

CP-ART-02-2015-001160 manuscript
REVISED Version: 19 March 2015

Supporting Information File for:

**Gas-phase VUV Photoionisation and Photofragmentation
of the Silver Deuteride Nanocluster $[\text{Ag}_{10}\text{D}_8\text{L}_6]^{2+}$ (L =
bis(diphenylphosphino)methane). A Joint Experimental
and Theoretical Study.**

Steven Daly, ^a Marjan Krstić, ^b Alexandre Giuliani, ^c Rodolphe Antoine, ^a Laurent Nahon, ^c
Athanasios Zavras, ^{d,e} George N. Khairallah, ^{d,e} Vlasta Bonačić-Koutecký, ^{*b,f} Philippe
Dugourd, ^{*a} and Richard A. J. O'Hair ^{*d,e}

^a Institut Lumière Matière, Université Lyon 1, CNRS UMR 5306, Lyon, France. E-mail:
philippe.dugourd@univ-lyon1.fr

^b Interdisciplinary Center for Advanced Science and Technology (ICAST) at University of
Split, Split, Croatia

^c SOLEIL, l'Orme des Merisiers, St Aubin, BP48, F-91192 Gif sur Yvette
Cedex, France

^d School of Chemistry and Bio21 Molecular Science and Biotechnology Institute, University
of Melbourne, 30 Flemington Rd, Parkville, Victoria 3010, Australia. E-mail:
rohair@unimelb.edu.au

^e ARC Centre of Excellence for Free Radical Chemistry and Biotechnology.

^f Humboldt-Universität Berlin, Institut für Chemie, Berlin, Germany. E-mail: vbk@cms.hu-
berlin.de

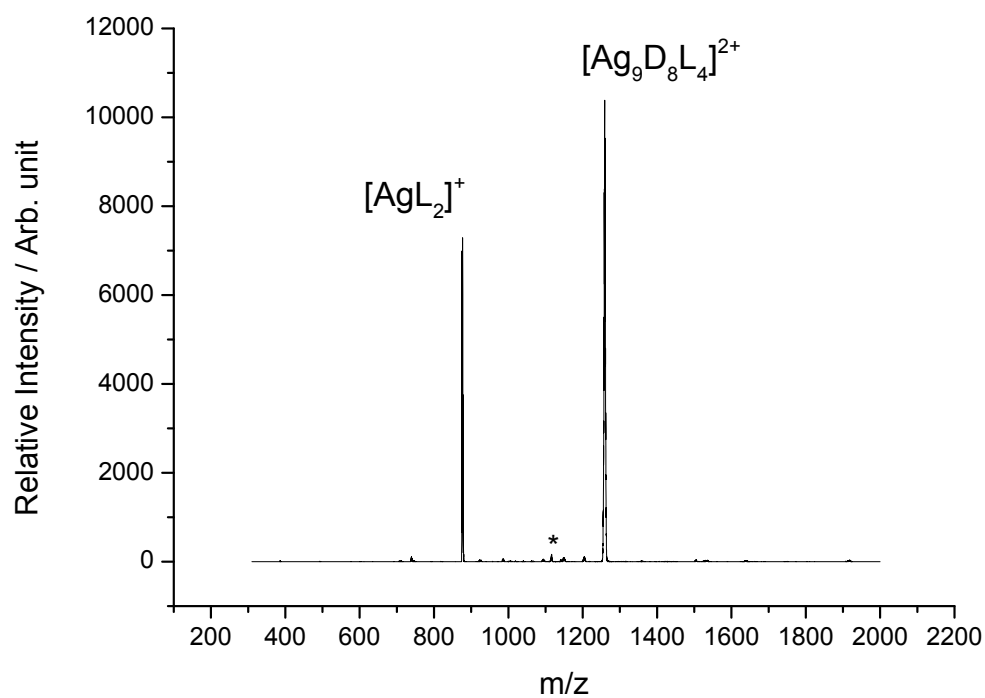


Figure S1. LTQ MS³ CID mass spectrum (100 ms 15% NCE) of the mass selected silver cluster trication, $[\text{Ag}_{10}\text{D}_8\text{L}_6]^{3+}$, formed via ionization of $[\text{Ag}_{10}\text{D}_8\text{L}_6]^{2+}$ at 15.5 eV (500 ms).

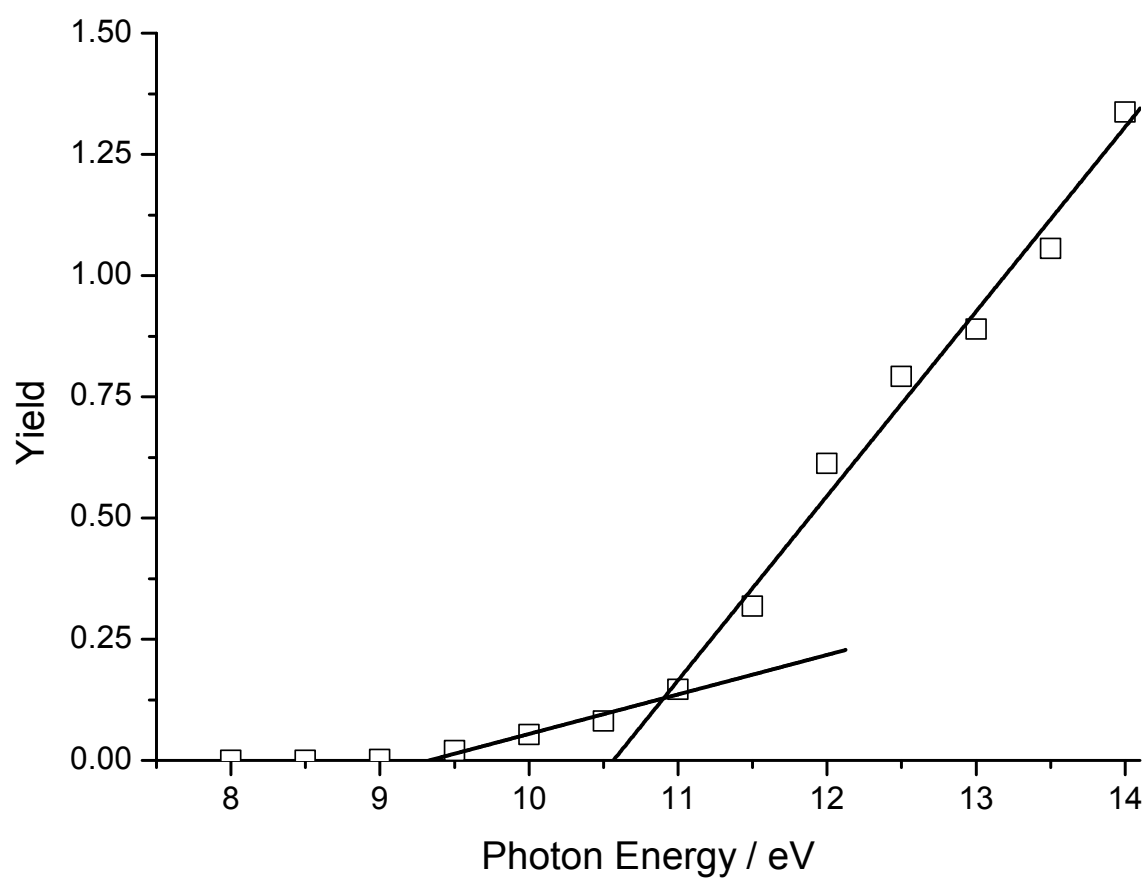


Figure S2. Determination of the onset of ionisation of $[\text{Ag}_{10}\text{D}_8\text{L}_6]^{2+}$ from a two curve linear fit of the yield of the product ion, $[\text{Ag}_{10}\text{D}_8\text{L}_6]^{3+}$, as a function of the VUV energy used, which was varied from 8 to 15.5 eV.

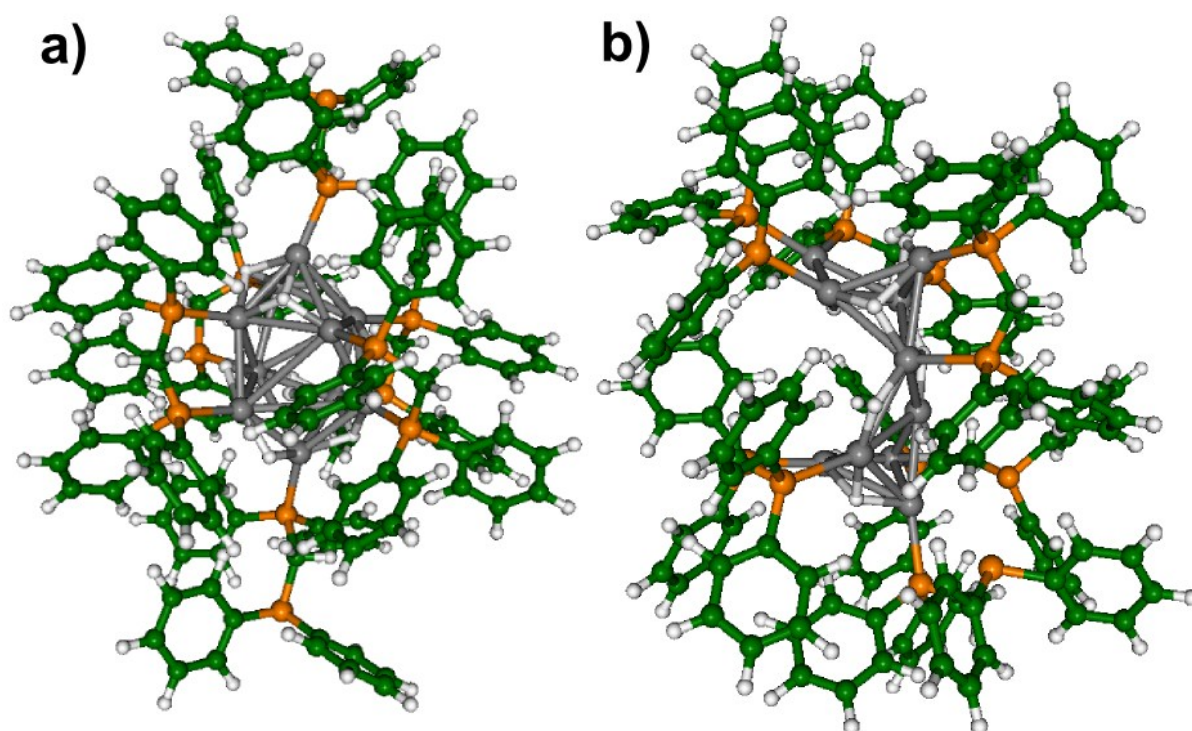


Figure S3. RI-PBE/RECP-def2-SVP optimised structure of the (a) isomer **II** and (b) isomer **III** of $[\text{Ag}_{10}\text{H}_8\text{L}_6]^{2+}$ structure. Grey, orange, white and green colors label silver, phosphorus, hydrogen and carbon atoms.

