-6.877785000	13.389526000
Ag	-2.934511000	-5.949958000	12.079965000
N	-5.110446000	-5.780147000	11.734896000
C	-5.990000000	-5.215775000	12.620720000
C	-7.326932000	-5.084966000	12.302213000
C	-7.761703000	-5.536996000	11.026340000
N	-6.883637000	-6.105384000	10.159516000
C	-5.626880000	-6.201118000	10.555377000
N	-9.046786000	-5.430446000	10.631980000
C	-9.519017000	-5.802846000	9.299219000
C	-9.272111000	-4.714266000	8.243100000
C	-9.391638000	-5.248846000	6.812729000
C	-9.096878000	-4.184553000	5.747427000
C	-8.780584000	-4.782693000	4.373311000
C	-8.437585000	-3.707316000	3.330697000
N	-7.774613000	-4.245264000	2.143639000
C	-5.427898000	-4.757661000	13.930091000
S	-4.418362000	-6.936286000	9.473684000
C	-5.436868000	-7.409452000	8.033450000
S	-0.820754000	-4.773910000	10.046908000
C	0.539374000	-4.201957000	8.970628000
N	3.348422000	-6.418181000	12.270379000
C	4.154379000	-5.942200000	11.147100000
C	4.210655000	-6.936645000	9.976970000
C	4.701605000	-6.286183000	8.680095000
C	4.712690000	-7.253934000	7.489300000
C	4.765421000	-6.538717000	6.135908000
C	4.723711000	-7.518391000	4.952756000
N	4.391579000	-6.874882000	3.682534000
C	3.132171000	-6.582045000	3.299838000

C	2.856591000	-5.881544000	2.093766000
C	1.539485000	-5.607157000	1.784193000
N	0.525798000	-6.012932000	2.611648000
C	0.889912000	-6.694789000	3.724123000
N	2.119122000	-6.990249000	4.107655000
S	-0.489810000	-7.199486000	4.730377000
C	0.339779000	-8.091149000	6.091265000
Ag	-1.608383000	-5.542891000	2.284177000
N	-3.756911000	-5.073233000	2.070467000
C	-4.409812000	-4.483639000	3.100590000
N	-5.698931000	-4.202346000	3.166661000
C	-6.456599000	-4.524240000	2.085959000
C	-5.864080000	-5.123769000	0.941097000
C	-4.510004000	-5.391146000	0.971082000
C	1.143506000	-4.863356000	0.547159000
S	-3.352994000	-4.090936000	4.478987000
C	-4.520012000	-3.294062000	5.635968000
C	-1.009961000	-7.312133000	14.422679000
H	5.150549000	-6.531042000	3.100915000
C	-3.792439000	-6.032497000	-0.175272000
H	-9.693875000	-4.965320000	11.262438000
H	3.809615000	-6.939444000	13.010728000
H	3.661655000	-5.559358000	1.433411000
H	5.692041000	-8.021194000	4.822448000
H	3.966048000	-8.292020000	5.141268000
H	-0.462574000	-8.387964000	6.777979000
H	0.855156000	-8.979125000	5.710547000
H	1.048218000	-7.428411000	6.599491000
H	2.019367000	-4.572377000	-0.044864000
H	0.490856000	-5.488946000	-0.082048000
H	0.582325000	-3.952771000	0.810583000
H	5.666111000	-5.906484000	6.065728000
H	3.895819000	-5.865855000	6.057460000
H	3.796885000	-7.871798000	7.519676000
H	5.558044000	-7.956637000	7.585796000
H	5.707977000	-5.856535000	8.822730000
H	4.036635000	-5.435224000	8.445456000
H	3.195274000	-7.332529000	9.811593000
H	4.848393000	-7.794852000	10.246537000
H	5.161038000	-5.729055000	11.532659000
H	3.718255000	-4.993463000	10.803854000
H	1.740245000	-7.388309000	14.218385000
H	0.051578000	-3.718070000	8.115440000
H	1.170402000	-3.480410000	9.499996000
H	1.137438000	-5.055192000	8.633385000
H	-0.428142000	-7.813128000	15.205490000
H	-1.596950000	-6.504939000	14.888601000
H	-1.719266000	-8.039054000	13.996110000
H	-6.461271000	-5.375845000	0.064859000
H	-9.342049000	-3.183479000	2.991732000
H	-7.765061000	-2.961714000	3.777831000
H	-3.932641000	-3.069130000	6.534764000
H	-4.915741000	-2.368366000	5.205225000

H	-5.337658000	-3.980848000	5.879205000
H	-9.623160000	-5.396271000	4.013482000
H	-7.913777000	-5.456470000	4.472111000
H	-8.228818000	-3.582280000	6.071635000
H	-9.945194000	-3.482526000	5.674925000
H	-10.394293000	-5.678308000	6.645486000
H	-8.677801000	-6.084077000	6.693611000
H	-8.254025000	-4.317391000	8.388240000
H	-9.968394000	-3.874307000	8.402979000
H	-10.589661000	-6.035289000	9.383643000
H	-8.996987000	-6.725017000	9.007373000
H	-8.025587000	-4.637216000	13.008896000
H	-4.733776000	-7.830004000	7.303910000
H	-6.177651000	-8.163852000	8.318357000
H	-5.933276000	-6.526727000	7.616589000
H	-6.203088000	-4.317527000	14.568578000
H	-4.973833000	-5.604738000	14.468094000
H	-4.641241000	-4.004015000	13.766727000
H	-4.476100000	-6.257391000	-1.002513000
H	-3.000027000	-5.365891000	-0.550673000
H	-3.315284000	-6.971216000	0.148134000
H	-8.348635000	-4.526336000	1.353704000

Coordinates of atoms for structure showed in figure 2f

110

Ag2C36N12H56S4

C	-0.163646000	-5.262853000	11.273791000
N	-0.855906000	-5.834240000	12.301173000
C	-0.126299000	-6.525208000	13.215367000
N	1.178942000	-6.721152000	13.199821000
C	1.874027000	-6.181277000	12.159777000
C	1.206613000	-5.416792000	11.167212000
Ag	-3.066308000	-5.851827000	12.346409000
N	-5.247552000	-5.809850000	11.984667000
C	-6.177203000	-5.265368000	12.830849000
C	-7.503169000	-5.173889000	12.456479000
C	-7.872053000	-5.640360000	11.165131000
N	-6.944671000	-6.195687000	10.341410000
C	-5.705399000	-6.257493000	10.792092000
N	-9.140037000	-5.562894000	10.712942000
C	-9.544475000	-5.952486000	9.363003000
C	-9.300120000	-4.854708000	8.315287000
C	-9.334947000	-5.397350000	6.883275000
C	-9.078541000	-4.317801000	5.822880000
C	-8.662331000	-4.900385000	4.468672000
C	-8.414222000	-3.817537000	3.404494000
N	-7.632720000	-4.291495000	2.266168000
C	-5.679234000	-4.785549000	14.157825000
S	-4.438539000	-6.998335000	9.778370000
C	-5.372118000	-7.460466000	8.277506000
S	-1.120065000	-7.195062000	14.528662000
C	0.112581000	-8.090867000	15.534616000
N	3.202758000	-6.406239000	12.148763000

C	4.102875000	-6.033474000	11.061364000
C	4.046620000	-6.998113000	9.864805000
C	4.642569000	-6.397150000	8.588012000
C	4.606742000	-7.368409000	7.400059000
C	4.753229000	-6.669521000	6.044947000
C	4.713289000	-7.659402000	4.869536000
N	4.451046000	-7.017553000	3.582273000
C	3.216476000	-6.697028000	3.144789000
C	3.007680000	-5.995839000	1.925742000
C	1.712181000	-5.681198000	1.565902000
N	0.656635000	-6.054692000	2.355297000
C	0.957796000	-6.750888000	3.476388000
N	2.160578000	-7.079099000	3.910242000
S	-0.477588000	-7.243738000	4.413554000
C	0.274066000	-8.122161000	5.828141000
Ag	-1.449012000	-5.463184000	2.029850000
N	-3.572537000	-4.854670000	2.118742000
C	-4.448040000	-5.197049000	1.138007000
N	-5.756600000	-5.024201000	1.151304000
C	-6.294176000	-4.447827000	2.262640000
C	-5.460087000	-4.032524000	3.333511000
C	-4.098888000	-4.250458000	3.222847000
C	1.383445000	-4.926636000	0.316248000
S	-3.654979000	-5.946760000	-0.265546000
C	-5.069106000	-6.329992000	-1.355097000
C	-0.952848000	-4.470161000	10.278401000
H	5.242153000	-6.695918000	3.031506000
C	-3.140002000	-3.839276000	4.296857000
H	-9.824882000	-5.110425000	11.312028000
H	3.553487000	-7.001609000	12.896647000
H	3.846674000	-5.699856000	1.296056000
H	5.664811000	-8.201519000	4.778990000
H	3.919160000	-8.400103000	5.038146000
H	-0.568604000	-8.446859000	6.451009000
H	0.837004000	-8.992959000	5.476602000
H	0.925024000	-7.445762000	6.392081000
H	2.287057000	-4.675159000	-0.251591000
H	0.720507000	-5.524818000	-0.328197000
H	0.854453000	-3.991886000	0.561469000
H	5.687496000	-6.084871000	6.009057000
H	3.923306000	-5.954315000	5.924138000
H	3.644606000	-7.911900000	7.406835000
H	5.390862000	-8.134982000	7.523464000
H	5.679605000	-6.066092000	8.768240000
H	4.071406000	-5.487375000	8.328421000
H	2.993039000	-7.263446000	9.673466000
H	4.561447000	-7.936732000	10.127696000
H	5.117961000	-5.990169000	11.478758000
H	3.857457000	-5.009682000	10.737449000
H	1.740847000	-4.958926000	10.337811000
H	-0.455569000	-8.524325000	16.366726000
H	0.581162000	-8.884570000	14.943451000
H	0.867122000	-7.394769000	15.915386000

H	-0.310251000	-4.068286000	9.485735000
H	-1.731814000	-5.097565000	9.815955000
H	-1.458968000	-3.628874000	10.777225000
H	-5.862023000	-3.554580000	4.223996000
H	-9.365042000	-3.434120000	3.010286000
H	-7.894859000	-2.955699000	3.852570000
H	-4.628886000	-6.798355000	-2.243866000
H	-5.752016000	-7.027871000	-0.859516000
H	-5.591649000	-5.409036000	-1.633732000
H	-9.423798000	-5.607332000	4.100596000
H	-7.735285000	-5.483164000	4.603249000
H	-8.274941000	-3.647454000	6.178014000
H	-9.975847000	-3.685820000	5.708857000
H	-10.300368000	-5.893126000	6.683722000
H	-8.563315000	-6.183173000	6.792247000
H	-8.307870000	-4.412266000	8.501691000
H	-10.039830000	-4.046796000	8.442079000
H	-10.607661000	-6.227125000	9.404727000
H	-8.974933000	-6.852943000	9.093587000
H	-8.242374000	-4.741858000	13.130956000
H	-4.635571000	-7.918004000	7.605453000
H	-6.153370000	-8.186149000	8.526100000
H	-5.808446000	-6.569817000	7.813176000
H	-6.489973000	-4.364296000	14.763982000
H	-5.220061000	-5.615902000	14.716715000
H	-4.908136000	-4.010942000	14.019788000
H	-3.661129000	-3.377053000	5.143901000
H	-2.574493000	-4.710722000	4.664434000
H	-2.410939000	-3.116161000	3.899008000
H	-8.120671000	-4.664984000	1.454247000

