

## Supporting Information

### **Temperature dependent chiroptical response of sigmoidal gold clusters: probing the stability of chiral metal clusters**

Ping Guo,<sup>a</sup> Biao Yang,<sup>a</sup> Li Zhang,<sup>b</sup> and Liang Zhao\*,<sup>a</sup>

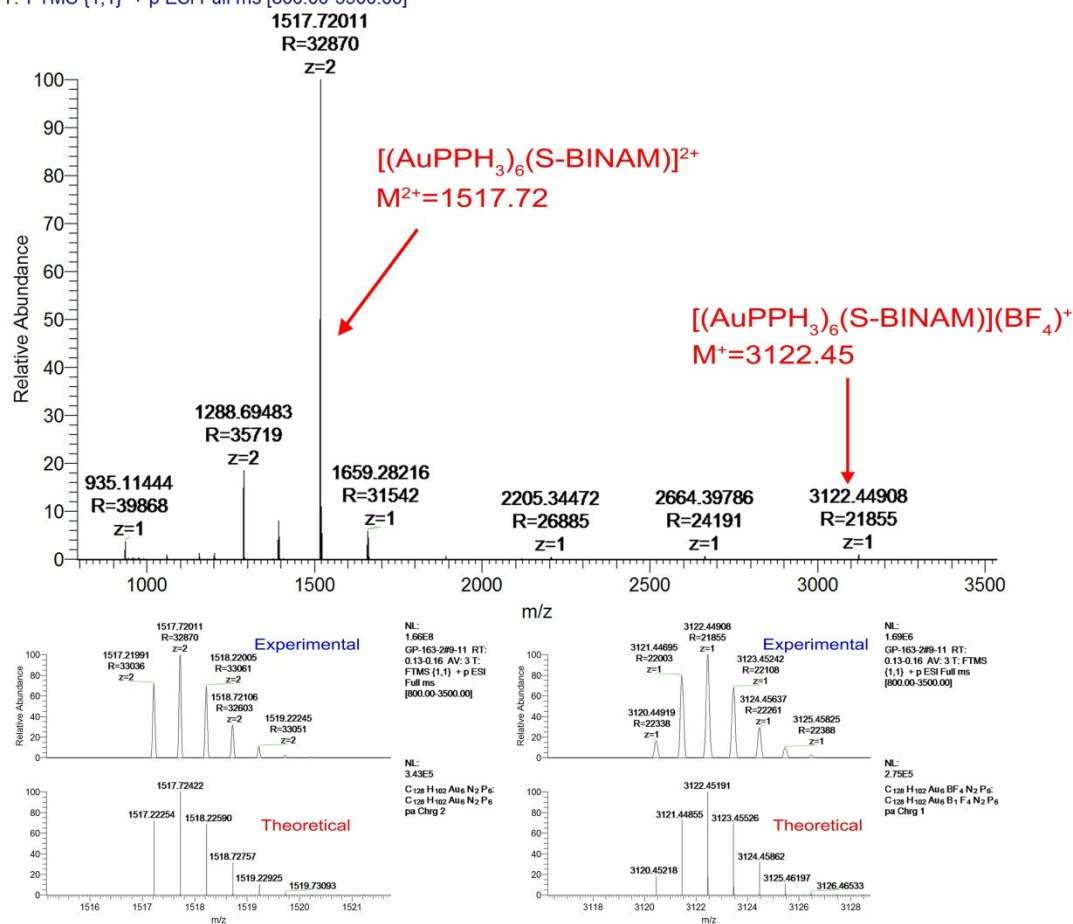
<sup>a</sup> The Key Laboratory of Bioorganic Phosphorus Chemistry & Chemical Biology (Ministry of Education), Department of Chemistry, Tsinghua University, Beijing 100084, China

<sup>b</sup> Beijing National Laboratory for Molecular Science, CAS Key Laboratory of Colloid, Interface and Chemical Thermodynamics, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.

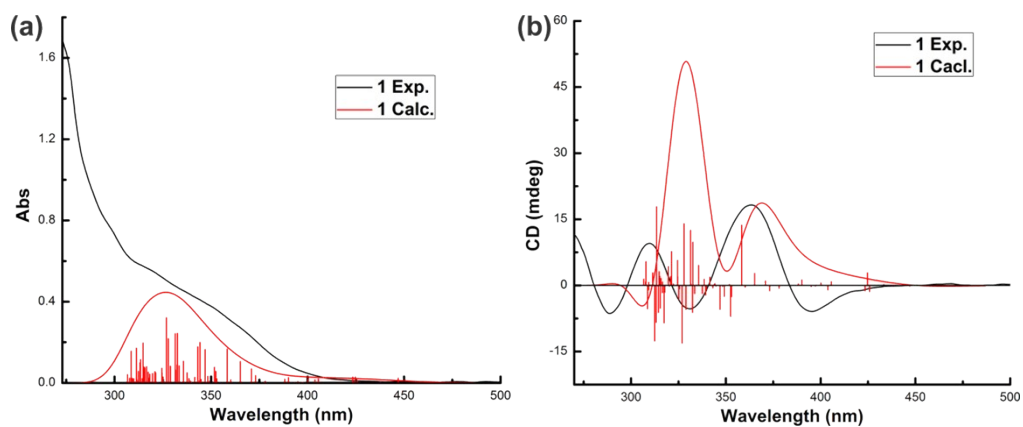
E-mail: zhaolchem@mail.tsinghua.edu.cn

## Supplementary Figures

GP-163-2 #9-11 RT: 0.13-0.16 AV: 3 NL: 1.66E8  
T: FTMS {1,1} + p ESI Full ms [800.00-3500.00]



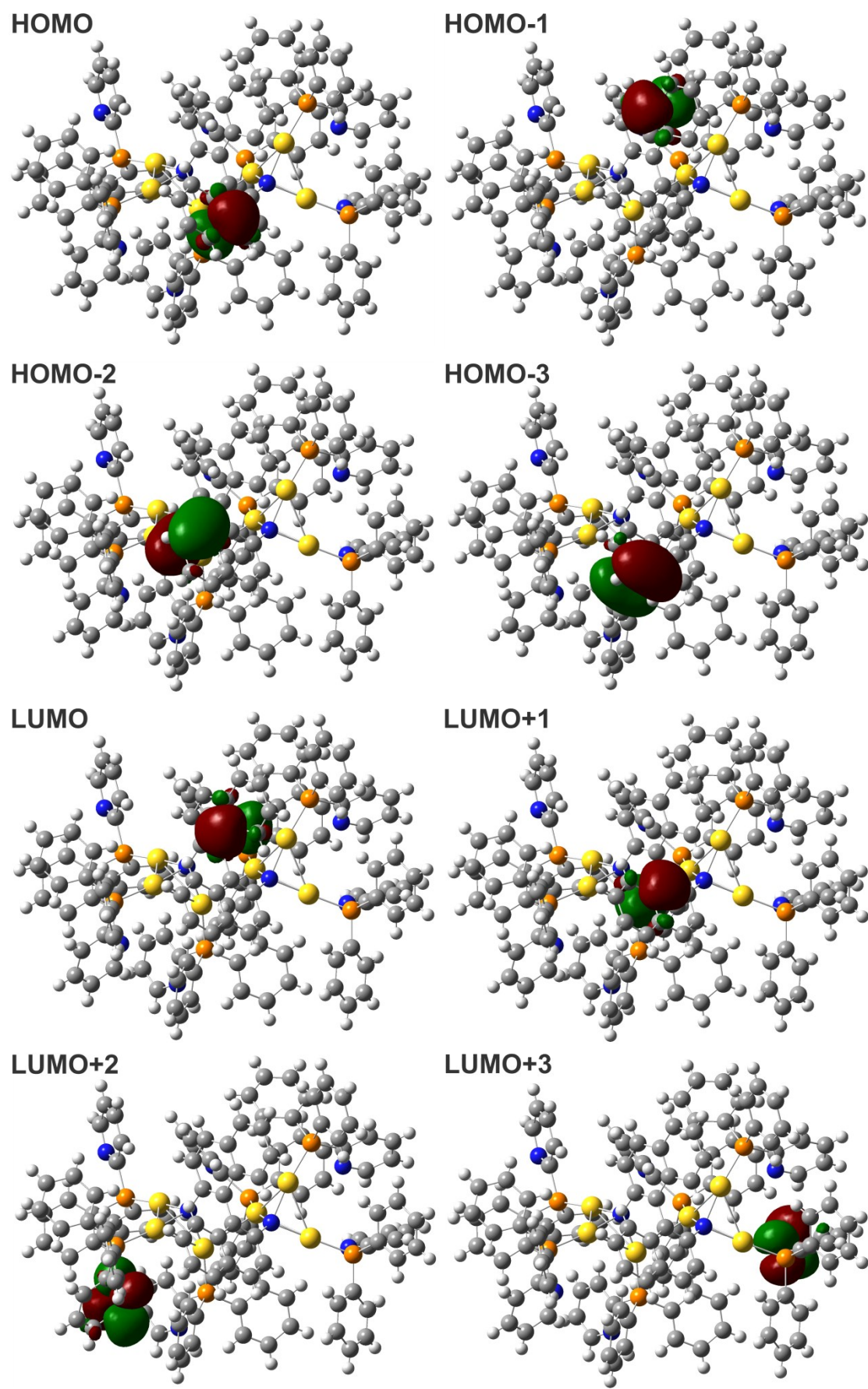
**Fig. S1** Top: ESI-MS spectra of the acetonitrile solution containing **1-(S<sub>a</sub>)**. Bottom: experimental (above) and theoretical (bottom) isotopic distribution of the ion fragment (left) **[(AuPPh<sub>3</sub>)<sub>6</sub>(S-BINAM)]<sup>2+</sup>**, (right) **[(AuPPh<sub>3</sub>)<sub>6</sub>(S-BINAM)](BF<sub>4</sub>)<sup>+</sup>** in ESI-MS spectra.