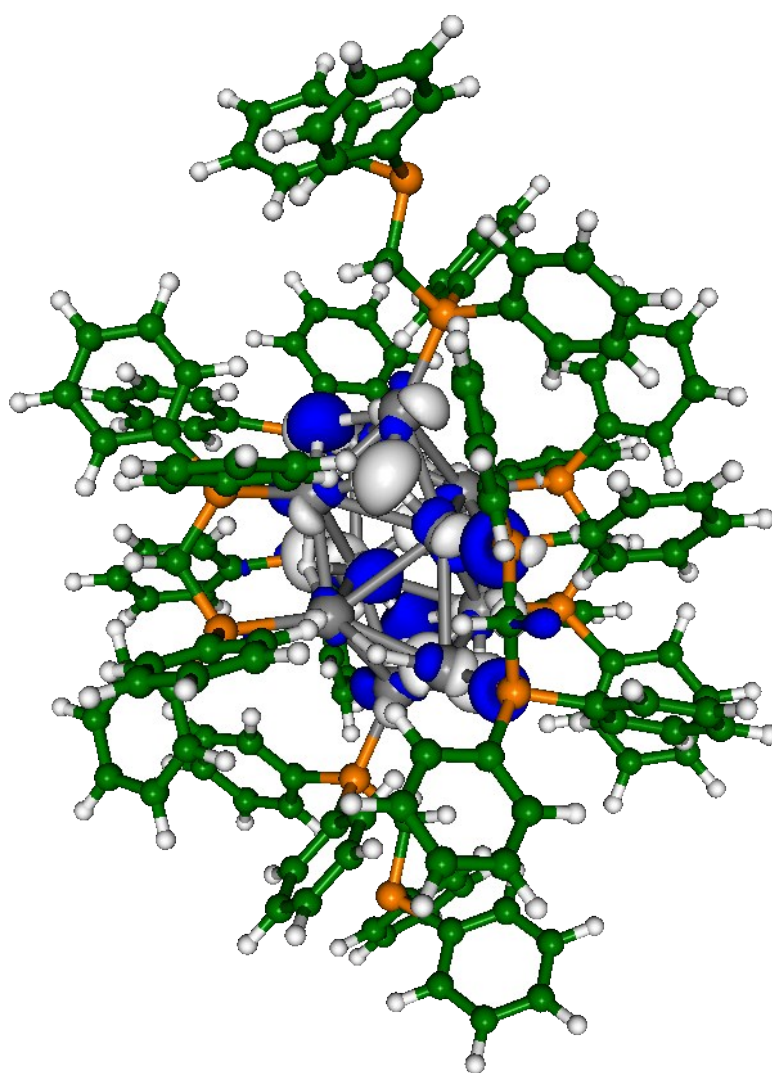


Figure S4. RI-PBE/RECP-def2-SVP calculated HOMO of the isomer **I** of [Ag₁₀H₈L₆]²⁺. Grey and blue colors label positive and negative lobes.

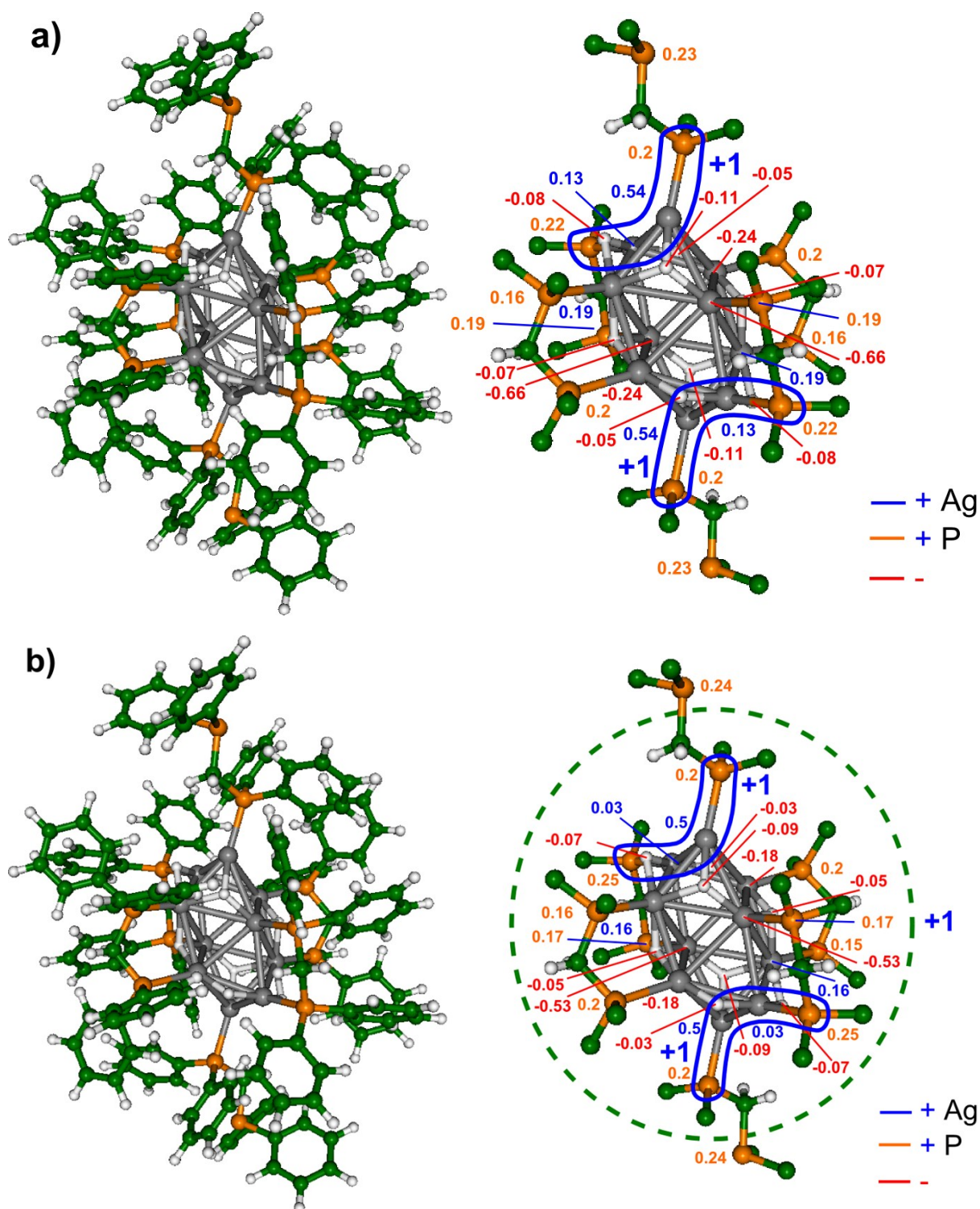


Figure S5. RI-PBE/RECP-def2-SVP optimized structures (left) and calculated Mulliken charges for silver core and surrounding atoms without phenyl rings (right) of a) isomer I of $[\text{Ag}_{10}\text{H}_8\text{L}_6]^{2+}$ and b) of $[\text{Ag}_{10}\text{H}_8\text{L}_6]^{3+}$. Blue symbols label positive charge on silver atoms. Green dashed line represent third charge delocalised on phenyl rings.

Cartesian Coordinates of isomers of $[\text{Ag}_{10}\text{H}_8\text{L}_6]^{2+}$

Isomer I (Figure 3):

Ag	0.55788200	0.65734500	-0.24981000
Ag	0.38338900	1.00195200	2.85261300
Ag	3.49476300	0.27378300	2.63567700
Ag	3.24584200	-0.43012200	-0.21470500
Ag	0.15411600	3.98040200	3.61572200
Ag	-0.09499600	3.27589100	0.76558600
Ag	3.01659200	2.54779500	0.54764900
Ag	2.84224200	2.89259400	3.65085400
Ag	1.81077500	5.12139600	1.54946000
Ag	1.58951100	-1.57197600	1.85155700
P	5.10977900	-0.08128400	4.53654700
P	4.93901400	2.96566800	5.23567000
P	4.87196200	2.72662900	-1.30000300
P	5.11198700	-0.37012400	-1.89676400
P	-1.71033200	3.63068700	-1.13525600
P	-1.53833200	0.58384100	-1.83537100
P	-1.71092700	3.92069300	5.29893800
P	-1.47205400	0.82416700	4.70065100
P	2.71995400	7.33132600	2.01637700
P	0.67996100	-3.78172200	1.38386100
C	-2.64179300	2.06126900	-1.51823000
C	6.04199200	1.48777200	4.91902600
C	5.11911200	1.37087300	-2.57068100
C	-1.71857200	2.17937200	5.97207600
C	1.62342500	8.58418200	1.17496700
C	1.77505100	-5.03562000	2.22558600
P	1.91926600	10.40663100	1.62883900

P	1.47932600	-6.85748100	1.76918900
H	4.23566000	1.42573600	-3.24056600
H	6.02618800	1.55891100	-3.18097000
H	-3.20920600	1.83744400	-0.59073700
H	-3.35950600	2.18803200	-2.35484700
H	-0.83511900	2.12379900	6.64190300
H	-2.62566700	1.99153700	6.58239700
H	6.60955000	1.71111200	3.99150600
H	6.75962700	1.36094900	5.75569800
H	0.59161900	8.28015400	1.44414400
H	1.73134500	8.42558400	0.08161400
H	2.80735400	-4.73145700	1.95851100
H	1.66531800	-4.87830900	3.31894100
C	-3.44983400	4.25852700	4.80001800
C	-3.16781100	0.63610500	3.97737400
C	4.60538300	2.86308600	7.05270000
C	4.42606500	-0.63233800	6.16268100
C	6.85073800	-0.70655900	-1.39622500
C	-1.20400600	0.68736400	-3.65223700
C	-1.02756400	4.18279500	-2.76140100
C	-3.05934600	4.86197700	-0.83826500
C	-2.72270100	-0.83309000	-1.74848200
C	-1.31011800	-0.66746600	5.78454900
C	-1.46321400	4.90646500	6.84379600
C	6.12367700	4.38224300	5.14748500
C	6.45817200	-1.31343000	4.24036700
C	4.70876900	4.21746100	-2.38483600
C	4.86616900	-1.35680300	-3.44138700
C	-4.56033900	3.86523700	5.57907500