Coordinates of atoms for structure showed in figure 2g

109
AgC36N12H56S4

N	3.105470000	-6.552911000	8.207444000
C	2.584450000	-7.604557000	8.893567000
C	1.481893000	-8.306343000	8.426424000
C	0.905593000	-7.887778000	7.200491000
N	1.417582000	-6.838643000	6.513786000
C	2.482287000	-6.250297000	7.062272000
N	-0.164553000	-8.533312000	6.665342000
C	3.267297000	-7.962492000	10.181348000
S	3.224388000	-4.859218000	6.214036000
C	2.183016000	-4.719825000	4.720671000
C	-0.861777000	-8.097789000	5.461531000
C	-1.894359000	-6.989907000	5.711230000
C	-2.525697000	-6.480347000	4.412823000
C	-3.552431000	-5.365484000	4.637390000
C	-4.108910000	-4.787705000	3.332913000
C	-5.132802000	-3.673492000	3.583623000
N	-5.628654000	-3.055227000	2.355851000
C	-5.040743000	-2.017824000	1.727013000

N	-3.954529000	-1.450526000	2.312756000
C	-3.407997000	-0.422237000	1.687740000
N	-3.807846000	0.124331000	0.514638000
C	-4.900307000	-0.443012000	-0.085526000
C	-5.544509000	-1.516005000	0.495633000
S	-1.986403000	0.386394000	2.391918000
C	-1.712877000	-0.571802000	3.922446000
C	-5.344517000	0.153723000	-1.384293000
S	-8.411296000	8.547638000	-7.540899000
C	-6.971678000	7.455211000	-7.279731000
C	-7.644093000	10.039103000	-8.166879000
N	-6.315739000	10.070809000	-8.290209000
C	-5.796715000	11.223898000	-8.775082000
C	-6.636778000	12.314801000	-9.113306000
C	-8.003519000	12.157324000	-8.929888000
N	-8.531350000	11.001038000	-8.447829000
N	-4.449080000	11.291227000	-8.942472000
C	-8.980017000	13.250837000	-9.251596000
C	-3.520894000	10.248744000	-8.522152000
C	-3.138771000	10.323193000	-7.037450000
C	-2.241494000	9.159079000	-6.608640000
C	-1.845368000	9.215142000	-5.129647000
C	-1.018016000	8.006903000	-4.681522000
C	-0.621661000	8.093085000	-3.202307000
N	0.127931000	6.928868000	-2.735686000
C	-0.425002000	5.809720000	-2.226735000
N	-1.771993000	5.784489000	-2.054331000
C	-2.286699000	4.683741000	-1.534394000
N	-1.615879000	3.566753000	-1.164039000
C	-0.257416000	3.581448000	-1.336898000
C	0.372845000	4.690136000	-1.863511000
S	-4.042645000	4.571785000	-1.261218000
C	-4.633436000	6.192296000	-1.861374000
C	0.489393000	2.348788000	-0.933200000
H	1.454362000	4.703213000	-1.998619000
H	0.005685000	8.979119000	-3.024867000
H	-1.519035000	8.184653000	-2.575591000
H	-5.722466000	6.167974000	-1.732682000
H	-4.200546000	6.999988000	-1.262123000
H	-4.380377000	6.317866000	-2.919313000
H	1.567613000	2.460624000	-1.098681000
H	0.320270000	2.129046000	0.132714000
H	0.135347000	1.480868000	-1.511694000
H	-0.107153000	7.925898000	-5.298824000
H	-1.595729000	7.081201000	-4.840306000
H	-2.758670000	9.279481000	-4.511649000
H	-1.278596000	10.143486000	-4.938118000
H	-1.328594000	9.144286000	-7.230466000
H	-2.764996000	8.206937000	-6.808291000
H	-4.063958000	10.317730000	-6.438354000
H	-2.631784000	11.282937000	-6.838631000
H	-2.622562000	10.332771000	-9.152245000
H	-3.989289000	9.276928000	-8.734270000

H	-6.221629000	13.244725000	-9.504721000
H	-7.381469000	6.521629000	-6.873471000
H	-6.458325000	7.256700000	-8.227055000
H	-6.272660000	7.902126000	-6.563956000
H	-8.475422000	14.147314000	-9.633721000
H	-9.704491000	12.901741000	-10.002712000
H	-9.554981000	13.520517000	-8.352867000
H	-6.415715000	-1.965946000	0.019555000
H	-6.004601000	-4.067739000	4.126121000
H	-4.683775000	-2.881363000	4.198213000
H	-0.825096000	-0.125821000	4.387297000
H	-2.576008000	-0.477072000	4.589437000
H	-1.525606000	-1.623192000	3.680298000
H	-6.229637000	-0.358861000	-1.779588000
H	-5.587259000	1.220087000	-1.253869000
H	-4.538329000	0.085483000	-2.131733000
H	-4.578738000	-5.588230000	2.736622000
H	-3.283373000	-4.379139000	2.726831000
H	-3.083620000	-4.554003000	5.222231000
H	-4.381881000	-5.750667000	5.256496000
H	-3.007210000	-7.318536000	3.878260000
H	-1.727379000	-6.108476000	3.745728000
H	-1.392514000	-6.156742000	6.229731000
H	-2.678351000	-7.366791000	6.390116000
H	-1.348272000	-8.982454000	5.023816000
H	-0.106460000	-7.742451000	4.745799000
H	1.072343000	-9.151718000	8.981320000
H	2.583042000	-3.863568000	4.162673000
H	2.253620000	-5.628115000	4.112104000
H	1.138119000	-4.535713000	4.994677000
H	2.787357000	-8.818883000	10.671811000
H	4.324225000	-8.204881000	9.994111000
H	3.252461000	-7.103130000	10.868593000
Ag	-2.717532000	1.852749000	-0.317477000
H	-6.409934000	-3.500235000	1.881989000
H	1.130634000	6.913549000	-2.901439000
H	-0.586065000	-9.269690000	7.222915000
H	-4.064495000	12.184354000	-9.234589000

Coordinates of atoms for structure showed in figure 2h

109
AgC36N12H56S4

N	3.105470000	-6.552911000	8.207444000
C	2.584450000	-7.604557000	8.893567000
C	1.481893000	-8.306343000	8.426424000
C	0.905593000	-7.887778000	7.200491000
N	1.417582000	-6.838643000	6.513786000
C	2.482287000	-6.250297000	7.062272000
N	-0.164553000	-8.533312000	6.665342000
C	3.267297000	-7.962492000	10.181348000
S	3.224388000	-4.859218000	6.214036000
C	2.183016000	-4.719825000	4.720671000

C	-0.861777000	-8.097789000	5.461531000
C	-1.894359000	-6.989907000	5.711230000
C	-2.525697000	-6.480347000	4.412823000
C	-3.552431000	-5.365484000	4.637390000
C	-4.108910000	-4.787705000	3.332913000
C	-5.132802000	-3.673492000	3.583623000
N	-5.628654000	-3.055227000	2.355851000
C	-5.040743000	-2.017824000	1.727013000
N	-3.954529000	-1.450526000	2.312756000
C	-3.407997000	-0.422237000	1.687740000
N	-3.807846000	0.124331000	0.514638000
C	-4.900307000	-0.443012000	-0.085526000
C	-5.544509000	-1.516005000	0.495633000
S	-1.986403000	0.386394000	2.391918000
C	-1.712877000	-0.571802000	3.922446000
C	-5.344517000	0.153723000	-1.384293000
S	-8.411296000	8.547638000	-7.540899000
C	-6.971678000	7.455211000	-7.279731000
C	-7.644093000	10.039103000	-8.166879000
N	-6.315739000	10.070809000	-8.290209000
C	-5.796715000	11.223898000	-8.775082000
C	-6.636778000	12.314801000	-9.113306000
C	-8.003519000	12.157324000	-8.929888000
N	-8.531350000	11.001038000	-8.447829000
N	-4.449080000	11.291227000	-8.942472000
C	-8.980017000	13.250837000	-9.251596000
C	-3.520894000	10.248744000	-8.522152000
C	-3.138771000	10.323193000	-7.037450000
C	-2.241494000	9.159079000	-6.608640000
C	-1.845368000	9.215142000	-5.129647000
C	-1.018016000	8.006903000	-4.681522000
C	-0.621661000	8.093085000	-3.202307000
N	0.127931000	6.928868000	-2.735686000
C	-0.425002000	5.809720000	-2.226735000
N	-1.771993000	5.784489000	-2.054331000
C	-2.286699000	4.683741000	-1.534394000
N	-1.615879000	3.566753000	-1.164039000
C	-0.257416000	3.581448000	-1.336898000
C	0.372845000	4.690136000	-1.863511000
S	-4.042645000	4.571785000	-1.261218000
C	-4.633436000	6.192296000	-1.861374000
C	0.489393000	2.348788000	-0.933200000
H	1.454362000	4.703213000	-1.998619000
H	0.005685000	8.979119000	-3.024867000
H	-1.519035000	8.184653000	-2.575591000
H	-5.722466000	6.167974000	-1.732682000
H	-4.200546000	6.999988000	-1.262123000
H	-4.380377000	6.317866000	-2.919313000
H	1.567613000	2.460624000	-1.098681000
H	0.320270000	2.129046000	0.132714000
H	0.135347000	1.480868000	-1.511694000
H	-0.107153000	7.925898000	-5.298824000
H	-1.595729000	7.081201000	-4.840306000

H	-2.758670000	9.279481000	-4.511649000
H	-1.278596000	10.143486000	-4.938118000
H	-1.328594000	9.144286000	-7.230466000
H	-2.764996000	8.206937000	-6.808291000
H	-4.063958000	10.317730000	-6.438354000
H	-2.631784000	11.282937000	-6.838631000
H	-2.622562000	10.332771000	-9.152245000
H	-3.989289000	9.276928000	-8.734270000
H	-6.221629000	13.244725000	-9.504721000
H	-7.381469000	6.521629000	-6.873471000
H	-6.458325000	7.256700000	-8.227055000
H	-6.272660000	7.902126000	-6.563956000
H	-8.475422000	14.147314000	-9.633721000
H	-9.704491000	12.901741000	-10.002712000
H	-9.554981000	13.520517000	-8.352867000
H	-6.415715000	-1.965946000	0.019555000
H	-6.004601000	-4.067739000	4.126121000
H	-4.683775000	-2.881363000	4.198213000
H	-0.825096000	-0.125821000	4.387297000
H	-2.576008000	-0.477072000	4.589437000
H	-1.525606000	-1.623192000	3.680298000
H	-6.229637000	-0.358861000	-1.779588000
H	-5.587259000	1.220087000	-1.253869000
H	-4.538329000	0.085483000	-2.131733000
H	-4.578738000	-5.588230000	2.736622000
H	-3.283373000	-4.379139000	2.726831000
H	-3.083620000	-4.554003000	5.222231000
H	-4.381881000	-5.750667000	5.256496000
H	-3.007210000	-7.318536000	3.878260000
H	-1.727379000	-6.108476000	3.745728000
H	-1.392514000	-6.156742000	6.229731000
H	-2.678351000	-7.366791000	6.390116000
H	-1.348272000	-8.982454000	5.023816000
H	-0.106460000	-7.742451000	4.745799000
H	1.072343000	-9.151718000	8.981320000
H	2.583042000	-3.863568000	4.162673000
H	2.253620000	-5.628115000	4.112104000
H	1.138119000	-4.535713000	4.994677000
H	2.787357000	-8.818883000	10.671811000
H	4.324225000	-8.204881000	9.994111000
H	3.252461000	-7.103130000	10.868593000
Ag	-2.717532000	1.852749000	-0.317477000
H	-6.409934000	-3.500235000	1.881989000
H	1.130634000	6.913549000	-2.901439000
H	-0.586065000	-9.269690000	7.222915000
H	-4.064495000	12.184354000	-9.234589000

The optimized structures of compound L4, its complexes and coordinates for geometry-optimized structures