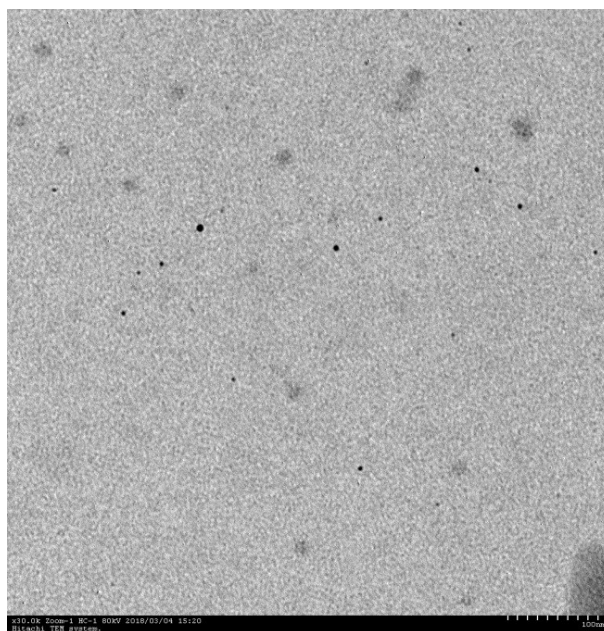
**Fig. S2** Experimental (black line) and calculated (red line) (a) UV-vis absorption and (b) CD spectra of **1-(S<sub>a</sub>)**.

**Table S1.** Mulliken population of **1-(S<sub>a</sub>)**.

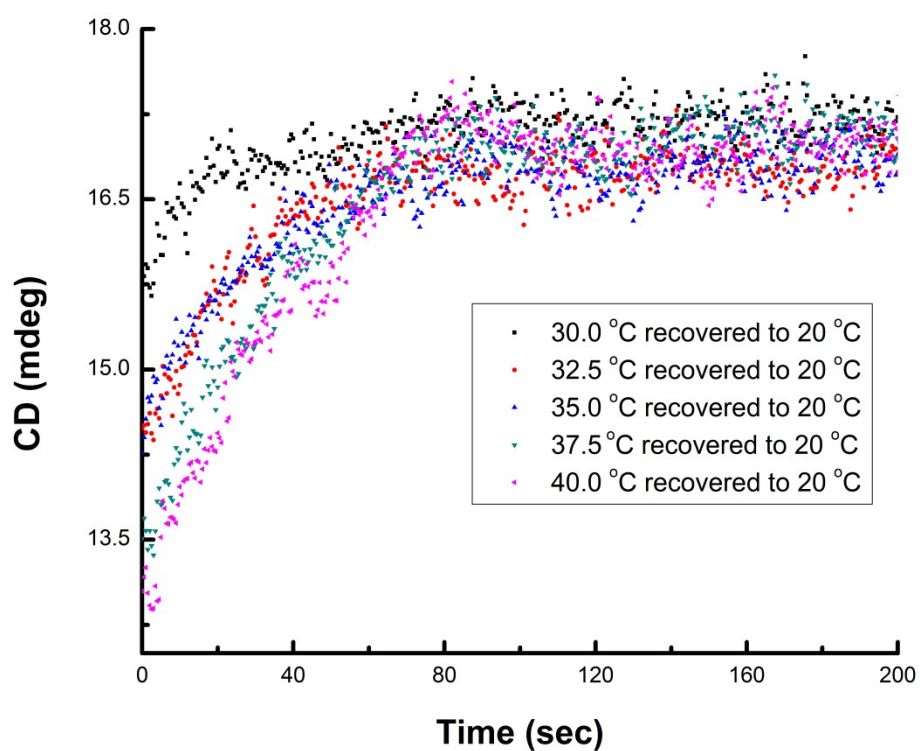
	LUMO+3	LUMO+2	LUMO+1	LUMO	HOMO	HOMO-1	HOMO-2	HOMO-3
<b>Au</b>	0.090	0.001	1.099	1.308	-0.410	0.077	0.586	0.039
<b>N</b>	0.000	0.000	-0.054	-0.044	-0.004	0.002	-0.008	0.000
<b>L</b>	0.001	0.000	99.127	98.816	99.082	99.288	99.350	99.610
<b>PPh<sub>3</sub></b>	99.909	99.999	-0.172	-0.008	1.332	0.633	0.072	0.351



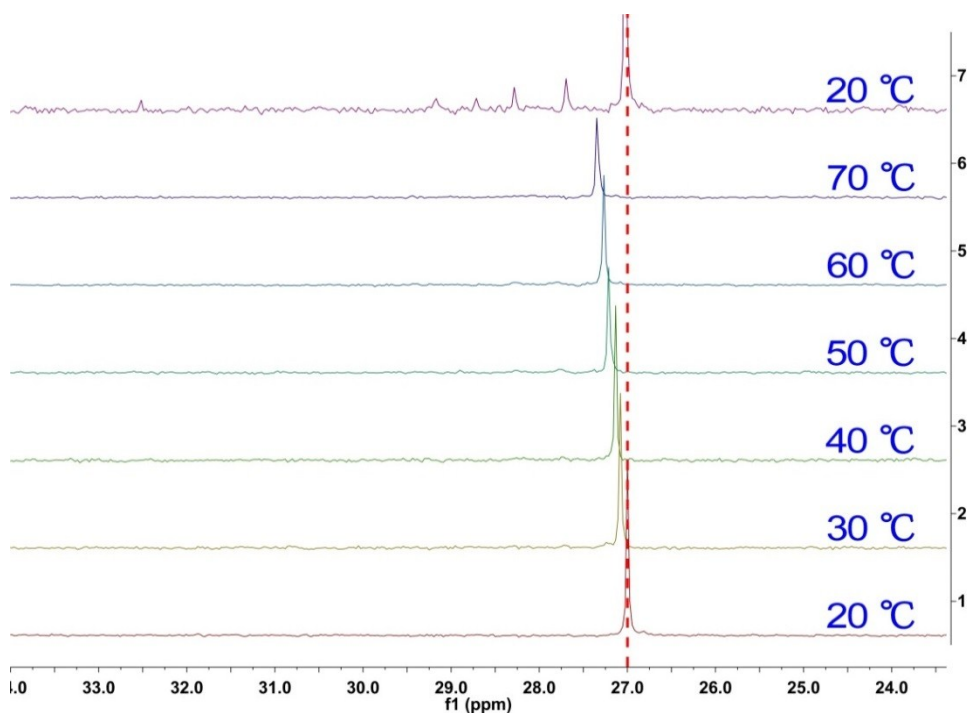
**Fig. S3** Plots of near-frontier transition-related orbitals of **1-(S<sub>a</sub>)**.



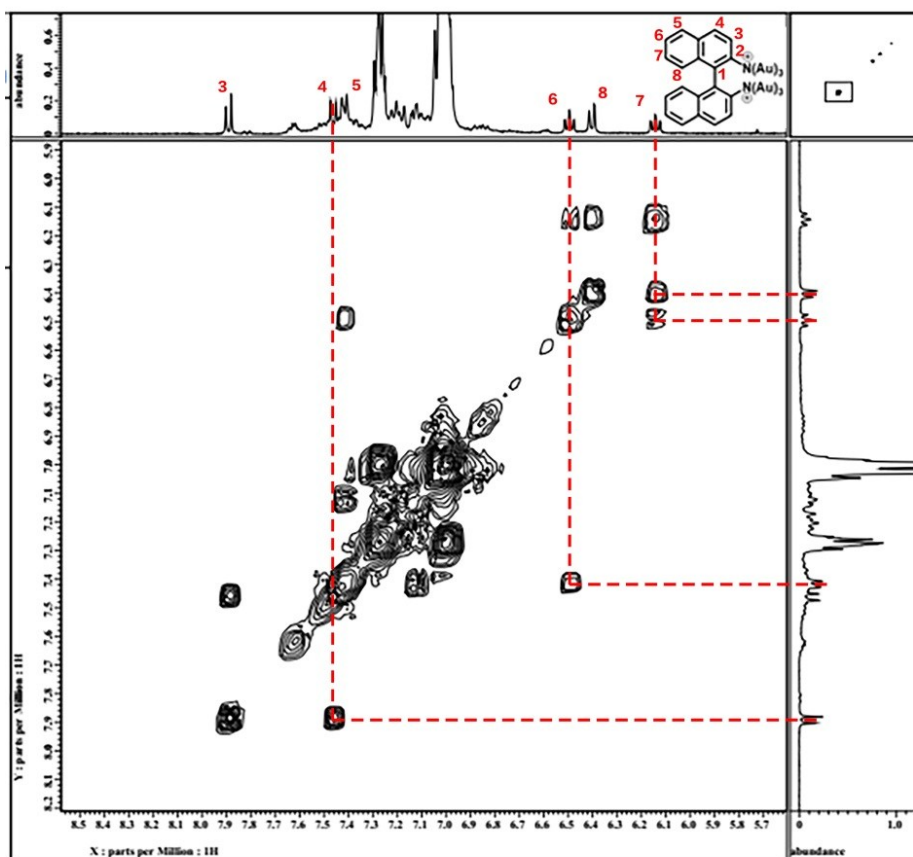
**Fig. S4** TEM image of the **1-(S<sub>a</sub>)** sample which was heated to 70 °C and then cooled back to 20 °C, indicating the formation of gold nanoparticles.