C	-5.86326400	4.14577700	5.14370600
C	-6.07059400	4.82647200	3.93146300
C	-4.97257900	5.22857300	3.15582900
C	-3.66653500	4.94365900	3.58650300
H	-4.41642400	3.34272100	6.53791000
H	-6.72267600	3.83337700	5.75620000
H	-7.09513100	5.04485000	3.59335300
H	-5.12590700	5.75974600	2.20443300
H	-2.80405100	5.24168200	2.96864100
C	-4.14013800	-0.21875000	4.53848600
C	-5.42551000	-0.29111400	3.97846300
C	-5.75658200	0.49310900	2.86142700
C	-4.79151900	1.34314400	2.29673900
C	-3.49892000	1.40437400	2.84068800
H	-3.89407800	-0.83563200	5.41607400
H	-6.17637500	-0.96117000	4.42470100
H	-6.76945700	0.44357900	2.43318100
H	-5.04900100	1.97477600	1.43181300
H	-2.73955200	2.05839500	2.38239600
C	5.62417700	3.07656700	8.00685500
C	5.33867400	2.98782600	9.37677300
C	4.03530000	2.68662700	9.80811800
C	3.01806300	2.47412800	8.86502300
C	3.29978300	2.56581700	7.49163700
H	6.64509500	3.32951700	7.67923400
H	6.13812200	3.15944600	10.11374000
H	3.81405300	2.61970700	10.88434100
H	1.99692600	2.23450500	9.19941000
H	2.50349800	2.40542600	6.74753400

C	5.26419200	-0.87322600	7.27288400
C	4.71439100	-1.29409400	8.49145700
C	3.32691600	-1.48995900	8.60909700
C	2.49020000	-1.26478200	7.50586400
C	3.03706200	-0.83565700	6.28462700
H	6.35498900	-0.74540100	7.18732900
H	5.37358300	-1.47758900	9.35347700
H	2.90008800	-1.82718400	9.56618800
H	1.40487900	-1.42719400	7.58756700
H	2.38041400	-0.65921500	5.41770900
C	6.56785300	2.91638000	-0.57740900
C	7.53959300	3.77099600	-1.13999200
C	8.82516600	3.84457600	-0.58066000
C	9.15709200	3.06181200	0.53717600
C	8.19263800	2.21209100	1.10331100
C	6.89978600	2.14965300	0.56003100
H	7.29284600	4.38673300	-2.01818800
H	9.57555100	4.51442500	-1.02802400
H	10.17017600	3.11232700	0.96484100
H	8.45077200	1.58159700	1.96888400
H	6.14089300	1.49582000	1.01939500
C	7.96166800	-0.31295700	-2.17455900
C	9.26442400	-0.59227900	-1.73788500
C	9.47117500	-1.27206600	-0.52501300
C	8.37276700	-1.67453400	0.24986200
C	7.06688000	-1.39081500	-0.18213800
H	7.81816700	0.20887900	-3.13383000
H	10.12421900	-0.27970300	-2.34976000
H	10.49557200	-1.48941700	-0.18581700

H	8.52560300	-2.20513000	1.20164900
H	6.20409300	-1.68912600	0.43516400
C	-1.86642500	4.42439800	-3.87091900
C	-1.31741900	4.84597600	-5.08959600
C	0.07000900	5.04178700	-5.20804500
C	0.90742400	4.81585300	-4.10550400
C	0.36135000	4.38608300	-2.88413600
H	-2.95716800	4.29663100	-3.78465600
H	-1.97715600	5.03006400	-5.95107400
H	0.49623400	5.37955800	-6.16521200
H	1.99271000	4.97815400	-4.18779100
H	1.01856800	4.20914100	-2.01775000
C	-2.22246600	0.47458200	-4.60692800
C	-1.93632300	0.56379800	-5.97667500
C	-0.63265200	0.86477900	-6.40733700
C	0.38422800	1.07657300	-5.46372500
C	0.10184800	0.98444100	-4.09049600
H	-3.24359300	0.22178000	-4.27982600
H	-2.73546500	0.39271600	-6.71410100
H	-0.41093000	0.93203900	-7.48343900
H	1.40561400	1.31598800	-5.79752100
H	0.89787500	1.14424400	-3.34599300
C	-2.66995400	6.11360800	-0.31015400
C	-3.61652400	7.12821900	-0.11003400
C	-4.96967800	6.90368700	-0.41811300
C	-5.36928900	5.65591800	-0.92071900
C	-4.42134600	4.63967800	-1.13107200
H	-1.61249100	6.28977700	-0.05394800
H	-3.29690400	8.10138800	0.29402900

H	-5.71226400	7.70129600	-0.26464000
H	-6.42741000	5.47102700	-1.16162400
H	-4.76066800	3.67480400	-1.53640200
C	-2.26124400	-2.08360400	-2.22272500
C	-3.09462600	-3.20996300	-2.18536400
C	-4.39528200	-3.11357400	-1.66260800
C	-4.85517800	-1.88226200	-1.17381500
C	-4.02630200	-0.74795000	-1.21511700
H	-1.24338800	-2.17855100	-2.63413600
H	-2.71835800	-4.17110700	-2.56565600
H	-5.04843100	-3.99864300	-1.63609500
H	-5.87264500	-1.79475500	-0.76278300
H	-4.41994000	0.20395900	-0.83053000
C	-2.37023700	5.90518400	7.25584100
C	-2.10661900	6.67015800	8.40421700
C	-0.94124500	6.44860800	9.15415500
C	-0.02557100	5.46512000	8.74175700
C	-0.27751900	4.70730700	7.58870600
H	-3.29019700	6.08617200	6.68071100
H	-2.82560100	7.44282700	8.71629800
H	-0.74440800	7.04469900	10.05800400
H	0.89769200	5.28933000	9.31525200
H	0.46879100	3.96555600	7.26115000
C	-0.90294200	-1.87502600	5.17422300
C	-0.78376300	-3.05125200	5.92948900
C	-1.05941900	-3.04023600	7.30676100
C	-1.45627700	-1.84420400	7.92489500
C	-1.58215100	-0.66524400	7.17074700
H	-0.67692200	-1.89700100	4.09666100

H	-0.47430100	-3.98389900	5.43486200
H	-0.96425200	-3.96335800	7.89833300
H	-1.67781200	-1.82508000	9.00290500
H	-1.90560700	0.25285000	7.68138900
C	5.66235000	5.63329300	5.62042300
C	6.49590800	6.75948600	5.58205900
C	7.79660500	6.66236100	5.05953900
C	8.25638700	5.43049600	4.57203600
C	7.42734100	4.29634900	4.61439700
H	4.64443000	5.72875400	6.03155200
H	6.11968200	7.72104600	5.96136300
H	8.44993400	7.54728100	5.03216700
H	9.27389400	5.34244700	4.16120300
H	7.82084900	3.34397800	4.23085600
C	6.06822700	-2.56473900	3.71191300
C	7.01421300	-3.57999700	3.51225800
C	8.36732700	-3.35641900	3.82119900
C	8.76749700	-2.10897200	4.32417500
C	7.82014400	-1.09208200	4.53403600
H	5.01079200	-2.74011100	3.45504300
H	6.69419800	-4.55290100	3.10788800
H	9.10946900	-4.15450000	3.66808600
H	9.82560800	-1.92487600	4.56572600
H	8.15993800	-0.12746900	4.93961700
C	4.30081500	5.42513100	-1.77524500
C	4.18075800	6.60078600	-2.53124600
C	4.45636000	6.58909100	-3.90853200
C	4.85400000	5.39295600	-4.52592900
C	4.98071800	4.21455200	-3.77103300

H	4.07486800	5.44764000	-0.69768700
H	3.87059600	7.53353300	-2.03725600
H	4.36050100	7.51178000	-4.50065300
H	5.07546300	5.37329600	-5.60394000
H	5.30479300	3.29636300	-4.28110600
C	5.77418600	-2.35524400	-3.85199800
C	5.51214000	-3.12096900	-5.00022000
C	4.34734700	-2.90049600	-5.75143400
C	3.43067300	-1.91735500	-5.34045900
C	3.68108200	-1.15875800	-4.18754400
H	6.69365600	-2.53536700	-3.27581900
H	6.23184000	-3.89339500	-5.31123200
H	4.15173000	-3.49718100	-6.65514500
H	2.50785600	-1.74245600	-5.91494200
H	2.93403200	-0.41728400	-3.86107200
C	4.42498700	7.62165200	1.38756300
C	2.75693200	7.86195600	3.78051200
C	1.86259400	11.20065800	-0.05610300
C	0.27488800	10.88452300	2.35386800
C	-1.02567400	-4.07166700	2.01116100
C	0.64421100	-4.31169900	-0.38046800
C	3.12371000	-7.33444800	1.04347300
C	1.53576600	-7.65382700	3.45306300
C	-2.01892700	-3.13362800	1.64740000
C	-3.33202800	-3.27006800	2.11916900
C	-3.66974600	-4.33996900	2.96560500
C	-2.68975000	-5.27331800	3.33449100
C	-1.37292400	-5.14315100	2.86134600
H	-1.76418400	-2.28601700	0.99071500

H	-4.09121800	-2.52886000	1.82882700
H	-4.69922800	-4.44416000	3.34075000
H	-2.94580200	-6.11487300	3.99585500
H	-0.62697800	-5.89380000	3.16125800
C	-0.22290700	-5.33267700	-0.82663000
C	-0.17609300	-5.75685400	-2.16395300
C	0.72973600	-5.16964400	-3.06308600
C	1.59141600	-4.15053500	-2.62581400
C	1.54555200	-3.72154000	-1.29023900
H	-0.93591000	-5.79510400	-0.12906000
H	-0.85103200	-6.55773400	-2.50353600
H	0.76277500	-5.50698300	-4.11036400
H	2.29894200	-3.68026900	-3.32527400
H	2.21319500	-2.90942900	-0.95304200
C	0.55268900	-8.63639400	3.70312300
C	0.50795400	-9.31141200	4.93444000
C	1.44561900	-9.00975700	5.93327300
C	2.42782500	-8.03191400	5.69765300
C	2.47346400	-7.35911200	4.46744600
H	-0.18269300	-8.87486600	2.91786500
H	-0.26198300	-10.07790300	5.11145300
H	1.41482300	-9.53872000	6.89799100
H	3.16894900	-7.79735600	6.47729500
H	3.25795000	-6.60486700	4.29936700
C	3.08135600	-8.26234500	-0.01911600
C	4.26495600	-8.72375900	-0.61753200
C	5.50857000	-8.25683000	-0.16690700
C	5.56387200	-7.32685100	0.88487200
C	4.38142700	-6.86999900	1.48543100