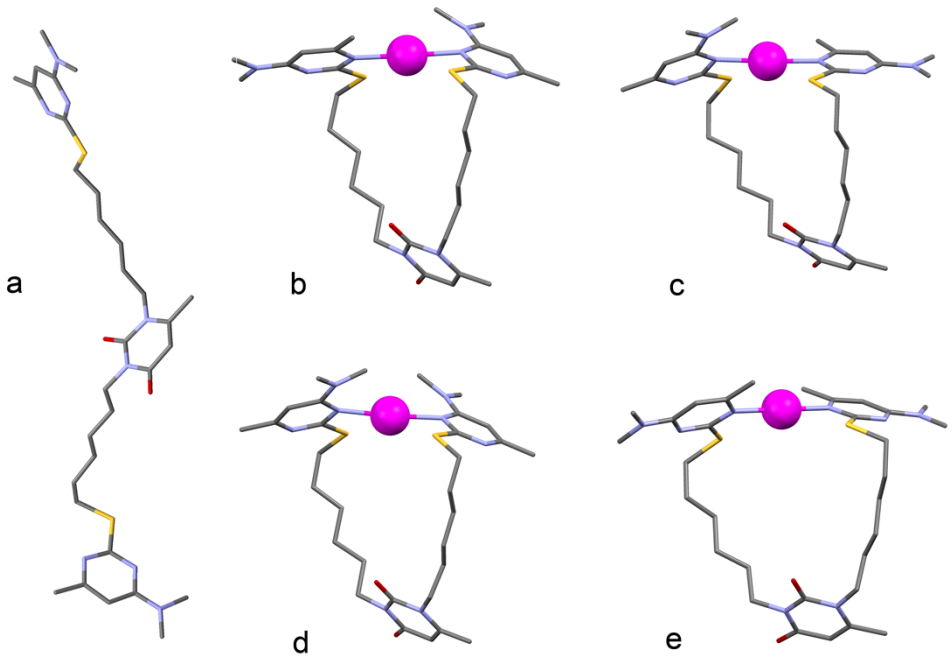


Fig. 3 The optimized structures of (a) compound L**4** and its complexes: [AgL**4**]$^{+}$ with the (b) N1-Ag^{+}-N3, (c) N3-Ag^{+}-N1, (d) N3-Ag^{+}-N3 and (e) N1-Ag^{+}-N1 coordination modes.

Coordinates of atoms for structure showed in figure 3a

91
C31N8H48S2O2

N	-11.633207000	-1.538340000	4.883985000
C	-10.428857000	-1.979896000	5.254444000
N	-10.123060000	-2.837106000	6.233675000
C	-11.159128000	-3.327043000	6.957020000
C	-12.491041000	-2.924025000	6.653856000
C	-12.674104000	-2.029279000	5.610049000
S	-8.974795000	-1.397104000	4.383625000
C	-9.693786000	-0.266661000	3.113230000
C	-8.631152000	0.695354000	2.584565000
C	-7.468236000	0.027677000	1.842543000
C	-6.488801000	1.039862000	1.241302000
C	-5.306491000	0.383344000	0.522221000
C	-4.376693000	1.429265000	-0.099482000
N	-3.217738000	0.842029000	-0.800758000
C	-3.443858000	0.453722000	-2.133276000
N	-2.365877000	-0.115858000	-2.803516000
C	-1.083660000	-0.329646000	-2.234353000
C	-0.964844000	0.073532000	-0.858901000
C	-1.999387000	0.643209000	-0.173831000
O	-4.541401000	0.617282000	-2.670319000
C	-1.840374000	1.084396000	1.250049000
O	-0.172371000	-0.830499000	-2.907772000
C	-2.580036000	-0.504329000	-4.209077000

C	-2.422218000	0.668019000	-5.181344000
C	-2.564558000	0.223872000	-6.640706000
C	-2.547297000	1.397134000	-7.625636000
C	-2.577071000	0.956829000	-9.091588000
C	-2.678269000	2.102482000	-10.097530000
S	-1.264533000	3.283293000	-10.075009000
C	-0.069432000	2.493504000	-11.153649000
N	-0.401712000	1.368533000	-11.789537000
C	0.563617000	0.854616000	-12.598669000
C	1.802133000	1.461502000	-12.748843000
C	2.041364000	2.660460000	-12.020722000
N	1.082965000	3.171707000	-11.209909000
C	0.213235000	-0.411978000	-13.323944000
N	3.215910000	3.340733000	-12.095770000
C	3.395162000	4.554124000	-11.300316000
N	-10.885022000	-4.199866000	7.964842000
C	-9.525706000	-4.638303000	8.258984000
C	-14.040018000	-1.547110000	5.215133000
H	-0.003351000	-0.080632000	-0.374275000
H	-0.850542000	0.786844000	1.613974000
H	-1.923430000	2.178322000	1.341592000
H	-2.600814000	0.637118000	1.906516000
H	-3.995906000	2.117227000	0.664572000
H	-4.926997000	2.022811000	-0.840262000
H	-1.838146000	-1.283232000	-4.424488000
H	-3.588133000	-0.932360000	-4.283536000
H	-5.675434000	-0.282241000	-0.274059000
H	-4.741438000	-0.244905000	1.231374000
H	-3.180499000	1.433142000	-4.949141000
H	-1.433069000	1.130976000	-5.030811000
H	-6.111005000	1.700691000	2.042062000
H	-7.029974000	1.691569000	0.532565000
H	-1.748869000	-0.477811000	-6.889711000
H	-3.506343000	-0.340459000	-6.763891000
H	-7.869902000	-0.615706000	1.039975000
H	-6.922103000	-0.641034000	2.530604000
H	-3.413356000	2.052595000	-7.422586000
H	-1.647243000	2.010687000	-7.450340000
H	-1.685975000	0.351308000	-9.324064000
H	-3.451183000	0.301058000	-9.258097000
H	-8.240603000	1.305042000	3.416911000
H	-9.141845000	1.394122000	1.899035000
H	-2.748334000	1.723118000	-11.124875000
H	-3.556420000	2.733553000	-9.893075000
H	-10.519000000	0.268634000	3.598108000
H	-10.112918000	-0.879821000	2.302676000
H	2.553364000	1.022164000	-13.402063000
H	-13.348166000	-3.298235000	7.209653000
H	-14.090722000	-0.450442000	5.292413000
H	-14.242953000	-1.803933000	4.164355000
H	-14.824245000	-1.984783000	5.845983000
H	1.040709000	-0.762347000	-13.954149000
H	-0.045218000	-1.201925000	-12.602548000

H	-0.673640000	-0.253185000	-13.956048000
C	-11.962791000	-4.771173000	8.762755000
C	4.303269000	2.843950000	-12.929868000
H	-8.831098000	-4.108805000	7.600632000
H	-9.273495000	-4.418149000	9.308149000
H	-9.425120000	-5.723327000	8.093478000
H	4.383880000	4.970236000	-11.521841000
H	2.626296000	5.302176000	-11.541549000
H	3.327635000	4.340278000	-10.222791000
H	-11.522029000	-5.424503000	9.523760000
H	-12.544379000	-3.989796000	9.277494000
H	-12.651111000	-5.374531000	8.148310000
H	5.144875000	3.540998000	-12.863995000
H	4.651979000	1.851693000	-12.598476000
H	4.001100000	2.770946000	-13.987232000

Coordinates of atoms for structure showed in figure 3b

92
AgC31N8H48S2O2

N	-8.762271000	-0.114218000	0.076976000
C	-8.576327000	-0.305891000	-1.213457000
N	-8.733067000	0.597057000	-2.214578000
C	-9.190828000	1.837055000	-1.860508000
C	-9.354257000	2.142084000	-0.480306000
C	-9.130953000	1.145323000	0.451565000
S	-8.097669000	-1.918699000	-1.828789000
Ag	-7.638438000	-0.000890000	-4.108366000
N	-6.577028000	-0.443032000	-6.013819000
C	-5.783041000	0.503147000	-6.574881000
N	-5.072045000	0.388102000	-7.677972000
C	-5.123864000	-0.802132000	-8.339947000
C	-5.948594000	-1.852315000	-7.842716000
C	-6.660012000	-1.634558000	-6.678116000
S	-5.790574000	2.039376000	-5.663901000
C	-4.508173000	3.048227000	-6.531569000
C	-3.072731000	2.738080000	-6.114057000
C	-2.776089000	3.019527000	-4.639599000
C	-1.376334000	2.581723000	-4.194259000
C	-1.230096000	2.598672000	-2.670185000
C	0.097790000	2.004170000	-2.179172000
N	0.002850000	1.564023000	-0.775984000
C	-0.636874000	0.348214000	-0.560534000
N	-0.837117000	-0.029827000	0.777466000
C	-0.397963000	0.751327000	1.833129000
C	0.252202000	1.926885000	1.586048000
C	0.467087000	2.423801000	0.252093000
O	-1.026309000	-0.361917000	-1.490988000
C	-1.661161000	-1.241802000	0.961557000
C	-3.158856000	-0.946838000	0.808286000
C	-3.995332000	-2.214831000	0.616760000
C	-5.470303000	-1.907454000	0.336045000
C	-6.285644000	-3.153765000	-0.012179000

C	-7.764121000	-2.895087000	-0.291922000
C	-0.636964000	0.268355000	3.231489000
O	1.001006000	3.505562000	-0.027398000
C	-7.546359000	-2.682520000	-6.080359000
N	-4.382729000	-0.941565000	-9.460574000
C	-3.552646000	0.138484000	-9.987989000
N	-9.484267000	2.738082000	-2.827802000
C	-9.652209000	2.357305000	-4.227160000
C	-9.305402000	1.373977000	1.920705000
H	0.606638000	2.541619000	2.410459000
H	-0.258165000	1.010427000	3.943106000
H	-1.707153000	0.111408000	3.432429000
H	-0.119128000	-0.684505000	3.420025000
H	-1.343374000	-1.960117000	0.195324000
H	-1.430098000	-1.671618000	1.942107000
H	0.911202000	2.737398000	-2.223406000
H	0.367304000	1.125500000	-2.779261000
H	-3.520968000	-0.378049000	1.681314000
H	-3.293633000	-0.301328000	-0.073900000
H	-2.053058000	2.002170000	-2.244923000
H	-1.341203000	3.623839000	-2.280916000
H	-3.579040000	-2.789310000	-0.229706000
H	-3.912032000	-2.865330000	1.504974000
H	-0.608712000	3.219176000	-4.665868000
H	-1.191976000	1.553246000	-4.552416000
H	-5.921588000	-1.404975000	1.208643000
H	-5.531970000	-1.190304000	-0.501120000
H	-3.519936000	2.482851000	-4.025123000
H	-2.918434000	4.094310000	-4.430444000
H	-2.410336000	3.345895000	-6.755627000
H	-2.849638000	1.684383000	-6.347456000
H	-5.827475000	-3.671321000	-0.871815000
H	-6.247127000	-3.867454000	0.830045000
H	-4.788908000	4.082980000	-6.285647000
H	-4.669520000	2.888357000	-7.605212000
H	-8.313483000	-3.834486000	-0.436324000
H	-8.246032000	-2.317359000	0.510466000
H	-6.028623000	-2.810335000	-8.350212000
H	-9.692757000	3.123693000	-0.159052000
H	-10.056011000	0.677984000	2.324456000
H	-8.361380000	1.166164000	2.447145000
H	-9.616339000	2.402810000	2.138954000
H	-7.559691000	-3.592921000	-6.691434000
H	-7.199363000	-2.945745000	-5.068855000
H	-8.577714000	-2.306830000	-5.989699000
C	-9.791440000	4.126218000	-2.479987000
C	-4.416851000	-2.187829000	-10.223237000
H	-8.720127000	2.474860000	-4.807496000
H	-10.010131000	1.322578000	-4.304136000
H	-10.412298000	3.009874000	-4.675281000
H	-2.511722000	-0.204482000	-10.083598000
H	-3.916444000	0.446542000	-10.980457000
H	-3.593490000	0.991994000	-9.306486000