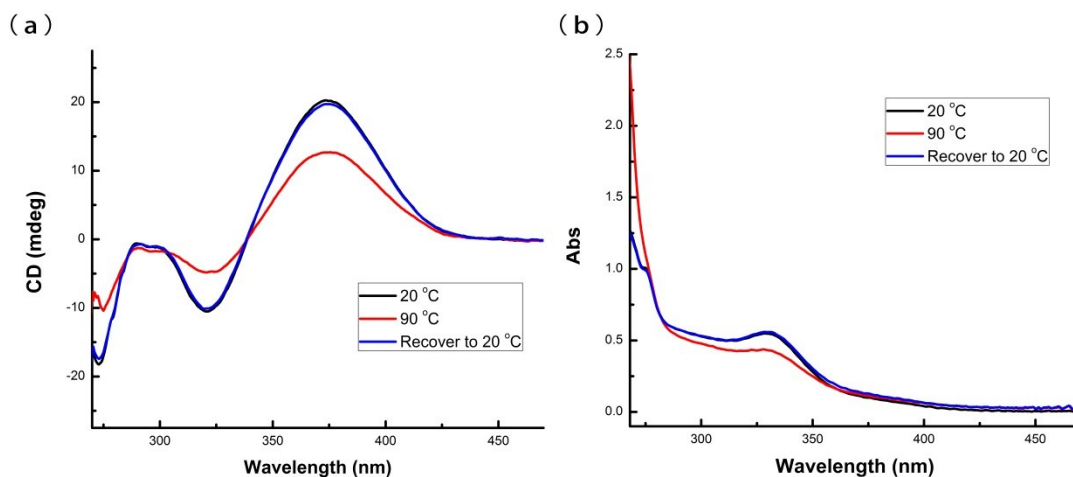
**Fig. S5** CD response of **1-(S<sub>a</sub>)** at 361 nm from different elevated temperatures recovered to 20 °C.



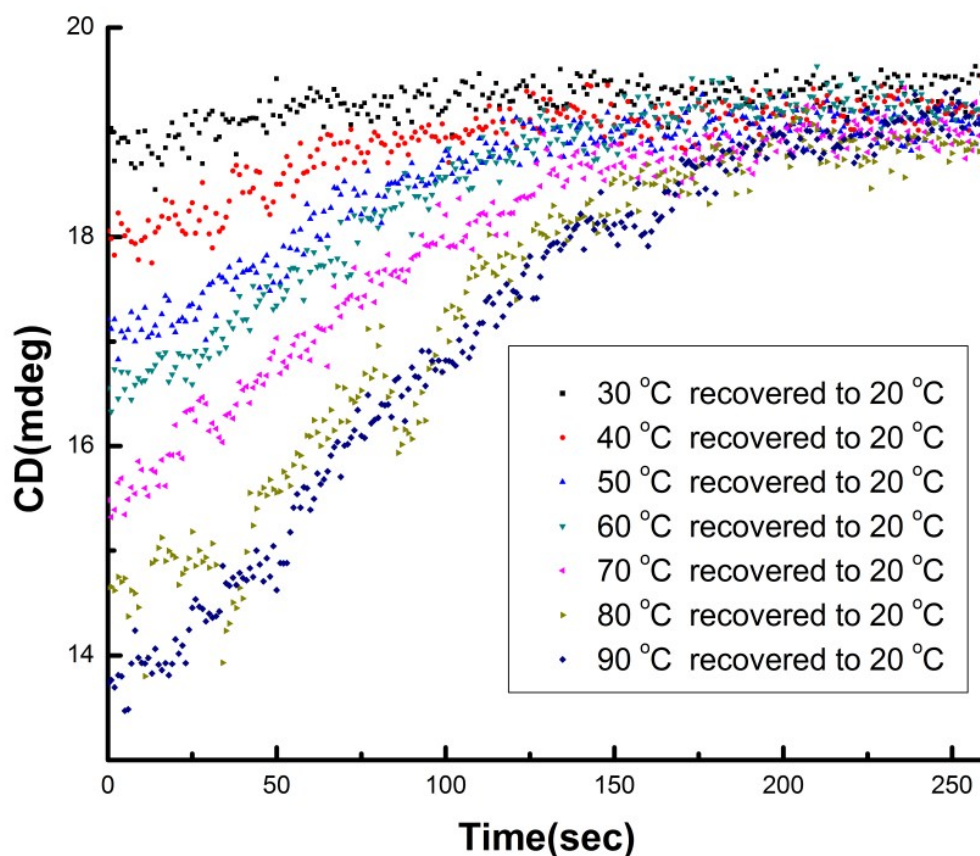
**Fig. S6** Variable temperature  $^{31}\text{P}$  NMR spectra (DMSO- $\text{d}_6$ ) of **1-(S<sub>a</sub>)** from 20 to 70 °C and back to 20 °C.



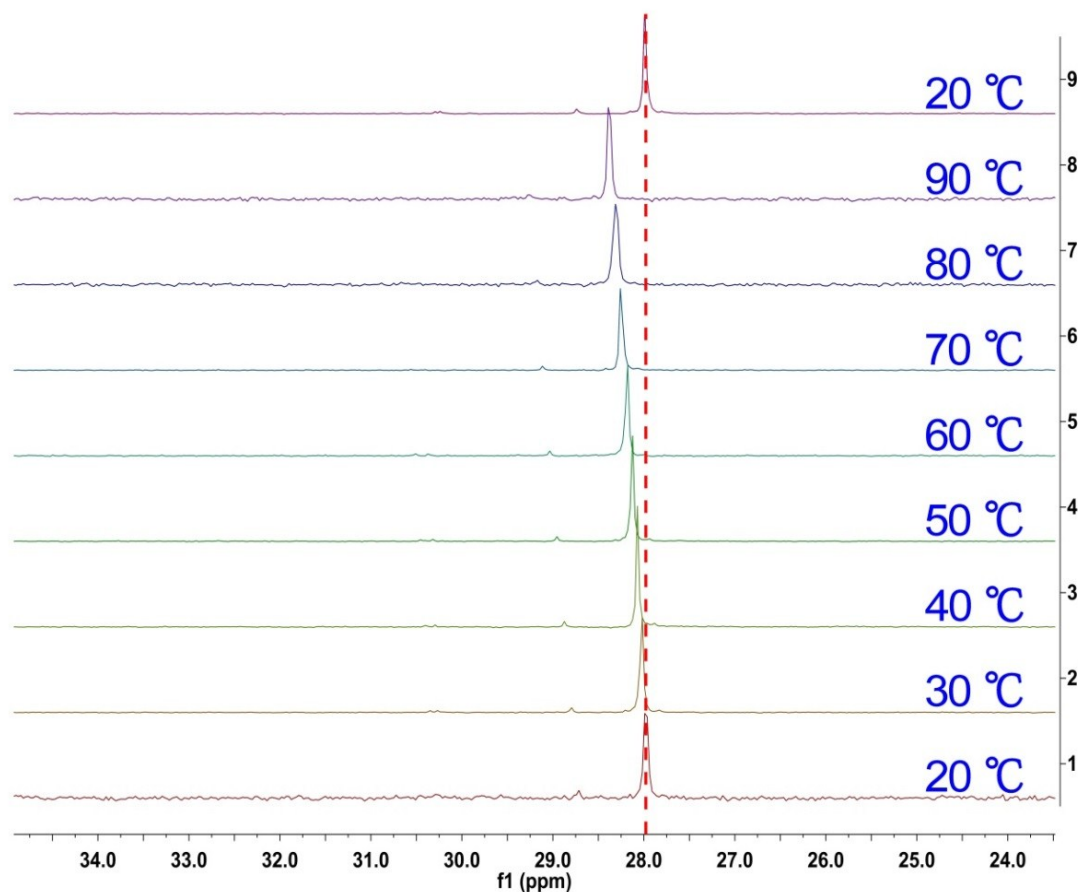
**Fig. S7** 2D  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1-(S<sub>a</sub>)** in DMSO- $\text{d}_6$  at 298K.



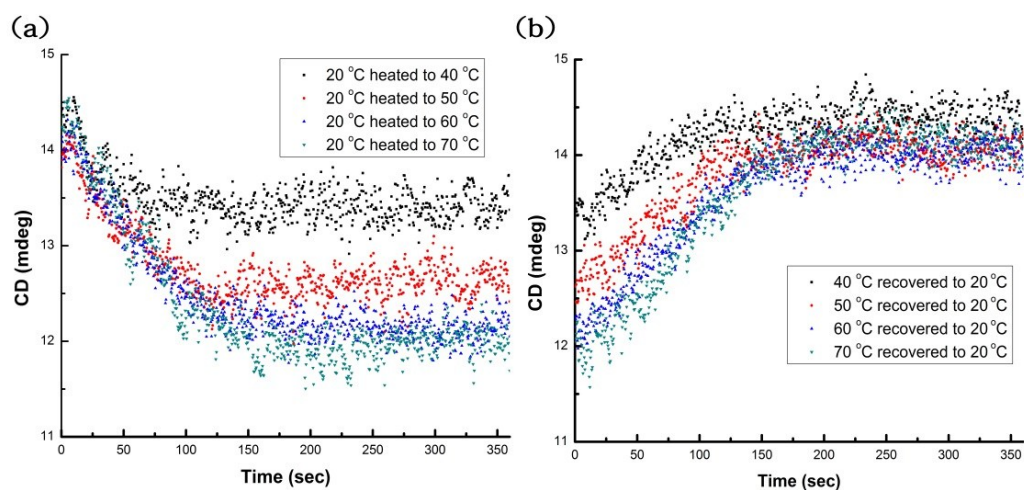
**Fig. S8** (a) CD and (b) UV-vis spectra of the DMSO solution ( $c = 2.5 \times 10^{-5}$  M) of **2-(R,R)** in 20 °C, heated to 90 °C, and cooled back to 20 °C.