H	2.10568600	-8.62522900	-0.37996900
H	4.21321800	-9.45035900	-1.44271100
H	6.43742200	-8.61734600	-0.63457900
H	6.53840300	-6.96037200	1.24432900
H	4.45188100	-6.14824500	2.31566000
C	3.62378600	8.88372800	4.22536300
C	3.57799700	9.30846700	5.56254800
C	2.67348900	8.72098800	6.46284200
C	1.81211100	7.70104400	6.02690200
C	1.85691500	7.27152200	4.69145100
H	4.33577000	9.34628800	3.52683000
H	4.25265400	10.11001000	5.90113100
H	2.64125600	9.05875900	7.51000300
H	1.10562800	7.23059000	6.72730500
H	1.18957900	6.45870400	4.35537500
C	5.41906000	6.68448300	1.75143600
C	6.73173300	6.82124300	1.27858000
C	7.06822100	7.89061800	0.43098600
C	6.08742000	8.82303800	0.06193300
C	4.77100800	8.69255500	0.53615500
H	5.16538000	5.83731200	2.40910100
H	7.49157800	6.08069800	1.56891500
H	8.09739000	7.99511000	0.05508800
H	6.34249900	9.66409800	-0.60043600
H	4.02446300	9.44254300	0.23604900
C	0.31729400	11.81319600	3.41575200
C	-0.86629000	12.27517700	4.01376100
C	-2.10991100	11.80802100	3.56339600
C	-2.16525300	10.87735300	2.51221900

C	-0.98283100	10.41993600	1.91205900
H	1.29300700	12.17621400	3.77633900
H	-0.81451300	13.00238600	4.83839500
H	-3.03875800	12.16889900	4.03079000
H	-3.13981300	10.51080900	2.15291300
H	-1.05328800	9.69768500	1.08225700
C	2.84455600	12.18408400	-0.30712400
C	2.88908200	12.85726500	-1.53946700
C	1.95238400	12.55283100	-2.53836200
C	0.97121900	11.57419100	-2.30173400
C	0.92575100	10.90326500	-1.07050600
H	3.57923700	12.42463800	0.47814900
H	3.65812300	13.62445500	-1.71726900
H	1.98311800	13.08022300	-3.50393600
H	0.23079700	11.33753400	-3.08140100
H	0.14207200	10.14835000	-0.90168200
H	1.49906200	3.43746100	4.68164500
H	1.62171100	-0.29950600	3.26180700
H	3.77908700	2.11302600	2.21797700
H	3.67924900	-1.15845800	1.39468000
H	1.77810300	3.84913300	0.13904000
H	1.90122800	0.11305100	-1.28081100
H	-0.27955100	4.70819300	2.00621000
H	-0.37983100	1.43674000	1.18261000

Isomer II (Figure S3a):

C	2.83885600	1.43816200	-0.55776500
P	1.58445000	2.79782300	-0.78015900
C	2.28642700	3.80132600	-2.16685900

P	2.47656300	0.32821000	0.90164300
C	4.05559700	-0.59994000	1.13103400
C	1.34021600	-0.95596200	0.22269000
Ag	1.93592700	1.64217500	3.00336100
Ag	2.86168400	4.30940700	4.03386900
P	4.37132700	6.40887500	3.49316100
C	5.82414000	6.37894500	4.63313600
C	0.14309400	2.00249900	-1.61649100
Ag	1.19557700	4.03257700	1.40525000
Ag	-1.54341200	4.74524700	2.09255600
P	-3.36453300	6.38954900	1.50343400
C	-4.73966400	6.50744100	2.72243700
Ag	0.55405600	6.25318800	3.24834900
Ag	-0.73789600	4.53494200	5.29845600
Ag	1.86548700	3.90637000	6.80158400
P	1.21554600	5.37044700	8.70366700
C	2.01634300	4.84563900	10.28777600
Ag	2.86723000	1.53636700	5.72462700
Ag	0.09488400	1.57869300	5.60606500
P	-1.25090800	-0.51805400	6.25025200
C	-0.35319000	-2.13584200	6.40054300
P	5.10133500	0.83785900	6.41211300
C	6.45035600	1.08615300	5.18063900
C	5.64802500	1.72417800	7.96570500
P	7.14452400	1.04642800	8.92694300
C	6.38374000	0.69353300	10.58087200
C	5.10479700	-0.95075800	6.86969200
P	1.94506700	8.33104200	3.03247600
C	2.40044100	8.98780600	1.36392600

C	1.25938800	9.83152600	3.85912500
C	3.57670000	8.05399300	3.88904800
P	-1.80842300	5.25612700	7.70797700
C	-3.20003200	4.27653500	8.43149500
Ag	-1.88147200	2.35101300	3.55003700
P	-3.27594400	0.24428500	3.88658300
C	-3.82635200	-0.75243600	2.42068800
C	-2.46889300	6.99054700	7.72241500
C	-0.58911100	5.23092100	9.14317800
C	-4.93167900	0.71184400	4.57280500
C	-2.54326100	-1.06106800	4.99900600
C	-2.94649900	8.13889700	1.07219700
C	-3.99046000	5.70878500	-0.12303700
P	-5.60037600	6.30449500	-0.90856300
C	-6.79209700	4.95729800	-0.45950400
C	-2.11217300	-0.35996200	7.87065700
C	1.61227900	7.16648900	8.62611800
C	5.17167800	6.66745900	1.84563600
C	8.09281300	2.60540400	9.26059200
C	-5.21452900	5.88131400	-2.67616000
H	1.35229400	2.11148300	6.98089800
H	1.53914300	0.71795800	4.49358600
H	2.59461200	3.36171800	2.48390300
H	3.12785000	4.65422900	5.76477400
H	-1.31344800	2.78324500	5.28607100
H	-0.02115100	6.12117100	4.93570200
H	-2.27020000	3.08394300	1.97369700
H	0.12900100	5.53059800	1.52582900
H	3.79451900	1.95188200	-0.31874900

H	2.97502200	0.84845000	-1.48752000
H	-1.97048500	-1.71571200	4.31035700
H	-3.30724200	-1.70742800	5.47772800
H	-0.66378300	4.20755000	9.56710400
H	-0.87470000	5.94402000	9.94463100
H	3.33993100	8.01542000	4.97436600
H	4.27715100	8.89370000	3.69837400
H	-3.94733600	4.60103300	-0.05991700
H	-3.19385800	6.00474400	-0.83727300
H	4.75603100	1.75539800	8.62466300
H	5.85287700	2.77077000	7.65601800
C	-0.55629300	-3.03882500	7.46436800
C	0.10326800	-4.28013300	7.47150300
C	0.96629800	-4.63124900	6.42129000
C	1.18713100	-3.72738200	5.36822900
C	0.53998200	-2.48317100	5.36092400
H	-1.23980900	-2.77940500	8.28671300
H	-0.07017600	-4.98186700	8.30154300
H	1.47275400	-5.60826200	6.42518200
H	1.87304900	-3.99062100	4.54875100
H	0.73364000	-1.77172500	4.54122100
C	-3.36318700	-0.93431300	8.17582500
C	-3.90012300	-0.82158300	9.46798800
C	-3.19042200	-0.14409600	10.47168000
C	-1.94584400	0.43494600	10.17649300
C	-1.41423600	0.33707600	8.88243900
H	-3.93248900	-1.48304700	7.41119900
H	-4.87869500	-1.27262800	9.69255400
H	-3.61127100	-0.06372200	11.48550300

H	-1.38616300	0.97213200	10.95739700
H	-0.44445500	0.80681400	8.64688000
C	-4.13486000	-2.12920700	2.48571600
C	-4.63031900	-2.79899000	1.35525200
C	-4.83213700	-2.10281400	0.15247300
C	-4.52266300	-0.73532800	0.07927800
C	-4.01634300	-0.06385700	1.20338200
H	-3.99945500	-2.69544600	3.41918600
H	-4.86840200	-3.87172900	1.41954600
H	-5.22895300	-2.62864000	-0.72922200
H	-4.66890500	-0.18719000	-0.86333300
H	-3.75809900	1.00582400	1.13930200
C	-5.80314100	-0.20941600	5.19088200
C	-7.10557200	0.17456000	5.54547600
C	-7.55784800	1.47799700	5.27445600
C	-6.69790800	2.40274300	4.66029500
C	-5.38936700	2.02255400	4.31678400
H	-5.48328900	-1.24653700	5.37709700
H	-7.77855500	-0.55440500	6.02208900
H	-8.58469600	1.77063900	5.54133200
H	-7.03909500	3.42662100	4.44545800
H	-4.71992200	2.75178200	3.83012500
C	4.16973000	-1.37016100	2.31094600
C	5.32177100	-2.13042500	2.55639100
C	6.38010500	-2.12368300	1.63301200
C	6.28104400	-1.35343100	0.46460300
C	5.12584300	-0.59478700	0.21113400
H	3.35034200	-1.36639000	3.04858300
H	5.39666200	-2.72098800	3.48232500

H	7.28652600	-2.71698700	1.82632100
H	7.10757600	-1.34505200	-0.26229700
H	5.07072300	-0.00665900	-0.71722900
C	1.77711600	-1.88473800	-0.74686700
C	0.89537400	-2.85807900	-1.23619200
C	-0.42472300	-2.91673800	-0.75722900
C	-0.86317000	-2.00072000	0.21091200
C	0.01683000	-1.02240300	0.70197100
H	2.81715100	-1.86256200	-1.10972800
H	1.24293400	-3.58212700	-1.98906500
H	-1.11367000	-3.68611300	-1.13783900
H	-1.89512500	-2.04534200	0.58756400
H	-0.32703800	-0.30327000	1.46416200
C	1.52081400	4.90967300	-2.59384700
C	1.94806300	5.69665400	-3.67172000
C	3.15573600	5.40164000	-4.32728700
C	3.92940100	4.31266500	-3.90004000
C	3.49850900	3.51260600	-2.82742800
H	0.57008300	5.14728400	-2.08836000
H	1.32923700	6.54312400	-4.00792600
H	3.48958700	6.01760700	-5.17580900
H	4.87320900	4.07148300	-4.41265600
H	4.11717600	2.65485200	-2.52478400
C	-1.15566400	2.29268800	-1.15520400
C	-2.27504300	1.78371800	-1.83450000
C	-2.10459500	0.97025700	-2.96389400
C	-0.80986700	0.66763000	-3.42106200
C	0.30931200	1.18897500	-2.75850300
H	-1.29437600	2.91617700	-0.25666600