H	-9.684991000	4.739599000	-3.381451000
H	-10.820458000	4.235483000	-2.099700000
H	-9.086235000	4.505563000	-1.729522000
H	-3.724439000	-2.095743000	-11.066334000
H	-4.098001000	-3.042224000	-9.607348000
H	-5.423593000	-2.388475000	-10.621787000

Coordinates of atoms for structure showed in figure 3c

92
AgC31N8H48S2O2

N	-8.102595000	0.528944000	-2.197800000
C	-8.062750000	-0.438283000	-1.248587000
N	-8.423866000	-0.322962000	0.012824000
C	-8.881846000	0.889799000	0.432206000
C	-8.986851000	1.963615000	-0.497848000
C	-8.588045000	1.744478000	-1.802564000
S	-7.477874000	-2.003597000	-1.887353000
C	-7.356238000	-3.080909000	-0.388694000
C	-5.922442000	-3.318687000	0.084056000
C	-5.206078000	-2.065267000	0.588856000
C	-3.731881000	-2.300045000	0.936176000
C	-2.987973000	-0.986857000	1.195504000
C	-1.470025000	-1.167738000	1.340340000
N	-0.744455000	0.090796000	1.072505000
C	-0.609049000	0.408950000	-0.289656000
N	-0.083750000	1.661064000	-0.588050000
C	0.323049000	2.615365000	0.379496000
C	0.184031000	2.177413000	1.743947000
C	-0.353178000	0.965189000	2.071961000
O	-0.956687000	-0.383724000	-1.168465000
C	-0.517878000	0.542089000	3.500129000
O	0.750974000	3.722706000	0.027412000
C	-0.042470000	2.024861000	-2.015440000
C	-1.412265000	2.494713000	-2.522274000
C	-1.511720000	2.495795000	-4.049872000
C	-2.907047000	2.891051000	-4.545794000
C	-3.096944000	2.677596000	-6.048820000
C	-4.467779000	3.079458000	-6.582368000
S	-5.893015000	2.119407000	-5.899792000
Ag	-7.385115000	0.114514000	-4.267052000
N	-6.743365000	-0.311852000	-6.405216000
C	-5.867110000	0.616924000	-6.869085000
N	-5.070417000	0.521490000	-7.915417000
C	-5.119516000	-0.658465000	-8.599790000
C	-5.994820000	-1.667870000	-8.243556000
C	-6.861133000	-1.463830000	-7.133303000
C	-4.191411000	-0.784429000	-9.767329000
N	-7.799569000	-2.377676000	-6.788036000
C	-8.879664000	-2.071767000	-5.855844000
N	-9.227685000	1.029079000	1.730800000
C	-9.179138000	-0.082886000	2.676581000
C	-8.661593000	2.817068000	-2.844039000

H	0.501563000	2.866149000	2.523693000
H	-0.185183000	1.350521000	4.160679000
H	-1.566461000	0.310034000	3.738976000
H	0.081219000	-0.353794000	3.723879000
H	-1.111069000	-1.900961000	0.607298000
H	-1.190856000	-1.524048000	2.337428000
H	0.712472000	2.813380000	-2.115696000
H	0.284698000	1.135749000	-2.569786000
H	-3.395416000	-0.481686000	2.087346000
H	-3.169342000	-0.317447000	0.339945000
H	-2.184189000	1.816222000	-2.124759000
H	-1.625231000	3.499450000	-2.121771000
H	-3.243714000	-2.817840000	0.091733000
H	-3.647617000	-2.973427000	1.806637000
H	-0.755733000	3.174151000	-4.482203000
H	-1.269992000	1.483834000	-4.420774000
H	-5.741369000	-1.658568000	1.463957000
H	-5.259536000	-1.289300000	-0.194564000
H	-3.661228000	2.295989000	-4.001642000
H	-3.104509000	3.948110000	-4.294219000
H	-2.354372000	3.277442000	-6.604888000
H	-2.900483000	1.625206000	-6.309798000
H	-5.337729000	-3.775222000	-0.732206000
H	-5.971507000	-4.075065000	0.887196000
H	-4.717678000	4.119024000	-6.323820000
H	-4.531052000	2.961673000	-7.671680000
H	-7.843738000	-4.021424000	-0.676696000
H	-7.971025000	-2.581157000	0.373052000
H	-6.041275000	-2.581488000	-8.830395000
H	-9.371750000	2.938807000	-0.210754000
H	-7.657556000	3.038802000	-3.238172000
H	-9.284119000	2.488284000	-3.691012000
H	-9.087098000	3.742211000	-2.437310000
H	-4.298252000	-1.752629000	-10.271335000
H	-4.385451000	0.021165000	-10.491465000
H	-3.149545000	-0.667806000	-9.432213000
C	-9.750486000	2.299985000	2.228036000
C	-7.826936000	-3.688918000	-7.438208000
H	-10.194913000	-0.336244000	3.018244000
H	-8.734243000	-0.954294000	2.189824000
H	-8.572505000	0.198789000	3.549814000
H	-9.743929000	-2.697944000	-6.108192000
H	-8.602892000	-2.285324000	-4.807842000
H	-9.186628000	-1.021618000	-5.951546000
H	-8.454470000	-4.358248000	-6.840253000
H	-8.244354000	-3.632788000	-8.456936000
H	-6.819744000	-4.123471000	-7.484983000
H	-9.882441000	2.218460000	3.311974000
H	-9.049680000	3.123900000	2.028561000
H	-10.725928000	2.540995000	1.776415000

Coordinates of atoms for structure showed in figure 3d

92
AgC31N8H48S2O2
N -8.496120000 -0.185398000 -0.054280000
C -8.335858000 -0.346108000 -1.352410000
N -8.535426000 0.572149000 -2.331330000
C -8.996871000 1.799290000 -1.939114000
C -9.126453000 2.074469000 -0.549325000
C -8.874558000 1.059869000 0.355633000
S -7.817644000 -1.931099000 -2.006446000
C -7.548016000 -2.970519000 -0.497726000
C -6.083164000 -3.210608000 -0.141578000
C -5.326866000 -1.963362000 0.316955000
C -3.858152000 -2.236091000 0.658509000
C -3.083599000 -0.946184000 0.941001000
C -1.577147000 -1.174236000 1.126638000
N -0.811999000 0.076281000 0.945334000
C -0.627904000 0.459417000 -0.393656000
N -0.077155000 1.717018000 -0.612646000
C 0.324109000 2.610573000 0.413247000
C 0.142314000 2.103955000 1.748686000
C -0.430399000 0.889331000 1.998969000
O -0.959940000 -0.281791000 -1.322058000
C -0.644297000 0.397707000 3.398346000
O 0.781170000 3.726332000 0.131163000
C -0.010773000 2.155837000 -2.017716000
C -1.379661000 2.634783000 -2.522406000
C -1.495636000 2.619284000 -4.048565000
C -2.909500000 2.965518000 -4.528225000
C -3.119813000 2.716760000 -6.022681000
C -4.524882000 3.026420000 -6.526609000
S -5.870233000 1.979753000 -5.805399000
Ag -7.547040000 0.002375000 -4.310539000
N -6.678448000 -0.454164000 -6.376059000
C -5.790575000 0.487604000 -6.787789000
N -4.936340000 0.407702000 -7.789260000
C -4.926559000 -0.771845000 -8.475530000
C -5.794326000 -1.801079000 -8.160339000
C -6.725518000 -1.612940000 -7.101187000
C -3.940065000 -0.876543000 -9.596322000
N -7.660309000 -2.548967000 -6.806549000
C -8.828185000 -2.258027000 -5.982088000
N -9.331252000 2.716344000 -2.878637000
C -9.584264000 2.356939000 -4.270680000
C -9.024399000 1.253168000 1.832499000
H 0.453667000 2.743697000 2.571471000
H -0.308577000 1.161547000 4.108556000
H -1.704712000 0.182846000 3.597948000
H -0.075318000 -0.524805000 3.590123000
H -1.211303000 -1.881806000 0.372059000
H -1.343402000 -1.584548000 2.114669000
H 0.738099000 2.954938000 -2.061095000
H 0.336134000 1.300328000 -2.611647000
H -3.498654000 -0.435430000 1.826211000

H	-3.222622000	-0.266420000	0.085655000
H	-2.153750000	1.965286000	-2.114566000
H	-1.584720000	3.643647000	-2.128493000
H	-3.380182000	-2.756524000	-0.190255000
H	-3.793742000	-2.921586000	1.521434000
H	-0.764988000	3.313585000	-4.498500000
H	-1.230733000	1.610071000	-4.410873000
H	-5.840026000	-1.522377000	1.188330000
H	-5.369547000	-1.203784000	-0.483181000
H	-3.635076000	2.356922000	-3.960352000
H	-3.136166000	4.020230000	-4.292038000
H	-2.428281000	3.350527000	-6.606266000
H	-2.868318000	1.673911000	-6.273239000
H	-5.561100000	-3.671447000	-0.997000000
H	-6.076823000	-3.966045000	0.664300000
H	-4.836039000	4.049295000	-6.267995000
H	-4.606142000	2.895717000	-7.613161000
H	-8.066553000	-3.912501000	-0.719068000
H	-8.087921000	-2.440657000	0.300501000
H	-5.791070000	-2.715580000	-8.747622000
H	-9.470386000	3.044415000	-0.199602000
H	-9.757604000	0.537787000	2.234376000
H	-8.067780000	1.046902000	2.336321000
H	-9.345096000	2.272336000	2.079944000
H	-4.002202000	-1.845952000	-10.105462000
H	-4.114629000	-0.073873000	-10.328596000
H	-2.918539000	-0.739289000	-9.210286000
C	-9.634739000	4.095810000	-2.496039000
C	-7.612340000	-3.868628000	-7.437909000
H	-8.702384000	2.521027000	-4.913321000
H	-9.909571000	1.311060000	-4.342537000
H	-10.400133000	2.986599000	-4.649261000
H	-9.665330000	-2.873707000	-6.334528000
H	-8.660862000	-2.493230000	-4.916692000
H	-9.122872000	-1.205486000	-6.090897000
H	-8.229051000	-4.556021000	-6.848495000
H	-8.000105000	-3.844994000	-8.469798000
H	-6.587115000	-4.259938000	-7.445911000
H	-9.544802000	4.728343000	-3.386386000
H	-10.657244000	4.196142000	-2.095637000
H	-8.916523000	4.460022000	-1.750917000

Coordinates of atoms for structure showed in figure 3e

92
AgC31N8H48S2O2

N	-8.401754000	0.496290000	-2.117250000
C	-8.327481000	-0.417111000	-1.118377000
N	-8.707094000	-0.248974000	0.132876000
C	-9.229320000	0.961512000	0.474193000
C	-9.379292000	1.977409000	-0.511772000
C	-8.952075000	1.706900000	-1.797877000
S	-7.673881000	-1.988028000	-1.666236000
C	-7.500524000	-2.959581000	-0.100808000
C	-6.047798000	-3.216028000	0.298909000
C	-5.259838000	-1.959809000	0.674419000
C	-3.781299000	-2.236472000	0.968942000
C	-2.965904000	-0.948546000	1.115763000
C	-1.458357000	-1.207950000	1.237761000
N	-0.664683000	0.005215000	0.954444000
C	-0.515273000	0.304813000	-0.410285000
N	0.100372000	1.512794000	-0.719315000
C	0.580986000	2.440873000	0.239646000
C	0.414477000	2.024429000	1.607633000
C	-0.206456000	0.855887000	1.946125000
O	-0.925269000	-0.465224000	-1.282302000
C	-0.392982000	0.455205000	3.378100000
O	1.089159000	3.510601000	-0.122128000
C	0.156324000	1.866480000	-2.148945000
C	-1.178953000	2.441531000	-2.639149000
C	-1.321819000	2.420137000	-4.163517000
C	-2.708395000	2.890386000	-4.616550000
C	-2.996486000	2.632098000	-6.097048000
C	-4.404700000	3.024507000	-6.537385000
S	-5.754176000	2.084984000	-5.694476000
C	-5.866956000	0.590641000	-6.664914000
N	-6.682680000	-0.338086000	-6.106381000
C	-6.874139000	-1.489271000	-6.818057000
C	-6.237621000	-1.690813000	-8.028176000
C	-5.378083000	-0.665556000	-8.515855000
N	-5.219407000	0.488280000	-7.808928000
Ag	-7.546705000	0.044973000	-4.106589000
C	-7.795466000	-2.507167000	-6.221117000
N	-4.696888000	-0.772859000	-9.676060000
C	-3.839227000	0.329069000	-10.119192000
N	-9.592562000	1.133233000	1.762752000
C	-9.420516000	0.036469000	2.718042000
C	-9.065583000	2.711005000	-2.902310000
H	0.783236000	2.694114000	2.381403000
H	-0.006854000	1.245822000	4.031095000
H	-1.453255000	0.292147000	3.622083000
H	0.148798000	-0.475162000	3.607318000
H	-1.151616000	-1.964110000	0.504150000
H	-1.186301000	-1.575057000	2.233100000
H	0.971097000	2.591210000	-2.260978000