**Fig. S9** CD response of **2-(R,R)** at 372 nm from different elevated temperatures recovered to 20 °C.

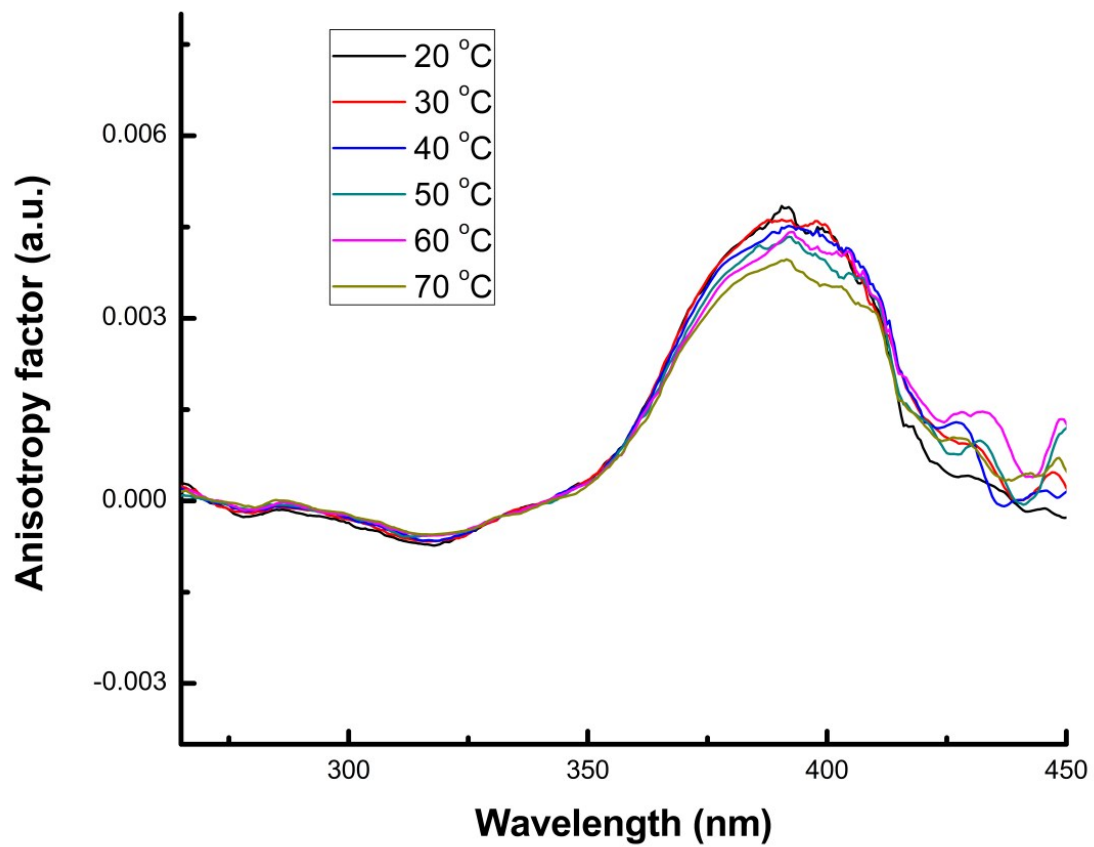


**Fig. S10** Variable temperature  $^{31}\text{P}$  NMR spectra (DMSO- $d_6$ ) of **2-(*R,R*)** from 20 to 90 °C and back to 20 °C.

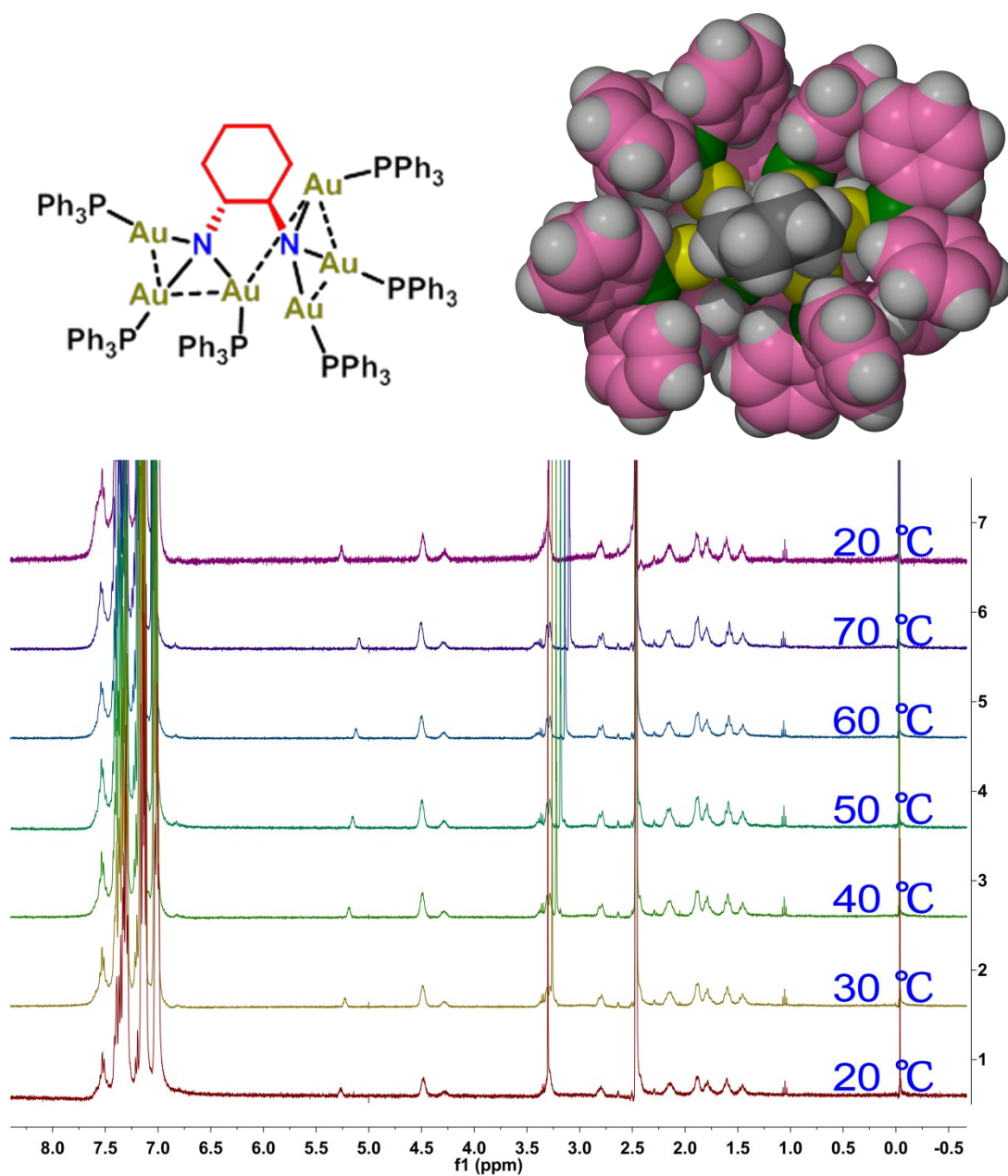


**Fig. S11** (a) CD response of **3-(*R,R*)** at 373 nm reaches a steady state at different temperatures. (b) CD response of **3-(*R,R*)** at 373 nm from different elevated temperatures recovered to 20 °C.