H	-3.28634700	2.03477900	-1.47880200
H	-2.98125400	0.57293200	-3.49813000
H	-0.67163900	0.03232900	-4.30880600
H	1.31538100	0.97074900	-3.14972400
C	6.14021600	7.39902800	5.55444600
C	7.24164700	7.26142400	6.41726900
C	8.03942100	6.10851200	6.36996000
C	7.73383100	5.08934000	5.45173000
C	6.63193600	5.22002800	4.59489700
H	5.53679100	8.31686200	5.60784300
H	7.47785700	8.06720100	7.12941900
H	8.89504200	5.99733300	7.05223300
H	8.35144700	4.17974600	5.40560700
H	6.39917600	4.40696200	3.88866100
C	6.15113200	7.66330200	1.64007100
C	6.73821300	7.82542700	0.37750900
C	6.35971700	6.99139100	-0.68914400
C	5.39556800	5.99204500	-0.49031800
C	4.80565400	5.82882700	0.77411200
H	6.46841000	8.30926900	2.47388100
H	7.50024400	8.60475200	0.22459800
H	6.82241400	7.12205400	-1.67921000
H	5.09109300	5.34142200	-1.32405700
H	4.04647300	5.04533500	0.93658900
C	1.97903800	10.64142200	4.76201700
C	1.39001700	11.79693200	5.30257200
C	0.08201800	12.15819700	4.94587700
C	-0.64346200	11.35174000	4.05210500
C	-0.06422100	10.19105900	3.51853600

H	3.00840000	10.38445000	5.05094000
H	1.96472100	12.42365700	6.00153100
H	-0.37176400	13.07004800	5.36270700
H	-1.66953200	11.62514000	3.76208700
H	-0.64399500	9.56902900	2.81790700
C	2.91972400	10.29094400	1.20328000
C	3.25399400	10.76591000	-0.07311600
C	3.07125500	9.94714200	-1.20051000
C	2.55112900	8.65259500	-1.04779900
C	2.21076100	8.17566900	0.22867300
H	3.05052500	10.94717000	2.07794300
H	3.65605300	11.78404500	-0.18854900
H	3.33271200	10.32339900	-2.20136200
H	2.41154500	8.00288800	-1.92488300
H	1.79191700	7.16326300	0.34665600
C	2.14697300	5.71753800	11.38990800
C	2.75237300	5.26909800	12.57394100
C	3.23842100	3.95405200	12.66618200
C	3.11570900	3.08082500	11.57281800
C	2.50657200	3.52529700	10.38776200
H	1.78487600	6.75499600	11.32077200
H	2.85101100	5.95521000	13.42901600
H	3.72238300	3.60731300	13.59171900
H	3.50806400	2.05420600	11.63909600
H	2.41168700	2.84554400	9.52426500
C	0.73840300	8.19183300	9.04155300
C	1.15211100	9.53436000	9.00654400
C	2.44429700	9.86413300	8.57258000
C	3.32058400	8.84719900	8.15456900

C	2.90505900	7.50808300	8.16664500
H	-0.27715500	7.95944100	9.39335500
H	0.45600200	10.32387800	9.32724600
H	2.77062900	10.91520500	8.56227100
H	4.34008700	9.09813300	7.82219000
H	3.59212400	6.71659500	7.82400200
C	-3.47900100	4.22192100	9.81648600
C	-4.57656300	3.48926100	10.29329100
C	-5.40645700	2.79788100	9.39635400
C	-5.13128800	2.83452900	8.02111900
C	-4.03354800	3.56683200	7.54199600
H	-2.84582100	4.75852300	10.53885900
H	-4.78530400	3.46246500	11.37376600
H	-6.26601300	2.22241900	9.77198600
H	-5.76777800	2.28566800	7.31233000
H	-3.81336300	3.57351500	6.46251200
C	-3.51168700	7.40632200	8.57957300
C	-3.96525800	8.73416800	8.55179800
C	-3.38755700	9.66112900	7.66884900
C	-2.35782900	9.25352000	6.80704600
C	-1.90479000	7.92490200	6.82650400
H	-3.98454000	6.68945600	9.26744200
H	-4.78024800	9.04398700	9.22388800
H	-3.74776600	10.70103400	7.64864200
H	-1.90023100	9.96854300	6.10696300
H	-1.10723500	7.60941900	6.13560600
C	7.82396200	0.98922800	5.50131100
C	8.79883800	1.19641300	4.51244800
C	8.41915100	1.50244300	3.19515400

C	7.05749700	1.60338300	2.86870100
C	6.08024900	1.39855300	3.85506600
H	8.13602800	0.75226100	6.53188700
H	9.86497500	1.11635100	4.77500700
H	9.18720900	1.66395100	2.42328800
H	6.75076900	1.84366600	1.83956700
H	5.01164600	1.48803100	3.59833300
C	6.22658700	-1.79566400	6.73268500
C	6.15928900	-3.13200000	7.16040900
C	4.98126200	-3.63509500	7.73519200
C	3.85745800	-2.80317500	7.86715300
C	3.91523500	-1.47206900	7.42682600
H	7.15734000	-1.41628100	6.28800800
H	7.04059000	-3.78207100	7.05048000
H	4.93760300	-4.68069800	8.07600500
H	2.92370600	-3.19348500	8.29895400
H	3.02130200	-0.83084000	7.51028800
C	9.47965000	2.58348200	9.00130700
C	10.27430300	3.71574500	9.24980800
C	9.68794400	4.88363600	9.76120700
C	8.30601100	4.91802100	10.02136000
C	7.51270100	3.78810300	9.77365300
H	9.94288300	1.66232000	8.61242400
H	11.35650800	3.68039600	9.05186700
H	10.31048400	5.76796300	9.96717200
H	7.84497000	5.83025000	10.43064800
H	6.43548500	3.82167100	10.00230800
C	6.99442700	1.12452900	11.77932600
C	6.47065900	0.74515700	13.02552500

C	5.33337600	-0.07417400	13.09952000
C	4.72826800	-0.52231300	11.91331900
C	5.25210800	-0.14975000	10.66552500
H	7.88796900	1.76538200	11.74306100
H	6.96173700	1.09331700	13.94732300
H	4.92769300	-0.37361800	14.07776400
H	3.84609600	-1.17982400	11.95747800
H	4.77912100	-0.53994900	9.75038100
C	-6.04124400	6.95466100	2.40099100
C	-7.02358200	7.04992300	3.39869700
C	-6.71619400	6.72016900	4.72895600
C	-5.42211400	6.28913100	5.06185300
C	-4.44183500	6.17607600	4.06309800
H	-6.29039700	7.24343400	1.36697500
H	-8.03474900	7.39386300	3.13273100
H	-7.48655500	6.80833300	5.51060800
H	-5.17004700	6.04348700	6.10455900
H	-3.42521700	5.83672100	4.32576600
C	-3.69576100	9.25123300	1.50719200
C	-3.31249600	10.55138600	1.13580000
C	-2.18045200	10.75658900	0.33206800
C	-1.41958700	9.65413900	-0.09357000
C	-1.79533000	8.35561200	0.28016400
H	-4.58616300	9.10637100	2.13601200
H	-3.91333500	11.41019700	1.47305200
H	-1.88472100	11.77630300	0.04246900
H	-0.51735500	9.80527200	-0.70582500
H	-1.17527900	7.50040900	-0.03488100
C	-8.08564000	5.06305500	-1.02345800

C	-9.08024700	4.12283600	-0.72275400
C	-8.80801400	3.06574700	0.16307100
C	-7.53550600	2.95888900	0.74314100
C	-6.53435600	3.89775500	0.43552800
H	-8.31434600	5.89293700	-1.71185600
H	-10.07769100	4.21974800	-1.17826700
H	-9.59074800	2.33033600	0.40342100
H	-7.31333500	2.13958300	1.44457300
H	-5.54851600	3.79236000	0.91359200
C	-4.83565600	6.94508500	-3.52338800
C	-4.50689100	6.70358300	-4.86696200
C	-4.56158000	5.39815000	-5.37982100
C	-4.94506300	4.33448200	-4.54543800
C	-5.27125500	4.57256100	-3.20170200
H	-4.81030400	7.97293900	-3.12661200
H	-4.22139200	7.54221200	-5.52033300
H	-4.31644300	5.20967700	-6.43635600
H	-4.99842500	3.31123000	-4.94879800
H	-5.58945500	3.73789500	-2.55740900

Isomer III (Figure S3b):

C	0.35525400	-7.20450500	3.24768400
P	1.32180100	-7.78074600	1.74801500
Ag	2.12163800	-5.93557800	0.34143900
Ag	1.34563600	-3.63652000	-1.23538500
P	-0.18987600	-3.82713300	-3.28906400
C	0.67532100	-3.26393700	-4.85854800
P	2.54147900	-3.34691800	-4.97707100
Ag	3.82097300	-3.15964800	-2.82782300

P	6.29961300	-3.56387300	-3.21638700
C	7.27402400	-3.36030200	-1.64441300
P	6.48430800	-4.12726800	-0.13318800
Ag	4.00696300	-3.76126200	0.02775400
Ag	2.08302600	-0.86945300	3.38248600
P	4.29457200	0.00803300	4.56528600
C	5.31004300	0.69367200	3.14260100
P	4.37157700	1.66381000	1.83144400
Ag	1.92366300	1.22080700	1.38705700
Ag	-0.50620600	0.66833900	2.93546900
P	-1.53246800	2.41283600	4.37707900
C	-2.72344100	1.59370800	5.54749400
P	-2.20308400	-0.15324200	6.00240300
Ag	1.68302900	-3.61422300	2.03945900
P	0.33021200	-5.34412600	3.59231600
Ag	-0.68640300	1.18207000	0.09429200
P	-2.41387700	2.22488400	-1.37095800
C	-4.07482100	1.38573000	-1.56485400
P	-4.80094600	0.63658800	0.01021400
Ag	0.01680700	-1.47920200	1.15779500
H	2.08696000	-5.45376300	-1.36809300
H	3.21252000	-4.61645200	1.50771300
H	3.09957500	-2.59228400	-1.23955300
H	2.44366400	-2.55996800	3.29070000
H	0.56167900	-3.05904000	0.47539600
H	1.35372200	0.77396900	3.30764200
H	-1.30920800	-0.18862700	1.35631200
H	1.02203500	1.84332700	-0.02184800
H	7.29705600	-2.26820500	-1.44872600