H	0.404367000	0.951517000	-2.702127000
H	-3.319710000	-0.365040000	1.982409000
H	-3.134497000	-0.328224000	0.221454000
H	-1.995244000	1.838529000	-2.209783000
H	-1.298520000	3.467844000	-2.255119000
H	-3.356393000	-2.827927000	0.138688000
H	-3.685924000	-2.859083000	1.875516000
H	-0.538863000	3.040150000	-4.633439000
H	-1.157609000	1.387261000	-4.518938000
H	-5.733001000	-1.471535000	1.543998000
H	-5.323476000	-1.239062000	-0.159330000
H	-3.470440000	2.365972000	-4.013918000
H	-2.827377000	3.966391000	-4.398823000
H	-2.290072000	3.205558000	-6.723256000
H	-2.827290000	1.568585000	-6.332663000
H	-5.528597000	-3.747725000	-0.516256000
H	-6.070798000	-3.914715000	1.153783000
H	-4.629106000	4.073754000	-6.295965000
H	-4.557159000	2.869407000	-7.613123000
H	-8.036894000	-3.900080000	-0.281280000
H	-8.047184000	-2.376407000	0.654491000
H	-6.398620000	-2.616545000	-8.575173000
H	-9.812136000	2.947268000	-0.279360000
H	-8.071938000	2.937571000	-3.320020000
H	-9.685278000	2.311027000	-3.720201000
H	-9.515723000	3.646482000	-2.549138000
H	-7.875909000	-3.397482000	-6.856212000
H	-7.432887000	-2.817637000	-5.228492000
H	-8.801872000	-2.080066000	-6.087968000
C	-10.182519000	2.396440000	2.201673000
C	-4.826493000	-1.972634000	-10.500514000
H	-10.031328000	-0.833856000	2.436678000
H	-8.369782000	-0.282664000	2.762439000
H	-9.731056000	0.387942000	3.706853000
H	-3.351529000	0.032514000	-11.052962000
H	-4.426985000	1.242059000	-10.293497000
H	-3.071307000	0.555147000	-9.366388000
H	-10.392637000	2.331785000	3.273360000
H	-9.492998000	3.238403000	2.035165000
H	-11.127943000	2.602290000	1.675729000
H	-4.193534000	-1.860076000	-11.385681000
H	-4.499297000	-2.870618000	-9.953862000
H	-5.865436000	-2.119483000	-10.834964000

The optimized structures of compound L5a, its complexes and coordinates for geometry-optimized structures

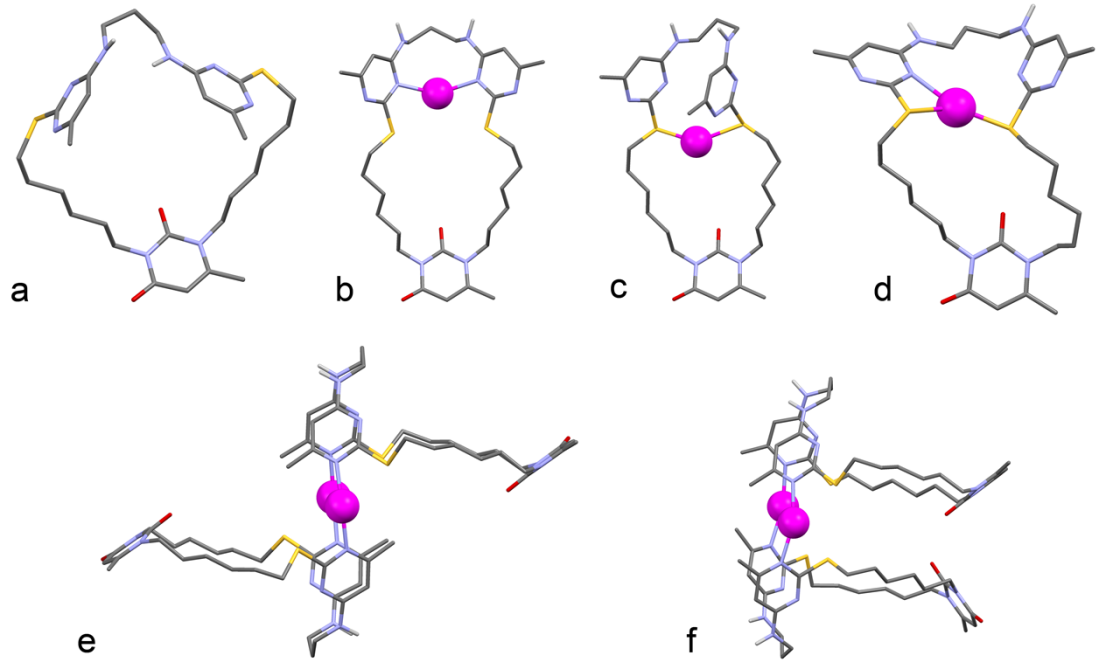


Fig. 4 The optimized structures of (a) compound L**5a** and its complexes: [AgL**5a**]$^{+}$ with the (b) N3-Ag^{+}-N3, (c) S-Ag^{+}-S, (d) N3,S-Ag^{+}-S coordination modes; isomers of complex [Ag_2L**5a**$_2$]$^{2+}$ with the (e) N1,N1-Ag^{+}-N1',N1' (*trans*) and (f) N1,N1-Ag^{+}-N1',N1'(*cis*) coordination modes. Only hydrogen atoms of NH groups are shown.

Coordinates of atoms for structure showed in figure 4a

86
C30N8H44S2O2

C	-0.409395000	0.274896000	-0.157821000
N	-0.698634000	-0.340421000	1.073346000
C	-0.269040000	-1.621904000	1.373177000
C	0.469918000	-2.324591000	0.465110000
C	0.810090000	-1.789702000	-0.825849000
N	0.347164000	-0.469539000	-1.058491000
C	-1.592257000	0.417643000	1.973018000
C	-0.611888000	-2.201822000	2.712448000
H	0.814693000	-3.329904000	0.696549000
O	1.453286000	-2.391829000	-1.697070000
C	0.630188000	0.147999000	-2.366220000
O	-0.806940000	1.412808000	-0.414412000
H	-0.238770000	-3.230543000	2.769107000
H	-0.150750000	-1.623998000	3.528078000
H	-1.697470000	-2.216644000	2.888331000
C	-3.071668000	0.208341000	1.637981000

H	-1.372531000	0.115157000	3.003515000
H	-1.327005000	1.476998000	1.869668000
C	-0.504773000	-0.063646000	-3.372666000
H	0.798431000	1.218715000	-2.194669000
H	1.557085000	-0.312707000	-2.729695000
C	-4.006831000	0.950018000	2.597702000
H	-3.250427000	0.553543000	0.607179000
H	-3.304586000	-0.869983000	1.658387000
C	-0.201543000	0.584813000	-4.726389000
H	-0.669338000	-1.145555000	-3.506068000
H	-1.434404000	0.361134000	-2.960310000
C	-5.477019000	0.808194000	2.192230000
H	-3.863462000	0.566424000	3.623937000
H	-3.735399000	2.020156000	2.625154000
C	-1.350794000	0.440918000	-5.729081000
H	0.014786000	1.657802000	-4.577127000
H	0.716742000	0.139843000	-5.149451000
C	-6.451569000	1.465478000	3.171091000
H	-5.615921000	1.248376000	1.190598000
H	-5.732256000	-0.260663000	2.092579000
C	-1.048537000	1.083768000	-7.084583000
H	-1.580943000	-0.628770000	-5.877832000
H	-2.260845000	0.899587000	-5.305841000
C	-2.206244000	1.031439000	-8.083514000
H	-0.730368000	2.130301000	-6.937026000
H	-0.190977000	0.568902000	-7.552728000
C	-7.920786000	1.371547000	2.752463000
H	-6.360707000	0.980724000	4.160068000
H	-6.177467000	2.524032000	3.319356000
S	-3.608103000	2.130585000	-7.596891000
H	-1.881022000	1.359775000	-9.079730000
H	-2.640062000	0.024496000	-8.168740000
S	-8.348504000	2.394067000	1.279159000
H	-8.207396000	0.341415000	2.497964000
H	-8.580668000	1.737909000	3.550769000
C	-5.015281000	1.025277000	-7.525329000
C	-8.320375000	1.218561000	-0.077833000
N	-4.883168000	-0.251161000	-7.879822000
C	-6.016372000	-1.002473000	-7.815720000
C	-7.226498000	-0.461429000	-7.408845000
C	-7.243233000	0.910497000	-7.047991000
N	-6.126426000	1.658004000	-7.111874000
C	-5.881467000	-2.442508000	-8.214590000
H	-8.132207000	-1.068137000	-7.364061000
N	-8.393708000	1.493615000	-6.580029000
N	-8.455935000	1.826338000	-1.267178000
C	-8.443792000	1.016136000	-2.347754000
C	-8.273973000	-0.388356000	-2.202929000
C	-8.156426000	-0.892370000	-0.919619000
N	-8.185421000	-0.080452000	0.175381000
N	-8.610064000	1.574604000	-3.573081000
H	-8.249078000	-1.044907000	-3.074061000
C	-7.989736000	-2.359611000	-0.651773000

H	-8.797708000	-2.719060000	0.003226000
H	-7.997506000	-2.945403000	-1.579891000
H	-7.041785000	-2.543016000	-0.123380000
H	-6.836381000	-2.977545000	-8.135943000
H	-5.515625000	-2.515400000	-9.249898000
H	-5.137778000	-2.942519000	-7.575934000
H	-8.451089000	0.990180000	-4.391522000
C	-8.719833000	3.009134000	-3.818551000
H	-9.247472000	0.969006000	-6.760864000
H	-7.723164000	3.487507000	-3.780493000
C	-9.383914000	3.302721000	-5.165777000
H	-9.311356000	3.445364000	-3.002353000
H	-9.577453000	4.385931000	-5.211428000
C	-8.554375000	2.941282000	-6.402217000
H	-10.369948000	2.809287000	-5.208847000
H	-9.026596000	3.374755000	-7.301081000
H	-7.544835000	3.365224000	-6.326470000