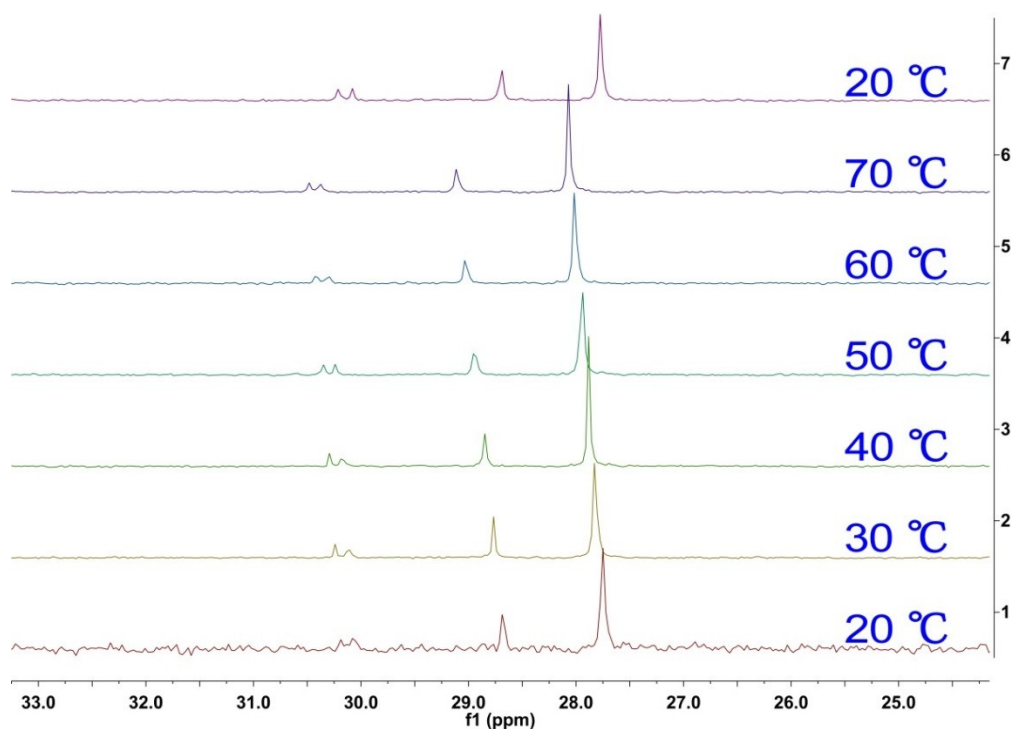




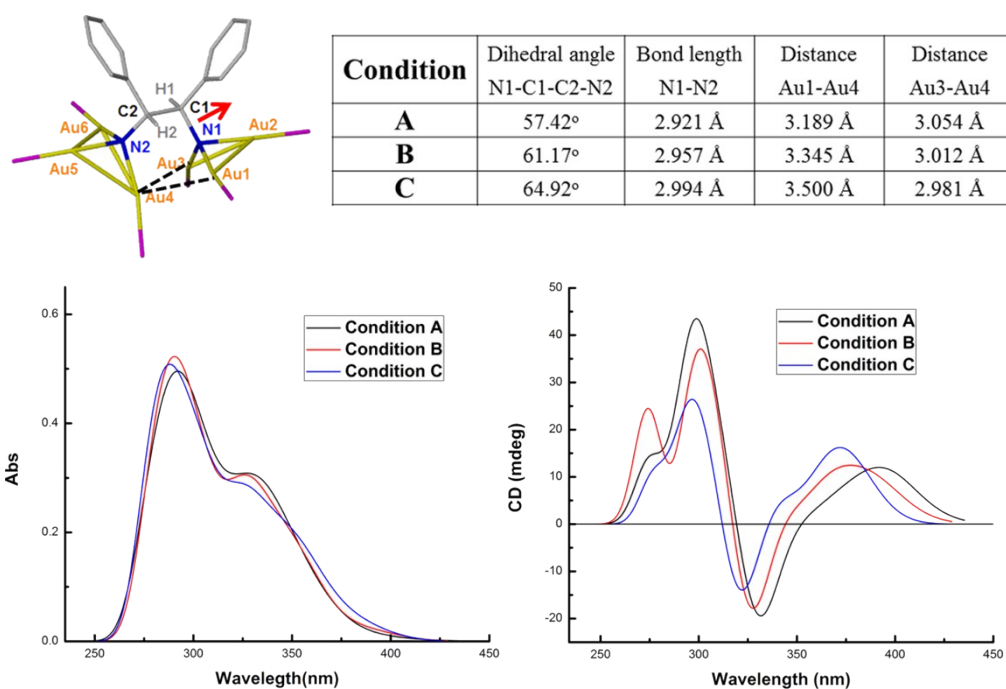
**Fig. S12** Unsynchronized variation of the anisotropy factors for different CD signals of **3-(R, R)**.



**Fig. S13** Variable temperature <sup>1</sup>H NMR spectra (DMSO-d<sub>6</sub>) of **3-(R,R)** from 20 to 70 °C and back to 20 °C. The environment of the central diamino ligand **L**<sup>3</sup> is shown in a space-filling model based on the crystal structure of **3-(R,R)**.

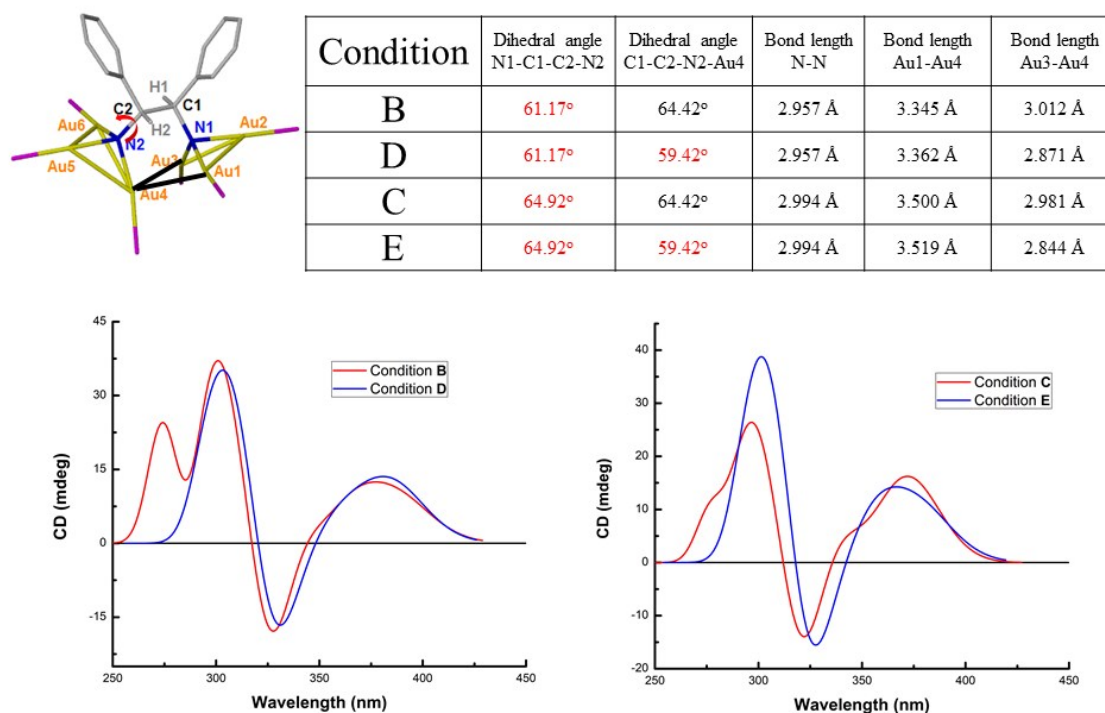


**Fig. S14** Variable temperature  $^{31}\text{P}$  NMR spectra (DMSO- $d_6$ ) of **3-(R,R)** from 20 to 70 °C and back to 20 °C.



**Fig. S15** Theoretical simulation of UV-vis and CD spectra of a model cluster complex based on the crystal structure of **2-(R,R)**. The conformational change of the model cluster is conducted by enlarging the N-C-C-N dihedral angle of

the diamino ligand  $L^2$  from  $57.4^\circ$  (in **2-(R,R)**) through  $61.2^\circ$  to  $64.9^\circ$ . In this process, the two  $[N(AuPPh_3)_3]$  moieties keep intact.



**Fig. S16** Theoretical simulation of CD spectra of a model cluster complex based on the crystal structure of **2-(R,R)**. The conformational change of the model cluster is conducted by enlarging the N1-C1-C2-N2 dihedral angle and decreasing the C1-C2-N2-Au4 angle. In this process, one of the two  $[N(AuPPh_3)_3]$  moieties is rotated around a N-C bond.

## Geometrical coordinates of the model complexes at condition A-E.

Condition A: N1-C1-C2-N2 dihedral angle is 57.42°.

C	0.63369500	-0.09653900	-2.12981300
H	0.35494300	-1.03400900	-2.09399300
C	-0.67893700	0.75997500	-2.14534600
H	-0.43015400	1.70744300	-2.13580600
C	1.43387900	0.06438300	-3.36336400
C	1.86936000	1.31140000	-3.87823100
H	1.64472000	2.08929500	-3.42093700
C	2.63671200	1.41275900	-5.06711000
H	2.96293600	2.23131500	-5.36263000
C	2.87798500	0.25885500	-5.76579600
H	3.35006300	0.31043300	-6.56701500
C	2.45077300	-0.97145900	-5.32906200
H	2.63527200	-1.73094300	-5.83302600
C	1.74617200	-1.08837600	-4.14228700
H	1.47311000	-1.92785900	-3.84975700
C	-1.52576300	0.49072800	-3.41475700
C	-2.22866400	1.53833300	-3.94852900
H	-2.14182600	2.38875200	-3.58358800
C	-3.07420200	1.33630300	-5.04019000
H	-3.56652200	2.04552100	-5.38282300
C	-3.18171600	0.09213700	-5.60804800
H	-3.73676800	-0.03243300	-6.34449600
C	-2.45720100	-0.99607400	-5.08314000
H	-2.52919600	-1.84127900	-5.46397300
C	-1.63826000	-0.78013100	-3.99119500
H	-1.15529600	-1.49048500	-3.63400000
C	0.87148800	5.47891600	-0.37173800
C	-0.39996700	5.01089600	-0.82074300
H	-0.50418600	4.10963000	-1.02012300
C	-1.47712000	5.85929100	-0.96548700
H	-2.26303600	5.55417700	-1.35756300
C	-1.37996500	7.17410800	-0.52183600
H	-2.12835300	7.72590100	-0.51157500
C	-0.08157500	7.67669700	-0.07103600
H	0.02869100	8.57180400	0.15485600
C	0.98634000	6.78336200	0.01350100
H	1.80167100	7.08671500	0.34268300
C	3.22870500	4.84033000	-1.81207200
C	4.07001400	3.87684500	-2.41900500
H	4.14295100	3.02657300	-2.05040300
C	4.77728700	4.19920200	-3.54642100
H	5.31565300	3.54446400	-3.92971800

C	4.73627000	5.40689700	-4.12993900
H	5.22836100	5.60397800	-4.89348600
C	3.88954600	6.36735800	-3.50359500
H	3.84689700	7.22577200	-3.86047100
C	3.14282300	6.08210300	-2.40742900
H	2.56960700	6.72536000	-2.05718300
C	3.25076500	4.79352200	1.08849600
C	2.64009500	5.09879200	2.31538900
H	1.71427500	5.17806200	2.35441500
C	3.39517400	5.28760400	3.48826600
H	2.99270900	5.45018000	4.31055800
C	4.83218000	5.21620500	3.34442600
H	5.37643600	5.41560900	4.07351900
C	5.38889000	4.87027500	2.18966000
H	6.31011900	4.74247100	2.17106300
C	4.67767700	4.68727300	0.99785300
H	5.10700300	4.50811900	0.19313900
C	6.64108600	-0.55699800	0.29777200
C	6.18440800	0.47175900	1.13277400
H	5.36348800	0.87331900	0.95983700
C	6.94042800	0.89874200	2.21429400
H	6.64251600	1.58588800	2.76320100
C	8.17199800	0.26274800	2.45408200
H	8.70691400	0.56564200	3.15208400
C	8.60097600	-0.77793500	1.70113400
H	9.40540500	-1.19923300	1.90508400
C	7.82831700	-1.22476200	0.60415400
H	8.10650800	-1.95165700	0.09336600
C	6.40616600	-0.49214200	-2.59208100
C	5.70933700	0.17709800	-3.53297300
H	4.82859300	0.42346800	-3.36152900
C	6.30021800	0.51326100	-4.78093400
H	5.78050200	0.87979300	-5.46023000
C	7.63895300	0.29352500	-4.97659400
H	8.07486700	0.58644600	-5.74500100
C	8.30167700	-0.37895600	-3.98761000
H	9.20192000	-0.57560200	-4.11787300
C	7.73062200	-0.77370300	-2.84075100
H	8.23120800	-1.23950500	-2.21043000
C	5.56663000	-2.85940100	-1.14783200
C	4.99303500	-3.40580600	-2.30024700
H	4.71278200	-2.84929300	-2.99099300
C	4.84369600	-4.78870100	-2.41358600
H	4.48612200	-5.15114700	-3.19043900