H	8.31782800	-3.71781200	-1.76148000
H	0.21722300	-3.73655500	-5.75102800
H	0.46518800	-2.17795300	-4.92472900
H	6.21989900	1.23250500	3.48211000
H	5.66901200	-0.21171100	2.60939600
H	-3.84296600	0.50552500	-2.20123500
H	-4.78662400	2.00942000	-2.14603800
H	-0.68904800	-7.56030400	3.16503600
H	0.80705900	-7.72392100	4.11345500
H	-3.64664200	1.48353400	4.93940500
H	-2.97610300	2.25248700	6.40491000
C	7.01365100	-5.89161200	-0.22166300
C	7.53510300	-3.38835700	1.19746500
C	7.21940400	-2.48402800	-4.40235500
C	6.70633100	-5.26253800	-3.80884100
C	-1.81551500	-2.96433200	-3.56955100
C	-0.66581300	-5.58055300	-3.66066800
C	2.88689100	-4.88330000	-5.93570000
C	2.82940400	-1.94787800	-6.14764600
C	-6.17746600	1.77671200	0.51689600
C	-5.82116400	-0.74627000	-0.72094200
C	-1.82397500	2.34001900	-3.12751400
C	-2.71714800	4.00179300	-0.97062300
C	5.42731300	-1.28153400	5.28163500
C	4.29018900	1.30075600	5.88172100
C	4.54975500	3.45563600	2.24209100
C	5.49422100	1.45276500	0.37318800
C	-2.57062000	3.79326500	3.70944400
C	-0.28660200	3.32416500	5.37862400

C	-1.31333200	0.08917800	7.62110700
C	-3.80896400	-0.84982200	6.62491200
C	-1.50376800	-5.04897300	3.70922400
C	0.86219800	-5.28798200	5.37560000
C	2.65165600	-8.80195200	2.52480300
C	0.20547000	-9.02511800	0.95347200
C	8.09863800	-4.18184600	2.21877900
C	8.85238500	-3.58915100	3.24392100
C	9.05407800	-2.20126600	3.26680900
C	8.48365300	-1.40305300	2.26244500
C	7.72017000	-1.98744800	1.24064100
H	7.95722200	-5.27269500	2.21073700
H	9.28992800	-4.22185900	4.03071500
H	9.65090300	-1.74188200	4.06881100
H	8.63548400	-0.31279400	2.26853300
H	7.27165000	-1.33554500	0.47359900
C	6.03030600	-6.89903900	-0.16873200
C	6.39284700	-8.25328900	-0.25553400
C	7.74128500	-8.61140600	-0.40149900
C	8.72951800	-7.61313800	-0.45677800
C	8.37013500	-6.26110100	-0.36589200
H	4.96911300	-6.61542600	-0.06905800
H	5.61427700	-9.02964100	-0.20817300
H	8.02684800	-9.67207200	-0.47291900
H	9.78871000	-7.88965900	-0.57039300
H	9.15732900	-5.49113400	-0.39680200
C	6.71268700	-2.39127000	-5.71832600
C	7.34960900	-1.58899800	-6.67518700
C	8.50181300	-0.86194700	-6.33266200

C	9.01534400	-0.94936500	-5.03022100
C	8.38120900	-1.75487400	-4.06856700
H	5.81389400	-2.96192700	-5.99944200
H	6.94065100	-1.52814000	-7.69507800
H	9.00239100	-0.23168700	-7.08306700
H	9.92570200	-0.39364500	-4.75765400
H	8.81443500	-1.81192600	-3.05937200
C	7.97465300	-5.56541800	-4.35044400
C	8.25814000	-6.86500900	-4.79257400
C	7.28003200	-7.87026100	-4.70190400
C	6.01688100	-7.57316700	-4.16868300
C	5.72704800	-6.27254400	-3.72600700
H	8.74072100	-4.77905300	-4.44154300
H	9.24774100	-7.09273400	-5.21734100
H	7.50362000	-8.88794300	-5.05732100
H	5.24499600	-8.35480300	-4.10353300
H	4.72929100	-6.04213400	-3.31728200
C	3.71802500	-4.88760700	-7.07727300
C	4.02185800	-6.09387100	-7.72895500
C	3.50183400	-7.30686400	-7.25317900
C	2.68435600	-7.31156300	-6.11118400
C	2.38796900	-6.11208500	-5.44729500
H	4.12120900	-3.94482600	-7.47657900
H	4.66562600	-6.08105300	-8.62175100
H	3.73435700	-8.24899800	-7.77186500
H	2.26747300	-8.25606600	-5.72892500
H	1.75951500	-6.14143300	-4.54389200
C	3.54205200	-0.82108100	-5.68690800
C	3.70655700	0.30550200	-6.51037300

C	3.16190700	0.31400500	-7.80405900
C	2.44954100	-0.80422000	-8.27246800
C	2.27920200	-1.92776200	-7.44987800
H	3.97255300	-0.82764000	-4.67202900
H	4.26899600	1.17528600	-6.13883900
H	3.29299900	1.19332400	-8.45281300
H	2.02300400	-0.80105500	-9.28710000
H	1.71779800	-2.79631200	-7.82819100
C	-0.54323800	-6.56077500	-2.65656100
C	-0.91891100	-7.89156500	-2.90955900
C	-1.41853700	-8.25451000	-4.16875900
C	-1.55542500	-7.28170200	-5.17440400
C	-1.18805200	-5.95334400	-4.92092000
H	-0.12400600	-6.28674500	-1.67649000
H	-0.81579900	-8.64509900	-2.11505900
H	-1.70826400	-9.29762600	-4.36911300
H	-1.95555000	-7.55880800	-6.16167100
H	-1.32658600	-5.20312800	-5.71508400
C	-3.03912900	-3.65947100	-3.45622700
C	-4.25254500	-3.01734800	-3.74798200
C	-4.26496300	-1.67806600	-4.16551800
C	-3.05586800	-0.96834000	-4.24850600
C	-1.84366300	-1.59956500	-3.92949600
H	-3.04746500	-4.71882300	-3.16202000
H	-5.19679600	-3.57426900	-3.66162300
H	-5.21767100	-1.18939900	-4.41884600
H	-3.04380000	0.08284700	-4.57386800
H	-0.91675800	-1.00860400	-3.98945600
C	-5.52994900	-2.05982400	-0.29951100

C	-6.30347800	-3.14546300	-0.74475000
C	-7.37240000	-2.93050900	-1.62803900
C	-7.66223900	-1.62679100	-2.06775300
C	-6.89691500	-0.54255300	-1.61246600
H	-4.68923000	-2.23002000	0.39132800
H	-6.07134500	-4.16303400	-0.39399700
H	-7.98820100	-3.77662100	-1.97045900
H	-8.50340400	-1.45177200	-2.75626400
H	-7.16147400	0.47550900	-1.93835200
C	-6.61691100	1.61479500	1.85098600
C	-7.67419800	2.38155200	2.36152100
C	-8.30524000	3.33709500	1.54910600
C	-7.88102300	3.50946100	0.22184500
C	-6.82916400	2.73183500	-0.29141100
H	-6.11821200	0.87391700	2.49761100
H	-8.00071000	2.23831600	3.40281800
H	-9.12833200	3.94748700	1.94981000
H	-8.37703500	4.25183600	-0.42222800
H	-6.53031700	2.87554000	-1.34155400
C	-0.55967100	1.80967700	-3.45587800
C	-0.07785200	1.88084600	-4.77424000
C	-0.85478100	2.48585700	-5.77423100
C	-2.11102000	3.02884800	-5.45276500
C	-2.59222300	2.96016400	-4.13694700
H	0.05645800	1.34956400	-2.66521400
H	0.91329600	1.46706900	-5.01936500
H	-0.47748200	2.54453900	-6.80656200
H	-2.71722600	3.51773200	-6.23070000
H	-3.56904900	3.40927200	-3.89803600

C	-1.64793900	4.71718400	-0.38801100
C	-1.75391100	6.09717900	-0.16268400
C	-2.93181400	6.77865400	-0.50686400
C	-4.00440500	6.07342600	-1.07460100
C	-3.89868800	4.69325900	-1.30705300
H	-0.72224700	4.18317800	-0.11599600
H	-0.91172800	6.64266000	0.28969300
H	-3.01565700	7.86152700	-0.32866900
H	-4.93287600	6.60090800	-1.34189000
H	-4.75163000	4.16312500	-1.75458200
C	5.17408800	-2.63115900	4.94996900
C	5.94109400	-3.65924800	5.52139800
C	6.96822400	-3.35435400	6.42781500
C	7.23167900	-2.01465000	6.75681900
C	6.46510700	-0.98394300	6.19196700
H	4.35602200	-2.87937800	4.25502700
H	5.71887600	-4.70658700	5.26515600
H	7.55856200	-4.16127400	6.88848700
H	8.03031000	-1.76821600	7.47351400
H	6.66444100	0.05627900	6.48811300
C	3.18929200	1.29109700	6.76488000
C	3.15889600	2.14200200	7.87968200
C	4.21916200	3.03030500	8.11690700
C	5.30930100	3.06682800	7.23281300
C	5.34718700	2.20460900	6.12571300
H	2.34486400	0.60871000	6.57977000
H	2.29282900	2.11081800	8.55698600
H	4.19697100	3.69964500	8.99059600
H	6.14292000	3.76309800	7.41309500

H	6.22609600	2.23009300	5.46451700
C	5.08767500	0.58342200	-0.66093300
C	5.91247600	0.38661400	-1.78150000
C	7.14317500	1.05609800	-1.88212100
C	7.55137900	1.92400300	-0.85452000
C	6.73093000	2.12502600	0.26644600
H	4.11806000	0.06276300	-0.59813300
H	5.58264700	-0.28799800	-2.58759900
H	7.77762600	0.90907600	-2.76932700
H	8.50955200	2.45991000	-0.93233200
H	7.04937800	2.82757400	1.05222900
C	3.64177500	4.33618200	1.61009500
C	3.72690700	5.72051400	1.81821000
C	4.71124000	6.24565200	2.67120400
C	5.61514000	5.37998800	3.30652900
C	5.53892200	3.99441600	3.08989900
H	2.86154600	3.92760600	0.94571200
H	3.01594600	6.39216900	1.31353400
H	4.77574200	7.33108500	2.83967900
H	6.39077500	5.78439100	3.97454900
H	6.26444200	3.33917200	3.59188300
C	2.39634100	-10.07586900	3.08041800
C	3.42382800	-10.78268200	3.72220600
C	4.71125100	-10.22754600	3.81986000
C	4.96924400	-8.96046700	3.27542700
C	3.94434600	-8.24920700	2.63015300
H	1.39323000	-10.52385100	3.00479700
H	3.21798000	-11.77619100	4.14925500
H	5.51431400	-10.78831100	4.32158700