Coordinates of atoms for structure showed in figure 4b

87
AgC30N8H44S2O2

C	0.516631000	0.991568000	0.329792000
N	0.419296000	0.549475000	1.660905000
C	1.399436000	-0.238051000	2.241453000
C	2.485010000	-0.624052000	1.507970000
C	2.608685000	-0.331790000	0.103487000
N	1.575393000	0.488615000	-0.418745000
C	-0.895654000	0.793873000	2.292821000
C	1.247080000	-0.629328000	3.680074000
H	3.270157000	-1.223555000	1.963288000
O	3.514490000	-0.747117000	-0.631570000
C	1.505244000	0.717124000	-1.874889000
O	-0.324734000	1.752584000	-0.153156000
H	2.117387000	-1.217556000	3.991741000
H	1.174079000	0.254436000	4.331796000
H	0.345561000	-1.239314000	3.842567000
C	-1.941468000	-0.178919000	1.732752000
H	-0.783743000	0.703547000	3.378219000
H	-1.180503000	1.828889000	2.066201000
C	0.444539000	-0.199178000	-2.498224000
H	1.253806000	1.772492000	-2.041747000
H	2.506753000	0.514990000	-2.271612000
C	-3.390829000	0.145665000	2.112588000
H	-1.861331000	-0.148884000	0.634695000
H	-1.692092000	-1.208147000	2.040215000
C	0.116317000	0.101069000	-3.964390000
H	0.767042000	-1.247982000	-2.392500000
H	-0.481574000	-0.086712000	-1.912016000
C	-4.368581000	-0.541763000	1.151999000
H	-3.597116000	-0.160803000	3.152235000
H	-3.552032000	1.236908000	2.068744000
C	-1.205383000	-0.561288000	-4.370289000

H	0.031756000	1.192086000	-4.111401000
H	0.933320000	-0.242282000	-4.621525000
C	-5.845994000	-0.379841000	1.516054000
H	-4.192681000	-0.134755000	0.139511000
H	-4.132263000	-1.618928000	1.091827000
C	-1.581002000	-0.391271000	-5.843993000
H	-1.167079000	-1.639193000	-4.132826000
H	-2.006255000	-0.138532000	-3.736244000
C	-2.967020000	-0.931846000	-6.187068000
H	-1.518074000	0.670097000	-6.135971000
H	-0.855757000	-0.933783000	-6.474646000
C	-6.795856000	-0.938723000	0.459674000
H	-6.053976000	-0.916245000	2.458014000
H	-6.083524000	0.680931000	1.699995000
S	-4.289050000	0.115367000	-5.414205000
H	-3.179161000	-0.902165000	-7.263387000
H	-3.101231000	-1.962427000	-5.830790000
S	-6.793686000	0.111428000	-1.069654000
H	-6.517656000	-1.959472000	0.163180000
H	-7.843836000	-0.941095000	0.787266000
C	-5.565586000	0.118871000	-6.656381000
C	-8.527004000	0.215729000	-1.477236000
N	-5.440686000	-0.590766000	-7.764999000
C	-6.483795000	-0.542633000	-8.641158000
C	-7.586119000	0.265758000	-8.407941000
C	-7.609193000	1.043189000	-7.227929000
N	-6.613233000	0.911850000	-6.314057000
C	-6.354273000	-1.380400000	-9.874189000
H	-8.394646000	0.343661000	-9.135241000
N	-8.628477000	1.919066000	-6.971756000
N	-8.751044000	1.004138000	-2.559263000
C	-10.046289000	1.193507000	-2.922717000
C	-11.073219000	0.483729000	-2.257413000
C	-10.728606000	-0.316976000	-1.180266000
N	-9.434545000	-0.427983000	-0.765068000
N	-10.331439000	2.055552000	-3.942940000
H	-12.113321000	0.609195000	-2.559595000
C	-11.746756000	-1.079130000	-0.391859000
H	-11.510776000	-2.153840000	-0.417169000
H	-11.715707000	-0.769974000	0.663672000
H	-12.760723000	-0.926761000	-0.780837000
H	-7.225010000	-1.274422000	-10.532393000
H	-5.446758000	-1.098535000	-10.428844000
H	-6.242081000	-2.439227000	-9.595520000
H	-11.327572000	2.104955000	-4.152387000
C	-9.638932000	3.341806000	-4.121988000
H	-9.339940000	1.917994000	-7.701624000
H	-8.636190000	3.259897000	-3.678512000
C	-9.539348000	3.821955000	-5.570913000
H	-10.177020000	4.104168000	-3.532238000
H	-9.388953000	4.912315000	-5.530625000
C	-8.389130000	3.258282000	-6.405640000
H	-10.500512000	3.673799000	-6.090638000

H	-8.185622000	3.951622000	-7.240297000
H	-7.469600000	3.218162000	-5.804608000
Ag	-7.082033000	1.143346000	-4.101262000

Coordinates of atoms for structure showed in figure 4c

87
AgC30N8H44S2O2

C	0.657628000	0.495756000	0.346699000
N	0.477586000	0.200213000	1.708865000
C	1.204599000	-0.793554000	2.342501000
C	2.108224000	-1.532247000	1.632805000
C	2.272235000	-1.389058000	0.209268000
N	1.507453000	-0.341529000	-0.366781000
C	-0.689021000	0.867321000	2.325476000
C	0.989022000	-1.015552000	3.808722000
H	2.698475000	-2.300341000	2.127594000
O	2.996703000	-2.100962000	-0.498564000
C	1.480188000	-0.188297000	-1.833172000
O	0.051657000	1.426128000	-0.190104000
H	1.657560000	-1.809657000	4.159442000
H	1.199478000	-0.103848000	4.388093000
H	-0.046391000	-1.318027000	4.026824000
C	-1.990768000	0.204820000	1.851954000
H	-0.576869000	0.833729000	3.413910000
H	-0.664317000	1.918925000	2.013968000
C	0.186099000	-0.781944000	-2.406310000
H	1.547799000	0.883208000	-2.061991000
H	2.370674000	-0.698480000	-2.217827000
C	-3.253843000	1.039378000	2.087546000
H	-1.896485000	0.034426000	0.767921000
H	-2.096294000	-0.787863000	2.320205000
C	-0.090017000	-0.400396000	-3.863211000
H	0.209580000	-1.878573000	-2.298219000
H	-0.652723000	-0.414599000	-1.793796000
C	-4.410532000	0.542042000	1.212613000
H	-3.544185000	1.015691000	3.151625000
H	-3.047746000	2.095376000	1.840879000
C	-1.542155000	-0.699758000	-4.252555000
H	0.102554000	0.677512000	-4.004238000
H	0.598690000	-0.933830000	-4.540276000
C	-5.726510000	1.291656000	1.428909000
H	-4.103995000	0.633499000	0.155181000
H	-4.576855000	-0.534451000	1.393137000
C	-1.875138000	-0.364909000	-5.708161000
H	-1.766479000	-1.764736000	-4.065124000
H	-2.200567000	-0.121211000	-3.577361000
C	-3.336951000	-0.582395000	-6.091954000
H	-1.580992000	0.672943000	-5.936797000
H	-1.276704000	-1.008550000	-6.374913000
C	-6.826412000	0.913174000	0.438593000
H	-6.113820000	1.070704000	2.437700000
H	-5.557407000	2.381519000	1.401645000

S	-4.415354000	0.715829000	-5.318154000
H	-3.496989000	-0.465688000	-7.170404000
H	-3.705172000	-1.571214000	-5.791471000
S	-6.548809000	1.741881000	-1.211934000
H	-6.869770000	-0.170974000	0.267251000
H	-7.807642000	1.269022000	0.777769000
C	-5.985254000	0.520545000	-6.229293000
C	-7.869801000	0.925590000	-2.172877000
N	-6.051988000	-0.450790000	-7.121748000
C	-7.232218000	-0.523250000	-7.812898000
C	-8.260577000	0.364703000	-7.564650000
C	-8.063003000	1.367149000	-6.573733000
N	-6.892098000	1.443528000	-5.894540000
C	-7.332077000	-1.606912000	-8.841979000
H	-9.199502000	0.307636000	-8.117490000
N	-9.053483000	2.249320000	-6.293040000
N	-8.922571000	1.657206000	-2.481275000
C	-9.863859000	1.051617000	-3.258119000
C	-9.759955000	-0.331778000	-3.559838000
C	-8.594429000	-0.990189000	-3.211801000
N	-7.597753000	-0.339040000	-2.534323000
N	-10.874250000	1.814219000	-3.728446000
H	-10.545551000	-0.844555000	-4.116167000
C	-8.332598000	-2.418069000	-3.576659000
H	-7.448808000	-2.486998000	-4.230140000
H	-8.111664000	-3.006519000	-2.673913000
H	-9.188571000	-2.865751000	-4.095591000
H	-8.311061000	-1.608023000	-9.337015000
H	-6.548055000	-1.477196000	-9.603420000
H	-7.165014000	-2.589657000	-8.375819000
H	-11.544250000	1.356785000	-4.341728000
C	-10.866400000	3.275747000	-3.705658000
H	-9.853828000	2.224035000	-6.920535000
H	-10.257386000	3.579239000	-2.845782000
C	-10.320891000	3.925347000	-4.990501000
H	-11.894963000	3.621445000	-3.528366000
H	-10.266015000	5.008065000	-4.798628000
C	-8.937852000	3.443458000	-5.454815000
H	-11.045186000	3.804661000	-5.814710000
H	-8.441675000	4.248016000	-6.024855000
H	-8.289114000	3.208988000	-4.600749000
Ag	-5.236396000	0.115024000	-2.964596000

Coordinates of atoms for structure showed in figure 4d

87
AgC30N8H44S2O2

C	-1.042262000	1.181882000	0.175796000
N	-0.809852000	1.034308000	1.554778000
C	0.452743000	0.760841000	2.057728000
C	1.501360000	0.557800000	1.207880000
C	1.346243000	0.591528000	-0.221343000
N	0.041477000	0.936113000	-0.662264000

C	-1.986895000	1.112208000	2.445626000
C	0.633876000	0.725887000	3.544689000
H	2.494003000	0.346474000	1.599229000
O	2.244355000	0.357605000	-1.041018000
C	-0.213726000	1.001455000	-2.111374000
O	-2.147513000	1.502863000	-0.267963000
H	1.678143000	0.493135000	3.780819000
H	0.386785000	1.699740000	3.995018000
H	-0.006159000	-0.029650000	4.021900000
C	-2.482058000	-0.267750000	2.952840000
H	-1.728448000	1.769688000	3.284624000
H	-2.766241000	1.615995000	1.863465000
C	-0.883253000	-0.272058000	-2.635510000
H	-0.850558000	1.875791000	-2.299157000
H	0.762490000	1.153272000	-2.587579000
C	-3.917784000	-0.633345000	2.547943000
H	-1.797550000	-1.052483000	2.590455000
H	-2.413431000	-0.286799000	4.051454000
C	-1.180345000	-0.204821000	-4.135974000
H	-0.233256000	-1.136285000	-2.421805000
H	-1.824617000	-0.425957000	-2.083134000
C	-4.105952000	-0.924406000	1.055248000
H	-4.217916000	-1.522532000	3.128774000
H	-4.603769000	0.175829000	2.855219000
C	-2.026476000	-1.387896000	-4.614926000
H	-1.713120000	0.735635000	-4.364710000
H	-0.233839000	-0.170032000	-4.702623000
C	-5.514082000	-1.424899000	0.721253000
H	-3.880781000	-0.019702000	0.467106000
H	-3.371165000	-1.687760000	0.740426000
C	-2.304792000	-1.376269000	-6.119256000
H	-1.529044000	-2.335644000	-4.344995000
H	-2.986309000	-1.380531000	-4.065211000
C	-3.277021000	-2.454113000	-6.587749000
H	-2.675996000	-0.385443000	-6.432263000
H	-1.360135000	-1.533479000	-6.668198000
C	-5.768429000	-1.621003000	-0.770737000
H	-5.685101000	-2.401596000	1.207256000
H	-6.276691000	-0.743111000	1.131589000
S	-5.031733000	-2.199961000	-6.047873000
H	-3.332697000	-2.518046000	-7.682558000
H	-3.017588000	-3.446629000	-6.192418000
S	-5.895351000	-0.011553000	-1.678458000
H	-4.944305000	-2.160468000	-1.259108000
H	-6.711213000	-2.147716000	-0.962582000
C	-5.531907000	-0.850828000	-7.146653000
C	-7.675327000	0.372808000	-1.547063000
N	-5.247902000	-0.938645000	-8.427026000
C	-5.682383000	0.099490000	-9.209799000
C	-6.418394000	1.136151000	-8.671502000
C	-6.691074000	1.130666000	-7.276183000
N	-6.204855000	0.125456000	-6.495408000
C	-5.327956000	0.028472000	-10.661504000