C	5.22866400	-5.63699800	-1.36422000
H	5.09708800	-6.55579700	-1.42498700
C	5.78641400	-5.09695000	-0.27283900
H	6.11188000	-5.66324500	0.38860600
C	5.90299200	-3.68985700	-0.08592600
H	6.19481600	-3.33805300	0.72441900
C	3.19666400	-3.22120400	2.57061500
C	4.01259400	-2.10245500	2.78734900
H	3.69671300	-1.26304200	2.53876800
C	5.25799500	-2.19567600	3.35078600
H	5.76000700	-1.43072700	3.51333300
C	5.75994800	-3.45476500	3.67597100
H	6.61984100	-3.53909900	4.01873500
C	4.96448900	-4.58939000	3.48407800
H	5.26747300	-5.42262900	3.76548600
C	3.72088400	-4.47247300	2.87196400
H	3.23599500	-5.23864200	2.66196900
C	0.51150100	-3.11609100	3.50772400
C	-0.83915900	-2.72991500	3.46461900
H	-1.18825300	-2.39335300	2.67189300
C	-1.66333000	-2.84065700	4.57570400
H	-2.56224600	-2.60730500	4.52722700
C	-1.10918200	-3.31404600	5.77750100
H	-1.63942200	-3.38224700	6.53927000
C	0.21653200	-3.67577600	5.82638100
H	0.57487000	-3.98958800	6.62579000
C	1.02488000	-3.58336500	4.71609600
H	1.91914700	-3.83260800	4.77280000
C	1.13643100	-4.61616800	1.13613400
C	0.05005300	-5.39746500	1.48611100
H	-0.53060500	-5.12499300	2.15993400
C	-0.16125300	-6.61266300	0.80695600
H	-0.89631200	-7.14338800	1.01344200
C	0.73409000	-7.01369700	-0.17156700
H	0.59041300	-7.81206600	-0.62850800
C	1.77931700	-6.28136600	-0.46152200
H	2.38684000	-6.58283100	-1.09862700
C	2.00301200	-5.03731000	0.17557200
H	2.73431300	-4.51284400	-0.05806600
C	-1.85056100	0.75505400	4.17558100
C	-1.72820100	0.74415600	5.54817200
H	-0.95557500	1.07728500	5.94406800
C	-2.73686300	0.24411400	6.33912900
H	-2.64544900	0.24038000	7.26477100

C	-3.91538600	-0.26386500	5.74127700
H	-4.59219100	-0.63517700	6.26060500
C	-4.03774500	-0.19245000	4.32598400
H	-4.83153100	-0.45810000	3.91978700
C	-2.99493600	0.26669000	3.54677300
H	-3.05539800	0.25071100	2.61884000
C	-0.61853600	3.25579500	3.41444200
C	-0.14118800	3.78604900	4.62765100
H	0.25042200	3.23781600	5.26841100
C	-0.27408500	5.16911200	4.84332000
H	0.04433900	5.53626400	5.63718200
C	-0.85373700	5.98525000	3.92490400
H	-0.95019100	6.89103000	4.10641400
C	-1.31117300	5.46176900	2.68955500
H	-1.68089500	6.02126200	2.04600800
C	-1.19494300	4.07418700	2.45747800
H	-1.50532900	3.70844200	1.66037300
C	1.06336100	0.99645500	3.85145400
C	1.25774600	0.00525800	4.80516700
H	0.53469500	-0.51265400	5.07950700
C	2.48643900	-0.22282100	5.35074600
H	2.58397400	-0.85679800	6.02430500
C	3.62314700	0.50141100	4.89297700
H	4.47303300	0.32448600	5.22942200
C	3.43130800	1.45025800	3.96238200
H	4.15793800	1.96038700	3.68397300
C	2.17827200	1.69914600	3.39489100
H	2.08735200	2.33022600	2.71774000
C	-6.59536400	1.24618900	-1.92938200
C	-7.90287700	0.73577200	-1.79145800
H	-8.26326600	0.60108100	-0.94537500
C	-8.65071200	0.43333100	-2.92546000
H	-9.49237200	0.04688300	-2.84129000
C	-8.11784500	0.72236100	-4.22139000
H	-8.60761800	0.54144200	-4.98982500
C	-6.86836900	1.27062100	-4.29677300
H	-6.51186000	1.47610800	-5.13204900
C	-6.11880200	1.52920200	-3.15591200
H	-5.27201300	1.90341100	-3.24149500
C	-6.00543100	3.35679300	-0.00770000
C	-7.30034700	3.83485900	-0.06750600
H	-8.00023700	3.25290600	-0.26039200
C	-7.56193600	5.16468100	0.15549100
H	-8.43675500	5.47210200	0.08455000



C	-6.56625400	6.05176200	0.47814600
H	-6.75639200	6.94180000	0.66942100
C	-5.23200200	5.55884700	0.50894600
H	-4.53211200	6.14080000	0.70183200
C	-4.95967500	4.22651400	0.25606900
H	-4.08297800	3.91765600	0.26350500
C	-6.30518600	0.58914900	0.84156700
C	-6.31096100	-0.78122900	0.65096400
H	-5.90300900	-1.13305300	-0.10690600
C	-6.89876100	-1.62749400	1.54034800
H	-6.89563100	-2.54312000	1.37752400
C	-7.50204400	-1.13624000	2.68818500
H	-7.91839300	-1.71236700	3.28749500
C	-7.47281500	0.22254100	2.92871600
H	-7.85467900	0.56422600	3.70357200
C	-6.87152700	1.08517800	2.01173100
H	-6.85008800	1.99864000	2.18246700
C	-4.52335600	-3.37228600	-1.77280800
C	-4.75482100	-2.32030900	-2.66325000
H	-4.08568100	-1.68609500	-2.78840300
C	-5.92223600	-2.18569800	-3.35902000
H	-6.00848800	-1.52786600	-4.01054000
C	-6.99659400	-3.05201100	-3.07525600
H	-7.82660200	-2.92128900	-3.47505500
C	-6.80335700	-4.07571500	-2.21843800
H	-7.49663000	-4.68197600	-2.08155700
C	-5.61174900	-4.26050200	-1.53103100
H	-5.52345900	-4.95626600	-0.92062000
C	-3.46528700	-4.33949400	0.65792700
C	-3.95037100	-3.52733900	1.66558700
H	-3.90213900	-2.60231500	1.58542900
C	-4.50080100	-4.09420700	2.78209100
H	-4.82617700	-3.54955500	3.46185000
C	-4.57731200	-5.49007800	2.91294900
H	-4.97943200	-5.87482400	3.65863600
C	-4.05533800	-6.26880900	1.93602700
H	-4.07983800	-7.19460000	2.02603300
C	-3.46912400	-5.69307300	0.76903200
H	-3.10109400	-6.22907300	0.10363300
C	-1.91648900	-4.59745400	-1.86802100
C	-2.37002600	-5.79730900	-2.43876200
H	-3.25210900	-6.06085800	-2.30567200
C	-1.53324200	-6.58948100	-3.19271200
H	-1.83744600	-7.40638300	-3.51874400

C	-0.22113300	-6.16604400	-3.47040400
H	0.33351700	-6.67673600	-4.01259500
C	0.23704200	-4.97357100	-2.92260900
H	1.10627100	-4.68683100	-3.08723500
C	-0.61703500	-4.20863300	-2.12298700
H	-0.30023200	-3.41824400	-1.75236800
N	1.40189700	0.16597200	-0.89377500
N	-1.50019800	0.48839600	-0.97770600
P	2.25831800	4.35649900	-0.35517300
P	5.56391700	-1.05198200	-1.06826500
P	1.49680400	-3.03798300	1.98071300
P	-0.53309100	1.45801400	3.11883400
P	-5.60103000	1.63117500	-0.45119300
P	-2.97216400	-3.52212800	-0.87904500
Au	1.75128100	2.16703500	-0.48437500
Au	3.44275400	-0.33581300	-0.98568000
Au	1.23704300	-1.27377000	0.61488100
Au	-0.82589500	0.95390500	0.94856900
Au	-3.43331400	1.16780400	-0.77350000
Au	-2.09365300	-1.46332300	-0.73398200

**Condition B:** N1-C1-C2-N2 dihedral angle is 61.17°.

C	0.62993100	-0.04457600	-2.07772800
H	0.33723300	-0.97752300	-2.03560300
C	-0.66905900	0.83255100	-2.06615700
H	-0.40601500	1.77397900	-2.00135300
C	1.40650300	0.10348600	-3.32786800
C	1.85071100	1.34338700	-3.85237700
H	1.64801600	2.12480800	-3.39086000
C	2.59446000	1.43242000	-5.05713700
H	2.92729000	2.24567400	-5.35984100
C	2.80278600	0.27473400	-5.76015300
H	3.25870800	0.31871800	-6.57112200
C	2.36546800	-0.94860900	-5.31394300
H	2.52734800	-1.71099600	-5.82128600
C	1.68415900	-1.05419000	-4.11259400
H	1.40408000	-1.88920800	-3.81398400
C	-1.49980900	0.64616800	-3.36081100
C	-2.17813800	1.73234600	-3.84717300
H	-2.08407700	2.56022800	-3.43522800
C	-3.00937200	1.60341900	-4.96068200
H	-3.48534700	2.33800000	-5.27149300
C	-3.12692200	0.39374900	-5.59696200