H	5.97591800	-8.52100300	3.34486700
H	4.14694800	-7.25065800	2.21011400
C	0.77819500	-10.07803400	0.20309800
C	-0.03754300	-11.01001700	-0.45544700
C	-1.43694000	-10.90037000	-0.38912000
C	-2.01393200	-9.84118400	0.32773900
C	-1.20074600	-8.90666300	0.98981700
H	1.87296400	-10.18290200	0.14601300
H	0.42486400	-11.83434700	-1.01937900
H	-2.07645100	-11.63804700	-0.89695900
H	-3.10858500	-9.74035900	0.37945600
H	-1.68431100	-8.08182900	1.53532300
C	0.87798100	3.75987700	4.70956800
C	1.79321400	4.60852300	5.34882500
C	1.56207100	5.01834500	6.67185900
C	0.42053300	4.56875200	7.35426700
C	-0.50252200	3.72772000	6.71221500
H	1.06741900	3.43569700	3.67306900
H	2.69293700	4.94407200	4.81064500
H	2.27886400	5.68372600	7.17630500
H	0.23784800	4.87977300	8.39434700
H	-1.39714000	3.39908900	7.26030400
C	-2.41053400	5.13230700	4.12428100
C	-3.26892600	6.12929300	3.63426400
C	-4.29392700	5.80034900	2.73480500
C	-4.45107500	4.47131800	2.30990700
C	-3.58683700	3.47321300	2.78359900
H	-1.61897900	5.40106600	4.83833300
H	-3.13702200	7.17018800	3.96773800

H	-4.97030500	6.58217200	2.35727000
H	-5.24587300	4.20755200	1.59822700
H	-3.70750500	2.43591400	2.42743700
C	-2.08845100	-4.09028500	2.85894600
C	-3.46997700	-3.83994600	2.90947300
C	-4.28528500	-4.55399700	3.79883600
C	-3.71182200	-5.51631300	4.64840800
C	-2.33055900	-5.75743800	4.61065500
H	-1.45373500	-3.52821100	2.15252000
H	-3.90555400	-3.07173800	2.25330400
H	-5.36685700	-4.35482000	3.84015600
H	-4.34467400	-6.07790100	5.35308400
H	-1.89740300	-6.49635500	5.30259200
C	1.46323100	-4.09808800	5.83848700
C	1.87997900	-3.97580200	7.17342000
C	1.70074000	-5.03820800	8.07159300
C	1.10345100	-6.22687400	7.62420500
C	0.68962900	-6.35272800	6.28886900
H	1.62741300	-3.26830700	5.13362000
H	2.36497900	-3.04569300	7.50753600
H	2.03093600	-4.94537700	9.11733500
H	0.95965600	-7.06785700	8.31903100
H	0.23013600	-7.30232100	5.97400000
C	-0.06255000	-0.53984800	7.78447700
C	0.63638500	-0.43595100	9.00017800
C	0.09420800	0.30252600	10.06280600
C	-1.15697000	0.92669500	9.91220300
C	-1.85836300	0.81395000	8.70323500
H	0.35550100	-1.13187100	6.95451000

H	1.60911100	-0.93779800	9.11850700
H	0.63883400	0.38180100	11.01620500
H	-1.59494500	1.49199300	10.74932300
H	-2.85425700	1.27746200	8.61440200
C	-3.86283300	-2.25221400	6.78553600
C	-5.01942600	-2.86947300	7.28457400
C	-6.14550000	-2.09843100	7.61579900
C	-6.10868500	-0.70608600	7.44388100
C	-4.94891900	-0.08457500	6.95287200
H	-2.98969700	-2.86790100	6.51473100
H	-5.04281100	-3.96296400	7.41004700
H	-7.05356800	-2.58201400	8.00652200
H	-6.98759100	-0.09448100	7.70002300
H	-4.94529300	1.00955400	6.83578200

Cartesian Coordinates of isomers of $[\text{Ag}_{10}\text{H}_8\text{L}_6]^{3+}$

Isomer I

Ag	0.50677300	0.68367400	-0.29501100
Ag	0.45339700	1.08575100	2.72805700
Ag	3.51027500	0.18272800	2.69402100
Ag	3.12877500	-0.52423400	-0.11632000
Ag	0.27164300	4.07406100	3.51661400
Ag	-0.11037000	3.36684800	0.70683100
Ag	2.94662400	2.46359200	0.67235400
Ag	2.89362100	2.86610500	3.69545800
Ag	1.91792000	5.19824500	1.46051100
Ag	1.48305900	-1.64901200	1.93976500
P	5.13487800	-0.14802900	4.59047400
P	4.89834300	2.88882500	5.31869800

P	4.74197400	2.63702400	-1.19903800
P	4.95771900	-0.49094400	-1.84894200
P	-1.73519700	3.69746300	-1.18945600
P	-1.49814100	0.66068800	-1.91812700
P	-1.55612100	4.04138100	5.25068000
P	-1.34180400	0.91352700	4.59965900
P	2.68639100	7.45327100	2.00618500
P	0.71328900	-3.90350300	1.39364100
C	-2.63041800	2.10810600	-1.57637700
C	6.03043800	1.44120200	4.97723900
C	4.93643900	1.27050800	-2.46236100
C	-1.53522200	2.27972600	5.86350300
C	1.56894800	8.66756900	1.14703000
C	1.82973800	-5.11874000	2.25279900
P	1.86286300	10.50101400	1.57601900
P	1.53564800	-6.95166700	1.82185000
H	4.05144200	1.34285700	-3.12770000
H	5.84332500	1.46465500	-3.07083900
H	-3.19119300	1.86087500	-0.65054600
H	-3.35280500	2.22814900	-2.40977300
H	-0.65003000	2.20677100	6.52851300
H	-2.44198200	2.08576500	6.47222100
H	6.59136200	1.68817600	4.05143300
H	6.75271100	1.32116900	5.81073000
H	0.53998100	8.36086400	1.42522200
H	1.67741500	8.49462800	0.05585100
H	2.85904400	-4.81193500	1.97597900
H	1.72019200	-4.94689600	3.34404600
C	-3.29818200	4.39534000	4.79324700

C	-3.03153700	0.77103800	3.86170600
C	4.54140100	2.76800300	7.12491500
C	4.46117800	-0.72774100	6.20567800
C	6.69958700	-0.84400200	-1.39027900
C	-1.14091900	0.78198500	-3.72424200
C	-1.06194900	4.27776300	-2.80462900
C	-3.10015300	4.89816700	-0.85969300
C	-2.62401900	-0.79745000	-1.82323000
C	-1.20864500	-0.58000400	5.67818800
C	-1.25601900	4.98473800	6.80731000
C	6.02419000	4.34698200	5.22316600
C	6.49956900	-1.34920400	4.26141500
C	4.60796500	4.13004000	-2.27813600
C	4.65905900	-1.43479300	-3.40559800
C	-4.38557700	3.99626900	5.60272900
C	-5.69901900	4.29662400	5.21560000
C	-5.93909300	5.00183500	4.02344000
C	-4.86354400	5.40882900	3.21935800
C	-3.54645200	5.10555900	3.60032100
H	-4.21584300	3.45957900	6.54940600
H	-6.54066000	3.98365700	5.85171100
H	-6.97185100	5.23764900	3.72481700
H	-5.04419600	5.95989300	2.28437100
H	-2.70377300	5.41059300	2.95988000
C	-4.00045000	-0.11080800	4.38754600
C	-5.29205400	-0.14633900	3.83884500
C	-5.63131800	0.69787800	2.76919600
C	-4.66916500	1.57368200	2.23953200
C	-3.37080000	1.60145300	2.77188000

H	-3.75051400	-0.77260100	5.23003000
H	-6.04177000	-0.83388000	4.25916000
H	-6.64951900	0.67589400	2.35189100
H	-4.93307800	2.25304300	1.41382100
H	-2.61784900	2.28002700	2.34077000
C	5.53505700	3.03880300	8.09122300
C	5.23571500	2.93452300	9.45722400
C	3.94561200	2.56073800	9.87113100
C	2.95397400	2.29035600	8.91514900
C	3.24841400	2.39753300	7.54595400
H	6.54461300	3.34874200	7.77807200
H	6.01366200	3.15145300	10.20492500
H	3.71435100	2.48242300	10.94431800
H	1.94401100	1.99394200	9.23742300
H	2.47297800	2.18729300	6.79238800
C	5.30693800	-0.95082500	7.31383300
C	4.77046300	-1.39850700	8.52866900
C	3.38992600	-1.63951800	8.64365100
C	2.54641400	-1.43264900	7.54179300
C	3.07913900	-0.97633000	6.32448800
H	6.39340100	-0.78966000	7.23020300
H	5.43484000	-1.56927000	9.38906400
H	2.97449200	-1.99891200	9.59748300
H	1.46710100	-1.62986200	7.62240800
H	2.41630600	-0.81421800	5.45976300
C	6.43159100	2.78082900	-0.46107200
C	7.40009400	3.66280100	-0.98749900
C	8.69170800	3.69927000	-0.43888100
C	9.03139100	2.85584500	0.63129500