H	-6.776464000	1.956627000	-9.294534000
N	-7.408142000	2.122517000	-6.711235000
N	-7.981563000	1.482461000	-2.217763000
C	-9.289176000	1.830533000	-2.195711000
C	-10.229736000	1.050652000	-1.469461000
C	-9.769249000	-0.070248000	-0.802143000
N	-8.448026000	-0.431628000	-0.843545000
N	-9.665294000	2.932358000	-2.888647000
H	-11.283319000	1.331361000	-1.437908000
C	-10.672060000	-0.954548000	0.000821000
H	-10.633195000	-1.984536000	-0.384753000
H	-10.330767000	-0.991264000	1.046438000
H	-11.711025000	-0.603478000	-0.022733000
H	-5.717374000	0.889100000	-11.218620000
H	-4.234498000	-0.011002000	-10.779701000
H	-5.730438000	-0.896368000	-11.101562000
H	-10.648838000	3.183812000	-2.858883000
C	-8.748239000	3.847444000	-3.562116000
H	-7.703870000	2.875026000	-7.327839000
H	-7.795012000	3.843213000	-3.014953000
C	-8.502653000	3.541489000	-5.046402000
H	-9.177951000	4.854858000	-3.476026000
H	-7.951624000	4.398725000	-5.469092000
C	-7.696767000	2.265213000	-5.288015000
H	-9.467663000	3.481270000	-5.575910000
H	-6.753889000	2.307890000	-4.715899000
H	-8.252529000	1.382423000	-4.935507000
Ag	-5.772968000	-0.378489000	-4.177742000

Coordinates of atoms for structure showed in figure 4e

174
Ag2C60N16H88S4O4

N	-7.697035000	-4.986637000	-4.056666000
C	-8.489459000	-6.043412000	-4.344885000
N	-8.102809000	-7.294933000	-4.543443000
C	-6.776884000	-7.553153000	-4.406316000
C	-5.874250000	-6.526402000	-4.012143000
C	-6.361988000	-5.243050000	-3.886160000
S	-10.218544000	-5.608266000	-4.497098000
C	-11.076654000	-7.113865000	-3.827760000
C	-12.567940000	-7.050797000	-4.160257000
C	-12.887268000	-7.428116000	-5.608452000
C	-14.332526000	-7.142061000	-6.032762000
C	-14.604030000	-7.679602000	-7.441544000
C	-15.842150000	-7.083957000	-8.122224000
N	-15.910217000	-7.515747000	-9.534590000
C	-14.985611000	-6.885584000	-10.385175000
N	-14.778609000	-7.475804000	-11.626321000
C	-15.502960000	-8.595835000	-12.114734000
C	-16.507783000	-9.094961000	-11.213267000
C	-16.667411000	-8.598743000	-9.951202000
O	-14.366200000	-5.881448000	-10.024150000

C	-17.665693000	-9.186197000	-9.000352000
O	-15.245744000	-9.073481000	-13.227387000
C	-13.632483000	-6.974552000	-12.407476000
C	-12.315252000	-7.481490000	-11.809674000
C	-11.061080000	-6.971137000	-12.524556000
C	-9.802098000	-7.250481000	-11.695329000
C	-8.491158000	-6.945883000	-12.423129000
C	-7.251897000	-7.070902000	-11.536536000
S	-7.081687000	-5.566392000	-10.460499000
C	-5.860300000	-6.081719000	-9.259063000
N	-5.052716000	-5.076386000	-8.850231000
C	-4.068940000	-5.402419000	-7.953341000
C	-3.928966000	-6.699923000	-7.507452000
C	-4.880966000	-7.665968000	-7.936170000
N	-5.837979000	-7.338265000	-8.841081000
C	-3.160097000	-4.299071000	-7.511652000
N	-4.874387000	-8.915094000	-7.426290000
C	-5.901897000	-9.935081000	-7.630375000
C	-6.277668000	-10.660485000	-6.331001000
C	-7.101325000	-9.867658000	-5.308535000
N	-6.328967000	-8.793836000	-4.686097000
C	-5.487806000	-4.077914000	-3.542666000
C	-5.163658000	1.508967000	-1.277126000
C	-6.582046000	1.165569000	-0.816651000
C	-7.619154000	1.226706000	-1.938809000
S	-7.498118000	-0.301081000	-2.988496000
C	-8.490447000	0.122182000	-4.416008000
N	-8.495659000	1.365698000	-4.873040000
C	-9.273851000	1.613361000	-5.957898000
C	-10.080051000	0.586224000	-6.523092000
C	-9.962208000	-0.689440000	-6.013506000
N	-9.150488000	-0.936114000	-4.937800000
N	-9.238480000	2.843251000	-6.509408000
C	-8.301367000	3.912154000	-6.168122000
C	-7.833043000	4.691895000	-7.402928000
C	-6.911062000	3.951568000	-8.381848000
N	-7.617909000	2.933401000	-9.157306000
C	-7.192797000	1.674757000	-9.393362000
C	-8.056870000	0.714632000	-9.988865000
C	-7.621995000	-0.591489000	-10.072121000
N	-6.358265000	-0.932979000	-9.666415000
C	-5.580793000	0.067821000	-9.192430000
N	-5.933997000	1.332617000	-9.019127000
S	-3.932997000	-0.463774000	-8.744365000
C	-2.903740000	1.030830000	-9.139950000
C	-1.514236000	0.891907000	-8.517416000
C	-1.477712000	1.200798000	-7.019333000
C	-0.130254000	0.907397000	-6.349355000
C	-0.107716000	1.426579000	-4.909104000
C	1.066684000	0.910192000	-4.070483000
N	0.981383000	1.427106000	-2.691898000
C	0.006677000	0.860911000	-1.878897000
N	-0.247450000	1.507321000	-0.656990000

C	0.513133000	2.582329000	-0.225998000
C	1.527579000	3.054892000	-1.008292000
C	1.786378000	2.539052000	-2.326748000
O	-0.635071000	-0.136106000	-2.220149000
C	-1.507912000	1.104978000	0.002803000
C	-2.709722000	1.717752000	-0.725968000
C	-4.072747000	1.213113000	-0.241327000
C	0.209638000	3.187309000	1.111037000
O	2.621245000	2.996649000	-3.117853000
C	-8.479066000	-1.689289000	-10.619017000
C	-10.712610000	-1.855403000	-6.576659000
H	2.142499000	3.885087000	-0.668001000
H	0.917300000	3.999262000	1.312159000
H	-0.808475000	3.603415000	1.149070000
H	0.296960000	2.443981000	1.917895000
H	-1.561137000	0.009629000	-0.030965000
H	-1.463444000	1.408837000	1.053772000
H	2.028475000	1.253082000	-4.469635000
H	1.062113000	-0.186701000	-4.025328000
H	-2.667026000	2.817013000	-0.648180000
H	-2.608683000	1.471111000	-1.794775000
H	-1.043757000	1.126955000	-4.411060000
H	-0.082992000	2.528831000	-4.915939000
H	-4.026974000	0.123411000	-0.068910000
H	-4.330510000	1.672589000	0.728159000
H	0.689290000	1.366045000	-6.928832000
H	0.051110000	-0.181909000	-6.359573000
H	-5.129284000	2.577299000	-1.553855000
H	-4.930565000	0.946198000	-2.197851000
H	-2.263588000	0.622745000	-6.502504000
H	-1.733395000	2.265185000	-6.873656000
H	-0.849689000	1.590481000	-9.052537000
H	-1.108650000	-0.115471000	-8.715152000
H	-6.602357000	0.170768000	-0.338880000
H	-6.902323000	1.877314000	-0.037868000
H	-3.444274000	1.903850000	-8.751391000
H	-2.852564000	1.093093000	-10.234142000
H	-8.642260000	1.256741000	-1.543951000
H	-7.459705000	2.086248000	-2.603116000
H	-9.055828000	0.990464000	-10.327163000
H	-10.735554000	0.788814000	-7.370247000
H	-10.017839000	-2.661991000	-6.860042000
H	-11.398759000	-2.267950000	-5.820940000
H	-11.298502000	-1.570559000	-7.458711000
H	-9.485527000	-1.330087000	-10.864651000
H	-8.026290000	-2.109256000	-11.530474000
H	-8.565700000	-2.510618000	-9.890284000
H	-9.895522000	3.023816000	-7.263511000
H	-8.524139000	3.188415000	-9.542139000
H	-7.450972000	3.452599000	-5.646593000
H	-8.775427000	4.613764000	-5.461229000
H	-7.280179000	5.571116000	-7.038124000
H	-8.705959000	5.097875000	-7.944622000

H -6.455078000 4.685765000 -9.066620000
H -6.092136000 3.448925000 -7.850816000
H -17.112997000 -9.931666000 -11.555007000
H -18.196652000 -10.008676000 -9.492397000
H -17.182176000 -9.583906000 -8.095263000
H -18.406467000 -8.437336000 -8.681531000
H -15.788637000 -5.988099000 -8.116131000
H -16.770410000 -7.379578000 -7.622432000
H -13.775752000 -7.336129000 -13.432481000
H -13.667692000 -5.877314000 -12.400675000
H -14.691025000 -8.778648000 -7.413948000
H -13.734036000 -7.445761000 -8.075399000
H -12.272941000 -7.166405000 -10.754719000
H -12.320889000 -8.583992000 -11.818278000
H -14.504542000 -6.051580000 -6.010516000
H -15.038427000 -7.584781000 -5.309435000
H -10.973792000 -7.444062000 -13.517801000
H -11.145520000 -5.884397000 -12.701909000
H -12.666229000 -8.500249000 -5.752694000
H -12.210432000 -6.881375000 -6.287952000
H -9.854126000 -6.661093000 -10.763273000
H -9.795377000 -8.311163000 -11.388059000
H -8.362283000 -7.653542000 -13.258971000
H -8.528154000 -5.943785000 -12.884471000
H -12.964096000 -6.047417000 -3.926656000
H -13.083888000 -7.742633000 -3.474043000
H -7.310608000 -7.938202000 -10.865867000
H -6.332784000 -7.133797000 -12.132348000
H -10.903023000 -7.118969000 -2.744516000
H -10.589067000 -7.988211000 -4.278638000
H -3.136412000 -6.964368000 -6.807197000
H -4.814894000 -6.736264000 -3.863394000
H -5.585828000 -3.284395000 -4.300528000
H -5.792854000 -3.644656000 -2.577564000
H -4.433181000 -4.370221000 -3.474298000
H -2.447737000 -4.643652000 -6.752604000
H -2.592988000 -3.905314000 -8.369248000
H -3.742872000 -3.462398000 -7.095376000
H -5.349066000 -8.979485000 -4.490098000
H -4.086577000 -9.161230000 -6.832079000
H -7.981420000 -9.410674000 -5.780580000
H -7.470698000 -10.560072000 -4.533468000
H -6.874641000 -11.541609000 -6.612118000
H -5.368301000 -11.063047000 -5.850107000
H -5.544028000 -10.677807000 -8.362678000
H -6.774897000 -9.436940000 -8.072023000
Ag -5.574116000 -3.013685000 -9.516512000
Ag -8.609695000 -2.957133000 -4.170188000