H	-3.67214900	0.31822900	-6.34728200
C	-2.42746600	-0.73283700	-5.12133900
H	-2.50635700	-1.55489200	-5.54864500
C	-1.62261400	-0.58960700	-4.00718500
H	-1.15623900	-1.32596100	-3.68203600
C	0.99249900	5.52672400	-0.32780700
C	-0.29532100	5.07876000	-0.74981600
H	-0.41790900	4.17921800	-0.94651700
C	-1.36175200	5.94403000	-0.87236200
H	-2.16043600	5.65129500	-1.24771900
C	-1.23457700	7.25722300	-0.43150200
H	-1.97378400	7.82076400	-0.40582400
C	0.08075300	7.73932800	-0.00828100
H	0.20984400	8.63262000	0.21480300
C	1.13597700	6.82925900	0.05428800
H	1.96271800	7.11975800	0.36614800
C	3.30861400	4.85076400	-1.81693900
C	4.12169900	3.87401500	-2.44090100
H	4.18892500	3.02276000	-2.07348600
C	4.81016600	4.18497800	-3.58306200
H	5.32997400	3.52175800	-3.97723800
C	4.77598000	5.39307200	-4.16619400
H	5.25499500	5.58223200	-4.93999100
C	3.95784200	6.36688500	-3.52271000
H	3.92126700	7.22580600	-3.87904100
C	3.22986900	6.09363800	-2.41098300
H	2.67434700	6.74592300	-2.04911400
C	3.39077100	4.80409900	1.08255100
C	2.81086500	5.11917800	2.32182900
H	1.88743300	5.21306000	2.38022200
C	3.59326600	5.29624200	3.47851900
H	3.21075300	5.46529000	4.30898900
C	5.02563200	5.20214200	3.30461000
H	5.58814100	5.39305200	4.02203000
C	5.55246900	4.84727300	2.13859600
H	6.47097400	4.70493900	2.10074800
C	4.81361400	4.67532200	0.96205700
H	5.22308500	4.48927800	0.14860600
C	6.67890700	-0.59940900	0.22357100
C	6.25613600	0.43657000	1.06745300
H	5.43820800	0.85101000	0.91157000
C	7.04131900	0.85174600	2.13266800
H	6.76586700	1.54360100	2.68735900
C	8.26745900	0.19642800	2.34689300

H	8.82161200	0.49095700	3.03337300
C	8.66407300	-0.85102300	1.58563400
H	9.46585500	-1.28493400	1.77287900
C	7.86161900	-1.28578100	0.50532100
H	8.11752900	-2.01706200	-0.01082600
C	6.38447300	-0.53133600	-2.66075200
C	5.67870800	0.14866300	-3.58715700
H	4.80575200	0.40893500	-3.39740400
C	6.24851300	0.47524700	-4.84740300
H	5.72051100	0.84982400	-5.51583300
C	7.57921500	0.23437100	-5.07098500
H	8.00348300	0.52024500	-5.84851000
C	8.25184400	-0.44832300	-4.09578100
H	9.14594200	-0.65917800	-4.24479600
C	7.69881400	-0.83381300	-2.93700200
H	8.20509900	-1.30735400	-2.31708500
C	5.53816700	-2.88480500	-1.19803400
C	4.93197400	-3.42228000	-2.33789400
H	4.64611000	-2.86152700	-3.02288800
C	4.75848700	-4.80266400	-2.44738700
H	4.37902100	-5.15955000	-3.21638900
C	5.15194800	-5.65675600	-1.40590200
H	5.00464400	-6.57337400	-1.46343800
C	5.74092100	-5.12539800	-0.32672700
H	6.07121300	-5.69664900	0.32803000
C	5.88358300	-3.72028900	-0.14300100
H	6.19785600	-3.37300000	0.66087000
C	3.24130700	-3.20852500	2.56947600
C	4.07915600	-2.10276000	2.76849300
H	3.77141600	-1.25850700	2.52617300
C	5.33447600	-2.21553600	3.30573600
H	5.85179500	-1.45858000	3.45733800
C	5.82320900	-3.48233800	3.62095000
H	6.68866500	-3.58017900	3.94564800
C	5.00609500	-4.60429600	3.44634700
H	5.30172900	-5.44216700	3.72175500
C	3.75192300	-4.46786300	2.86038900
H	3.25070600	-5.22631700	2.66099100
C	0.57838500	-3.06087800	3.56263700
C	-0.76662000	-2.65343500	3.54767400
H	-1.12691100	-2.31153600	2.76227500
C	-1.56894800	-2.75096600	4.67585300
H	-2.46488900	-2.50346000	4.64612200
C	-0.99725100	-3.23284200	5.86600100

H	-1.51240600	-3.29253600	6.63875600
C	0.32332300	-3.61544800	5.88724900
H	0.69335400	-3.93474400	6.67912400
C	1.10956100	-3.53599600	4.76021000
H	2.00077700	-3.79931600	4.79827200
C	1.12968200	-4.57103100	1.17921200
C	0.03869100	-5.33502200	1.55228400
H	-0.52333300	-5.05330400	2.23800000
C	-0.20596400	-6.54684600	0.87831500
H	-0.94481300	-7.06586600	1.10043600
C	0.66221600	-6.96212900	-0.11856900
H	0.49640600	-7.75820700	-0.57199800
C	1.71255700	-6.24643900	-0.43074400
H	2.30174900	-6.55756400	-1.08029900
C	1.96917000	-5.00596200	0.20089800
H	2.70359400	-4.49314600	-0.04828600
C	-1.93998800	0.50394900	4.22698200
C	-1.83943300	0.41671100	5.59861400
H	-1.06813700	0.71540800	6.02351800
C	-2.86794200	-0.10915100	6.34607200
H	-2.79117900	-0.16451600	7.27139700
C	-4.04452700	-0.56493600	5.70397200
H	-4.73501700	-0.95289800	6.19218300
C	-4.14348500	-0.41496400	4.29300100
H	-4.93474300	-0.64539100	3.86117100
C	-3.08164700	0.06887500	3.55555200
H	-3.12773000	0.10418400	2.62732800
C	-0.65808200	3.02209700	3.62152900
C	-0.19185000	3.47806500	4.86877600
H	0.18120500	2.88967700	5.48450400
C	-0.30698700	4.84936900	5.15741000
H	0.00447100	5.16778200	5.97473400
C	-0.85957500	5.72331000	4.27625300
H	-0.94502900	6.61935800	4.50534300
C	-1.30544800	5.27498300	3.00756500
H	-1.65640400	5.87441200	2.38999500
C	-1.20678500	3.90032500	2.70205600
H	-1.51013400	3.58336300	1.88169100
C	0.98202300	0.71559900	3.95990100
C	1.14620800	-0.32883000	4.86103300
H	0.41110100	-0.84913600	5.09597700
C	2.36253200	-0.60590000	5.41162300
H	2.43975700	-1.27693700	6.05105000
C	3.51723500	0.12367400	5.01093300

H	4.35891800	-0.08489000	5.34986600
C	3.35458500	1.12452600	4.13061500
H	4.09321400	1.63722400	3.89123800
C	2.11458600	1.42395200	3.55891800
H	2.04398700	2.09218500	2.91584500
C	-6.58003700	1.40157200	-1.91216800
C	-7.89720200	0.90555600	-1.82171700
H	-8.27288200	0.73103200	-0.98968100
C	-8.63162400	0.67709900	-2.98151100
H	-9.48030900	0.30026400	-2.93104400
C	-8.07406900	1.02731700	-4.25170800
H	-8.55438900	0.89622000	-5.03605900
C	-6.81533300	1.55866100	-4.27852100
H	-6.44262100	1.80334500	-5.09597200
C	-6.07995700	1.74292800	-3.11424100
H	-5.22630900	2.10753800	-3.16670900
C	-5.98826300	3.39515500	0.13012600
C	-7.27462500	3.89655300	0.07715700
H	-7.98019800	3.33725600	-0.15752100
C	-7.51935100	5.21637600	0.36829300
H	-8.38814700	5.54123900	0.30117300
C	-6.51543900	6.06851600	0.75354700
H	-6.69494900	6.94982600	0.99013500
C	-5.18952100	5.55323000	0.77733400
H	-4.48394800	6.11252700	1.01201300
C	-4.93362800	4.23234700	0.45639000
H	-4.06197600	3.90946000	0.46005500
C	-6.34358700	0.59074000	0.82292000
C	-6.36729000	-0.76702400	0.55793900
H	-5.95287900	-1.08378300	-0.21180100
C	-6.98187600	-1.65066800	1.39108600
H	-6.99016800	-2.55605500	1.17872700
C	-7.59558100	-1.21268900	2.55485200
H	-8.03006400	-1.81366800	3.11564600
C	-7.54939300	0.13041200	2.86940000
H	-7.93814500	0.43570800	3.65593500
C	-6.92063800	1.03168100	2.00978800
H	-6.88794100	1.93408300	2.23029500
C	-4.58153100	-3.25137300	-1.97639700
C	-4.78285500	-2.14909300	-2.81160200
H	-4.10221900	-1.51988800	-2.89206800
C	-5.93698000	-1.95818900	-3.51631900
H	-6.00290700	-1.26471100	-4.13227600
C	-7.02877800	-2.82119100	-3.29616200