C	8.06964500	1.97994400	1.16150700
C	6.77128500	1.95125100	0.62922800
H	7.14983200	4.32396400	-1.83037600
H	9.44108500	4.38687800	-0.85963600
H	10.04959600	2.87855200	1.04853800
H	8.33392400	1.30119700	1.98761600
H	6.01865400	1.27256200	1.06075800
C	7.78747100	-0.44478600	-2.19906900
C	9.10069300	-0.74434900	-1.81090400
C	9.34025800	-1.44898800	-0.61826800
C	8.26425600	-1.85618400	0.18519200
C	6.94739600	-1.55367200	-0.19688200
H	7.61814400	0.09149100	-3.14611900
H	9.94269400	-0.43125800	-2.44649800
H	10.37289700	-1.68420800	-0.31879500
H	8.44450500	-2.40684700	1.12049300
H	6.10432200	-1.85890200	0.44303000
C	-1.90847600	4.50143100	-3.91245900
C	-1.37236500	4.94942800	-5.12728200
C	0.00818600	5.19018100	-5.24288000
C	0.85218000	4.98272400	-4.14150300
C	0.31979400	4.52608900	-2.92411800
H	-2.99480100	4.34046100	-3.82828900
H	-2.03711400	5.12066200	-5.98733600
H	0.42325400	5.54980300	-6.19676600
H	1.93148700	5.17969700	-4.22255000
H	0.98313500	4.36353100	-2.05972600
C	-2.13452000	0.51209200	-4.69083000
C	-1.83490200	0.61655300	-6.05670300

C	-0.54462600	0.98959500	-6.47031700
C	0.44722400	1.25914600	-5.51411000
C	0.15235200	1.15175900	-4.14497400
H	-3.14438900	0.20265700	-4.37791700
H	-2.61292300	0.40029600	-6.80458600
H	-0.31306100	1.06806600	-7.54346400
H	1.45729300	1.55495800	-5.83611800
H	0.92784900	1.36124900	-3.39122500
C	-2.72324200	6.16015500	-0.34796400
C	-3.68459400	7.15903500	-0.13879600
C	-5.03823200	6.90708200	-0.42206400
C	-5.42423800	5.64870800	-0.90880500
C	-4.46246300	4.64772300	-1.12874900
H	-1.66414000	6.36213800	-0.11890100
H	-3.37563000	8.14214500	0.24886300
H	-5.79226300	7.69310200	-0.26484800
H	-6.48249000	5.44488800	-1.13273100
H	-4.79179800	3.67590200	-1.52538300
C	-2.11577400	-2.02885400	-2.30020200
C	-2.91044800	-3.18301700	-2.27105900
C	-4.21696900	-3.13124200	-1.75571500
C	-4.72154100	-1.91854500	-1.26382200
C	-3.93151200	-0.75652800	-1.29439100
H	-1.09498000	-2.08625100	-2.71088300
H	-2.50177600	-4.12955000	-2.65440700
H	-4.84147700	-4.03697400	-1.73977500
H	-5.74531500	-1.86728700	-0.86284200
H	-4.35957400	0.18068900	-0.90995300
C	-2.13163400	6.00735500	7.23161500

C	-1.84995000	6.73707100	8.39800800
C	-0.69872600	6.45734400	9.15086200
C	0.18609900	5.45224300	8.72360600
C	-0.08225200	4.72783600	7.55330100
H	-3.04196600	6.23192200	6.65654300
H	-2.54453300	7.52619000	8.72341700
H	-0.48923900	7.02508900	10.06985000
H	1.09722900	5.23188900	9.30084300
H	0.64131300	3.96691800	7.21985100
C	-0.88924600	-1.81025300	5.06130100
C	-0.82926100	-2.99146400	5.81526600
C	-1.08100600	-2.96327600	7.19703900
C	-1.39155800	-1.74519500	7.82125700
C	-1.45548200	-0.55996000	7.06948200
H	-0.69404200	-1.85083000	3.97769600
H	-0.59182700	-3.94159300	5.31474600
H	-1.03716000	-3.89124400	7.78692900
H	-1.59596500	-1.71298500	8.90212300
H	-1.71550800	0.37396700	7.58685400
C	5.51570700	5.57860300	5.69926500
C	6.31037600	6.73281000	5.66948300
C	7.61691500	6.68084700	5.15442400
C	8.12173000	5.46788000	4.66340600
C	7.33177600	4.30571000	4.69459600
H	4.49487400	5.63620000	6.10968700
H	5.90149700	7.67958800	6.05215800
H	8.24135100	7.58660700	5.13797200
H	9.14555700	5.41642900	4.26264300
H	7.75998000	3.36836400	4.31089200

C	6.12252500	-2.61104400	3.74941500
C	7.08354800	-3.61029800	3.54086500
C	8.43706000	-3.35894200	3.82502900
C	8.82333900	-2.10071600	4.31209000
C	7.86180600	-1.09939500	4.53137200
H	5.06341700	-2.81256700	3.51963900
H	6.77441900	-4.59329400	3.15298100
H	9.19091400	-4.14528600	3.66827700
H	9.88149300	-1.89736500	4.53671000
H	8.19129600	-0.12765100	4.92823600
C	4.28788300	5.36042500	-1.66180800
C	4.22723900	6.54122400	-2.41628500
C	4.47900900	6.51264800	-3.79799600
C	4.79026200	5.29440500	-4.42171800
C	4.85481300	4.10961200	-3.66945900
H	4.09268100	5.40132900	-0.57819500
H	3.98922100	7.49148200	-1.91617400
H	4.43466000	7.44031600	-4.38831300
H	4.99469400	5.26190300	-5.50257700
H	5.11537200	3.17556400	-4.18641600
C	5.53542100	-2.45711700	-3.82907000
C	5.25478600	-3.18720100	-4.99553500
C	4.10400300	-2.90815800	-5.74920400
C	3.21842600	-1.90332300	-5.32275400
C	3.48567600	-1.17854700	-4.15241700
H	6.44543100	-2.68115600	-3.25335100
H	5.94996200	-3.97610700	-5.32029800
H	3.89536600	-3.47617000	-6.66821300
H	2.30759400	-1.68351400	-5.90066500

H	2.76157200	-0.41788000	-3.81960100
C	4.39317700	7.76274900	1.39648300
C	2.68302300	7.97010500	3.76983600
C	1.77947500	11.26700800	-0.11779400
C	0.23190200	10.97403400	2.32872000
C	-0.99385200	-4.21260800	2.00253900
C	0.71736200	-4.41964300	-0.37013600
C	3.16628100	-7.42395200	1.06779200
C	1.61967200	-7.71948300	3.51476200
C	-2.00712300	-3.31639200	1.59003700
C	-3.32441800	-3.48050100	2.04077500
C	-3.64675100	-4.53648200	2.91054400
C	-2.64665700	-5.42853600	3.32549700
C	-1.32422100	-5.27029000	2.87699100
H	-1.76807600	-2.48588700	0.90569200
H	-4.10116100	-2.77535500	1.70989400
H	-4.68078900	-4.66576600	3.26439500
H	-2.89213700	-6.26160600	4.00125200
H	-0.56315600	-5.99101400	3.21062100
C	-0.13466500	-5.44986700	-0.82540000
C	-0.04933600	-5.89091400	-2.15528800
C	0.88008400	-5.31316800	-3.03581100
C	1.72634200	-4.28502300	-2.58889600
C	1.64223200	-3.83829200	-1.26140500
H	-0.86191800	-5.90931900	-0.14081000
H	-0.71088300	-6.69943000	-2.50268400
H	0.94526300	-5.66620100	-4.07622300
H	2.45254700	-3.82499800	-3.27534500
H	2.30449100	-3.02422100	-0.91703700

C	0.69597900	-8.75917900	3.76286800
C	0.68083300	-9.42567400	4.99942600
C	1.58584200	-9.05643500	6.00588200
C	2.50738200	-8.02080900	5.77244600
C	2.52595100	-7.35742200	4.53637400
H	-0.01493500	-9.05088600	2.97313400
H	-0.04037300	-10.23834800	5.17476900
H	1.57748200	-9.57874000	6.97450500
H	3.22352500	-7.73481800	6.55815600
H	3.26545800	-6.55823000	4.37095200
C	3.10353500	-8.32745600	-0.01445400
C	4.27763500	-8.79376200	-0.62819200
C	5.52975500	-8.35498500	-0.17317900
C	5.60448000	-7.44963500	0.89917100
C	4.43226000	-6.98906800	1.51649600
H	2.12131800	-8.67178200	-0.37573000
H	4.21175600	-9.50497200	-1.46548300
H	6.45088100	-8.72249700	-0.65033400
H	6.58683400	-7.11172200	1.26489300
H	4.51651500	-6.29578400	2.36963500
C	3.53437900	9.00093700	4.22416100
C	3.44974900	9.44240500	5.55407000
C	2.52133300	8.86402800	6.43536900
C	1.67563300	7.83516100	5.98937500
C	1.75910600	7.38804800	4.66180300
H	4.26087900	9.46088800	3.53899800
H	4.11085700	10.25145400	5.90070000
H	2.45663000	9.21726900	7.47574800
H	0.95029600	7.37469200	6.67635800

H	1.09737200	6.57341100	4.31821500
C	5.40698600	6.86736900	1.80926700
C	6.72409200	7.03172600	1.35798700
C	7.04559500	8.08728900	0.48729900
C	6.04492400	8.97851800	0.07206600
C	4.72271700	8.81998700	0.52111500
H	5.16860800	6.03723100	2.49432000
H	7.50124500	6.32722200	1.68908700
H	8.07944700	8.21679400	0.13302900
H	6.28974600	9.81122300	-0.60439200
H	3.96119500	9.54006700	0.18718900
C	0.29406500	11.87779600	3.41099500
C	-0.88021100	12.34452700	4.02362600
C	-2.13217700	11.90612400	3.56770300
C	-2.20640100	11.00068100	2.49545400
C	-1.03388200	10.53964800	1.87916700
H	1.27622800	12.22178100	3.77290000
H	-0.81483500	13.05590800	4.86091400
H	-3.05358000	12.27407800	4.04409800
H	-3.18863800	10.66311200	2.12898200
H	-1.11764700	9.84629600	1.02591400
C	2.70204900	12.30765500	-0.36596900
C	2.71753400	12.97312600	-1.60313800
C	1.81401500	12.60181600	-2.61008500
C	0.89347700	11.56504300	-2.37661000
C	0.87476800	10.90291200	-1.13994600
H	3.41191600	12.60100200	0.42415200
H	3.43785000	13.78653000	-1.77844900
H	1.82255300	13.12320500	-3.57919700

H	0.17856000	11.27744500	-3.16268500
H	0.13606900	10.10276700	-0.97454400
H	1.55061700	3.54838000	4.64874900
H	1.61227400	-0.28936900	3.20040000
H	3.79614200	2.03950700	2.29257700
H	3.77687700	-1.16715900	1.41835300
H	1.78735100	3.83872300	0.20038400
H	1.85006700	0.00241400	-1.24851100
H	-0.37935400	4.71553100	1.98298800
H	-0.39606600	1.50980300	1.10782800