Coordinates of atoms for structure showed in figure 4f

174
Ag2C60N16H88S4O4
N -6.281993000 -4.934669000 -9.416561000

C	-5.197922000	-5.716285000	-9.202588000
N	-5.191150000	-6.937832000	-8.686998000
C	-6.395261000	-7.471175000	-8.362132000
C	-7.601266000	-6.769418000	-8.640365000
C	-7.502694000	-5.489144000	-9.141898000
S	-3.668391000	-4.921422000	-9.665590000
C	-2.514433000	-6.342419000	-9.961106000
C	-1.069341000	-5.941393000	-9.661782000
C	-0.734030000	-5.933812000	-8.169244000
C	0.640616000	-5.341248000	-7.838743000
C	0.977207000	-5.510694000	-6.353848000
C	2.132249000	-4.625721000	-5.871556000
N	2.292445000	-4.718639000	-4.405494000
C	1.315776000	-4.029953000	-3.664449000
N	1.267033000	-4.294694000	-2.299990000
C	2.165597000	-5.152767000	-1.615754000
C	3.184483000	-5.737653000	-2.448023000
C	3.216454000	-5.554710000	-3.801032000
O	0.528255000	-3.256184000	-4.213437000
C	4.247850000	-6.226028000	-4.656559000
O	2.036842000	-5.358205000	-0.401113000
C	0.108416000	-3.744946000	-1.570171000
C	-1.141548000	-4.591655000	-1.836780000
C	-2.435985000	-3.979118000	-1.294422000
C	-3.660259000	-4.750070000	-1.798253000
C	-4.999655000	-4.200636000	-1.303896000
C	-6.211230000	-4.947422000	-1.857876000
S	-6.468853000	-4.534581000	-3.661189000
C	-7.602541000	-5.873486000	-4.115098000
N	-8.885367000	-5.485120000	-4.256046000
C	-9.790648000	-6.464213000	-4.575987000
C	-9.374431000	-7.768717000	-4.752203000
C	-7.987306000	-8.061006000	-4.634357000
N	-7.105132000	-7.085216000	-4.291300000
C	-11.220731000	-6.044522000	-4.702879000
N	-7.511661000	-9.299436000	-4.888859000
C	-6.109192000	-9.715750000	-4.821260000
C	-5.603166000	-10.356391000	-6.123654000
C	-5.247978000	-9.395078000	-7.260122000
N	-6.420103000	-8.669769000	-7.747156000
C	-8.708295000	-4.652960000	-9.443152000
C	-5.700795000	1.383832000	-1.208582000
C	-7.108379000	1.128069000	-0.666691000
C	-8.186518000	1.115774000	-1.751285000
S	-8.190021000	-0.503400000	-2.654763000
C	-8.794938000	-0.072980000	-4.277772000
N	-8.672181000	1.166144000	-4.733565000
C	-9.158236000	1.411518000	-5.975825000
C	-9.834495000	0.395399000	-6.706958000
C	-9.877398000	-0.871083000	-6.164025000
N	-9.334538000	-1.126539000	-4.933978000
N	-8.963132000	2.633069000	-6.509873000
C	-8.143965000	3.691474000	-5.921428000

C	-7.654157000	4.686587000	-6.975623000
C	-6.687891000	4.135429000	-8.036550000
N	-7.359386000	3.369140000	-9.088532000
C	-7.085210000	2.094637000	-9.442697000
C	-7.821906000	1.444032000	-10.470903000
C	-7.565603000	0.111080000	-10.723010000
N	-6.593023000	-0.552452000	-10.020153000
C	-5.915712000	0.166108000	-9.102659000
N	-6.107383000	1.430933000	-8.770889000
S	-4.629808000	-0.767798000	-8.232335000
C	-3.116234000	-0.058805000	-9.064839000
C	-1.855390000	-0.416815000	-8.280560000
C	-1.705882000	0.357003000	-6.969326000
C	-0.474050000	-0.029638000	-6.144329000
C	-0.397609000	0.792957000	-4.854960000
C	0.672169000	0.309756000	-3.868787000
N	0.543470000	1.021100000	-2.582391000
C	-0.489858000	0.604407000	-1.750106000
N	-0.757406000	1.407598000	-0.627245000
C	0.020456000	2.509443000	-0.312526000
C	1.073998000	2.848505000	-1.112639000
C	1.368949000	2.147901000	-2.335326000
O	-1.164845000	-0.399115000	-1.990341000
C	-2.026494000	1.097511000	0.063384000
C	-3.225905000	1.614495000	-0.739184000
C	-4.585111000	1.188059000	-0.175632000
C	-0.308542000	3.294168000	0.921287000
O	2.252333000	2.469028000	-3.141940000
C	-8.300396000	-0.674143000	-11.762646000
C	-10.540470000	-2.018650000	-6.861812000
H	1.699742000	3.702712000	-0.863710000
H	0.404505000	4.119139000	1.028845000
H	-1.322183000	3.720225000	0.876097000
H	-0.249949000	2.667284000	1.824025000
H	-2.083473000	0.006133000	0.164039000
H	-1.989369000	1.529338000	1.069031000
H	1.683032000	0.517293000	-4.238954000
H	0.564402000	-0.765917000	-3.681165000
H	-3.177591000	2.714189000	-0.809040000
H	-3.133645000	1.223883000	-1.764703000
H	-1.376538000	0.737948000	-4.351395000
H	-0.216454000	1.853853000	-5.095378000
H	-4.548606000	0.123769000	0.117107000
H	-4.813186000	1.755641000	0.742992000
H	0.442297000	0.114209000	-6.742952000
H	-0.518229000	-1.102903000	-5.890994000
H	-5.656358000	2.412551000	-1.607599000
H	-5.510068000	0.713141000	-2.064462000
H	-2.606853000	0.203762000	-6.350747000
H	-1.669948000	1.437102000	-7.197645000
H	-0.998797000	-0.197879000	-8.940795000
H	-1.822909000	-1.503867000	-8.091694000
H	-7.135103000	0.184631000	-0.094467000

H	-7.377899000	1.919981000	0.051970000
H	-3.264023000	1.029603000	-9.101022000
H	-3.087295000	-0.458719000	-10.086000000
H	-9.190574000	1.237232000	-1.325633000
H	-8.020634000	1.890868000	-2.511882000
H	-8.589212000	1.977934000	-11.032935000
H	-10.276647000	0.602197000	-7.681736000
H	-9.857436000	-2.881038000	-6.917318000
H	-11.430086000	-2.341151000	-6.298552000
H	-10.855054000	-1.748383000	-7.877248000
H	-9.055693000	-0.063211000	-12.270884000
H	-7.595103000	-1.062372000	-12.513156000
H	-8.799642000	-1.543237000	-11.306452000
H	-9.374085000	2.810217000	-7.421810000
H	-8.031628000	3.868772000	-9.666728000
H	-7.291993000	3.219160000	-5.410589000
H	-8.721107000	4.231613000	-5.152063000
H	-7.128495000	5.489324000	-6.436545000
H	-8.514076000	5.171927000	-7.469133000
H	-6.155459000	4.976773000	-8.507412000
H	-5.936661000	3.477156000	-7.582713000
H	3.916359000	-6.380168000	-1.963533000
H	4.901641000	-6.838314000	-4.025495000
H	3.788320000	-6.881017000	-5.412112000
H	4.870784000	-5.490086000	-5.187288000
H	1.925177000	-3.574537000	-6.109653000
H	3.082146000	-4.899313000	-6.342777000
H	0.378754000	-3.750210000	-0.507723000
H	-0.050148000	-2.711609000	-1.903288000
H	1.207280000	-6.568023000	-6.140142000
H	0.086838000	-5.249875000	-5.760615000
H	-1.246500000	-4.711416000	-2.927439000
H	-0.994477000	-5.599083000	-1.413063000
H	0.641863000	-4.268042000	-8.099490000
H	1.418365000	-5.813872000	-8.463107000
H	-2.421223000	-3.972398000	-0.190574000
H	-2.503012000	-2.924928000	-1.613969000
H	-0.789631000	-6.968966000	-7.788645000
H	-1.504937000	-5.362856000	-7.622977000
H	-3.650191000	-4.745974000	-2.901752000
H	-3.577795000	-5.808758000	-1.494172000
H	-5.052390000	-4.282942000	-0.204751000
H	-5.081510000	-3.123709000	-1.531946000
H	-0.847266000	-4.958041000	-10.111140000
H	-0.416986000	-6.661349000	-10.183722000
H	-6.061426000	-6.035025000	-1.808223000
H	-7.132698000	-4.680022000	-1.326054000
H	-2.643982000	-6.635265000	-11.010631000
H	-2.862453000	-7.158284000	-9.312901000
H	-10.092285000	-8.551941000	-4.999107000
H	-8.573708000	-7.215911000	-8.431936000
H	-8.623182000	-3.667544000	-8.958389000
H	-8.787258000	-4.479100000	-10.527692000

H	-9.632154000	-5.137163000	-9.103820000
H	-11.868280000	-6.891087000	-4.959903000
H	-11.571773000	-5.604297000	-3.757162000
H	-11.327380000	-5.271533000	-5.479865000
H	-7.333186000	-9.070764000	-7.553676000
H	-8.202516000	-10.028874000	-5.051746000
H	-4.505966000	-8.655980000	-6.924330000
H	-4.785533000	-9.963278000	-8.084847000
H	-4.687110000	-10.916231000	-5.881381000
H	-6.328883000	-11.109965000	-6.475952000
H	-6.002157000	-10.442200000	-4.000224000
H	-5.517960000	-8.829037000	-4.560799000
Ag	-9.000484000	-3.204805000	-4.158091000
Ag	-6.005522000	-2.752358000	-9.852620000

Enthalpy and entropy of formation for complex isomers $[Ag_nL_m]^{n+}$

Table S1. Enthalpy (kcal/mol) and entropy (kcal/(mol·K)) of formation for complex isomers $[Ag_nL_m]^{n+}$.

Composition (coordination mode)	Figure	ΔH^o_{298}	ΔS_{298}
$Ag^+ + 2L$**1** [a]			
$[AgL$**1**$(N3)_2]^+$	1c	-9.64	-37.73
$[AgL$**1**$(N1)_2]^+$	1d	-21.82	-43.96
$Ag^+ + L$**3** [a]			
$[AgL$**3**$(N3,N3)]^+$	2b	-2.64	32.96
$[AgL$**3**$(N3,N3)]^+$	2c	-1.74	31.73
$[AgL$**3**$(N3,S)]^+$	2d	-2.74	24.96
$[Ag_2L$**3**$(N1,N1)_2]^{2+}$	2e	-19.74	-5.73
		(-9.87) [b]	(-2.86)[b]
$[Ag_2L$**3**$(N1,N1)_2]^{2+}$	2f	-18.92	-0.36
		(-9.46) [b]	(-0.18)[b]
$[AgL$**3**$(N1)_2]^+$	2g	-17.24	-35,95
$[Ag_2L$**3**$(N1,N1)L$**3**$(N1)_2]^{2+}$	2h	-28.76	-73,41
		(-14.38) [b]	(-36.70)[b]
$Ag^+ + L$**4** [a]			
$[AgL$**4**$(N1,N3)]^+$	3b	-10.77	28.05
$[AgL$**4**$(N1,N3)]^+$	3c	-11.15	23.21
$[AgL$**4**$(N3,N3)]^+$	3d	-4.84	21.43
$[AgL$**4**$(N1,N1)]^+$	3e	-17.52	16.02
$Ag^+ + L$**5a** [a]			
$[AgL$**5a**$(N3,N3)]^+$	4b	3.79	12.60
$[AgL$**5a**$(S,S)]^+$	4c	6.68	21.38
$[AgL5$**a**$(S,N3,S)]^+$	4d	-4.57	19.23
$[Ag_2L$**5a**$(N1,N1)_2]^2$	4e	-10.08	-46.57
		(-5.04) [b]	(-23.28)[b]
$[Ag_2L$**5a**$(N1,N1)_2]^{2+}$	4f	-8.34	-44.26
		(-4.17) [b]	(-22.13)[b]

[a] Equimolar mixtures of Ag^+ ion and ligand L in $CDCl_3$–DMSO-d_6 =1 : 1 (v/v) at 303 K;

[b] per one Ag^+ ion