H	-7.85029600	-2.65564300	-3.70056700
C	-6.86471200	-3.89280400	-2.49355700
H	-7.56923300	-4.49434800	-2.40021900
C	-5.68703500	-4.13374100	-1.79956100
H	-5.61900200	-4.86289500	-1.22668200
C	-3.57675700	-4.36580700	0.41357000
C	-4.06518400	-3.60174700	1.45661000
H	-4.00157300	-2.67463600	1.42765200
C	-4.64171600	-4.21935200	2.53228200
H	-4.96939700	-3.70717000	3.23576000
C	-4.74158900	-5.61885000	2.58580800
H	-5.16122800	-6.03691600	3.30337500
C	-4.21625400	-6.35179800	1.57582500
H	-4.25630500	-7.28059200	1.61492700
C	-3.60301600	-5.72318000	0.45075900
H	-3.23278500	-6.22818900	-0.23727700
C	-1.99250500	-4.51140700	-2.09933300
C	-2.45527300	-5.67110700	-2.74123100
H	-3.34326500	-5.92724100	-2.63583400
C	-1.61892000	-6.43462900	-3.52464200
H	-1.93039500	-7.22765600	-3.89915200
C	-0.29628800	-6.01795300	-3.75930400
H	0.25896500	-6.50737800	-4.32017100
C	0.17136600	-4.86445400	-3.14064700
H	1.04735700	-4.58325100	-3.27645900
C	-0.68341100	-4.13031900	-2.31337800
H	-0.36044700	-3.36638200	-1.89560700
N	1.42793800	0.20598200	-0.85820300
N	-1.51265300	0.51135400	-0.92739000
P	2.36148700	4.38255700	-0.33976900
P	5.56564400	-1.07755500	-1.11932900
P	1.53255000	-2.99859000	2.01526000
P	-0.59546200	1.24183500	3.22980200
P	-5.60333300	1.68981800	-0.40057200
P	-3.04707200	-3.47439500	-1.06911700
Au	1.81736600	2.20134800	-0.45721800
Au	3.45824600	-0.32797500	-0.99263600
Au	1.27206800	-1.23072500	0.65429600
Au	-0.86172800	0.86086500	1.03119500
Au	-3.43814200	1.20974300	-0.71531100
Au	-2.13961100	-1.44089400	-0.79913300

**Condition C:** N1-C1-C2-N2 dihedral angle is 64.92°.

C	0.62688800	0.01671800	-2.02227900
H	0.32273700	-0.91251000	-1.97910500
C	-0.65973700	0.91085700	-1.97787800
H	-0.38462200	1.84274700	-1.85309000
C	1.37841800	0.16186500	-3.28797000
C	1.82779800	1.39885300	-3.81494300
H	1.64547600	2.18015300	-3.34480300
C	2.54669800	1.48514400	-5.03489100
H	2.88379100	2.29569600	-5.34011300
C	2.72445700	0.32896600	-5.74870100
H	3.16345500	0.37169700	-6.56902100
C	2.28051000	-0.89109700	-5.30006200
H	2.42130200	-1.65255400	-5.81503300
C	1.62373600	-0.99473700	-4.08496000
H	1.33899900	-1.82772500	-3.78508500
C	-1.47238300	0.81414500	-3.29365400
C	-2.12767100	1.93729200	-3.72446600
H	-2.02859100	2.73773400	-3.26250200
C	-2.94286900	1.88716900	-4.85601900
H	-3.40354500	2.64593200	-5.12955400
C	-3.06721300	0.71933900	-5.56502200
H	-3.60147800	0.69667700	-6.32660000
C	-2.39119600	-0.44381600	-5.14702200
H	-2.47478400	-1.23775500	-5.62374400
C	-1.60218500	-0.37906200	-4.01436700
H	-1.15135900	-1.14030400	-3.72677000
C	1.10115200	5.57233300	-0.24934500
C	-0.20127300	5.14392600	-0.64608600
H	-0.34003600	4.24725800	-0.84514700
C	-1.25844300	6.02392400	-0.74083200
H	-2.06881700	5.74399100	-1.10057300
C	-1.10434600	7.33270200	-0.29545100
H	-1.83524900	7.90580500	-0.25073400
C	0.22606000	7.79487400	0.10210200
H	0.37180700	8.68505300	0.32736500
C	1.27014500	6.87058300	0.13687600
H	2.10717800	7.14828500	0.43252100
C	3.37562200	4.87459800	-1.79167400
C	4.16205400	3.89087900	-2.43843100
H	4.22576800	3.03665900	-2.07732500
C	4.82999200	4.19943700	-3.59336200
H	5.33234500	3.53173700	-4.00233000
C	4.79945000	5.41129200	-4.16884300
H	5.26426600	5.59865900	-4.95168200



C	4.00834500	6.39202800	-3.50247500
H	3.97561200	7.25344200	-3.85311700
C	3.30076400	6.12188300	-2.37691000
H	2.76187200	6.77931200	-1.99953500
C	3.51922000	4.80976900	1.10507400
C	2.97024000	5.12518000	2.35827500
H	2.04960400	5.23091500	2.43702500
C	3.77952300	5.28506800	3.49885800
H	3.41717100	5.45426100	4.33829200
C	5.20645400	5.17306800	3.29368400
H	5.78669400	5.35229300	3.99990800
C	5.70341900	4.81814000	2.11464500
H	6.61892200	4.66390200	2.05626900
C	4.93731100	4.66290700	0.95331100
H	5.32674900	4.47626100	0.13021800
C	6.71581600	-0.63157900	0.14534700
C	6.32507200	0.40490700	1.00391500
H	5.50959700	0.83103600	0.86797100
C	7.13835600	0.80338400	2.05432100
H	6.88410100	1.49554100	2.61867400
C	8.35994900	0.13066400	2.23846900
H	8.93255500	0.41379200	2.91452200
C	8.72615900	-0.91743600	1.46300100
H	9.52590600	-1.36300300	1.63053700
C	7.89502600	-1.33517400	0.39776300
H	8.13004500	-2.06672200	-0.12785700
C	6.36061900	-0.54262900	-2.73155600
C	5.64431500	0.15208800	-3.63875300
H	4.77917100	0.42275500	-3.42882700
C	6.19130800	0.47853000	-4.90910100
H	5.65415800	0.86398500	-5.56392000
C	7.51358400	0.22140500	-5.16257500
H	7.92488200	0.50622200	-5.94742400
C	8.19777400	-0.47585500	-4.20589500
H	9.08558200	-0.69763000	-4.37527000
C	7.66459000	-0.86082100	-3.03767900
H	8.17767000	-1.34465700	-2.43145000
C	5.51450200	-2.89328000	-1.26420600
C	4.87692200	-3.41597000	-2.39377100
H	4.58396300	-2.84746100	-3.06931000
C	4.68272700	-4.79327100	-2.50724700
H	4.28215400	-5.14057200	-3.26990700
C	5.08697000	-5.65861100	-1.47926400
H	4.92625000	-6.57284600	-1.53876000

C	5.70595400	-5.14145300	-0.41003400
H	6.04254000	-5.72086800	0.23426100
C	5.87125300	-3.73946000	-0.22154100
H	6.20727400	-3.40109800	0.57732500
C	3.29473200	-3.20880000	2.54992000
C	4.15133000	-2.11540000	2.73708200
H	3.84976400	-1.26573900	2.50616800
C	5.41625000	-2.24792400	3.24658300
H	5.94675100	-1.49877900	3.39127400
C	5.89467500	-3.52291100	3.54411400
H	6.76550300	-3.63409600	3.84958400
C	5.05911100	-4.63292000	3.38082300
H	5.34936900	-5.47623500	3.64511200
C	3.79461100	-4.47647100	2.82272700
H	3.27916400	-5.22704500	2.62989700
C	0.65589500	-3.03181800	3.60089100
C	-0.68356500	-2.60654800	3.61712000
H	-1.05599900	-2.25529500	2.84157500
C	-1.46278100	-2.70010900	4.76171600
H	-2.35577100	-2.44061000	4.75263500
C	-0.87221000	-3.19650500	5.93658300
H	-1.37145000	-3.25393500	6.71988400
C	0.44329400	-3.59665300	5.92730100
H	0.82590400	-3.92547300	6.70923800
C	1.20620700	-3.52096300	4.78409000
H	2.09444000	-3.79626200	4.80151300
C	1.13582800	-4.53505800	1.19773800
C	0.04297900	-5.28674400	1.58988100
H	-0.50042300	-5.00166600	2.28908600
C	-0.23220000	-6.49123600	0.91454200
H	-0.97298300	-7.00174400	1.14957600
C	0.60881600	-6.91207900	-0.10308200
H	0.42272700	-7.70321000	-0.55729900
C	1.66168700	-6.20850900	-0.43374100
H	2.23263100	-6.52356500	-1.09754100
C	1.94829600	-4.97527700	0.19918700
H	2.68399300	-4.47075500	-0.06284400
C	-2.03473500	0.22777500	4.26468700
C	-1.95716500	0.05768200	5.63002600
H	-1.18860300	0.31907500	6.08350700
C	-3.00464200	-0.49629800	6.32927700
H	-2.94333900	-0.60769900	7.25069700
C	-4.17715600	-0.89553900	5.64356300
H	-4.88065200	-1.30150500	6.09735300

C	-4.25162800	-0.66051500	4.24272700
H	-5.03908400	-0.85305800	3.78610500
C	-3.17157600	-0.14957100	3.55145800
H	-3.20244000	-0.05847400	2.62640700
C	-0.70832600	2.75808300	3.82982400
C	-0.25559800	3.13212100	5.10890100
H	0.09939100	2.50268600	5.69395400
C	-0.35611900	4.48540800	5.47707000
H	-0.05323800	4.75000700	6.31651100
C	-0.88240300	5.41830900	4.64143400
H	-0.95894700	6.30033000	4.92226400
C	-1.31433000	5.05286800	3.34171900
H	-1.64704000	5.69310300	2.75581600
C	-1.23005700	3.69748200	2.95626000
H	-1.52476400	3.43439100	2.11399000
C	0.89381400	0.41137800	4.05454500
C	1.02908200	-0.68709000	4.89412500
H	0.28314400	-1.20943400	5.08656300
C	2.23253500	-1.01448100	5.44537700
H	2.29022800	-1.72341100	6.04472000
C	3.40352800	-0.27966200	5.10628200
H	4.23673400	-0.52051400	5.44474900
C	3.26885600	0.77405300	4.28490000
H	4.01828000	1.28901400	4.08763600
C	2.04238100	1.12536400	3.71355900
H	1.99133000	1.83161400	3.11051000
C	-6.56388300	1.55769900	-1.87885000
C	-7.88912000	1.07685700	-1.83790900
H	-8.28034400	0.85880500	-1.02349200
C	-8.60818500	0.92870000	-3.02014600
H	-9.46274800	0.56221300	-3.00497900
C	-8.02572400	1.34544800	-4.25868600
H	-8.49533700	1.26836900	-5.05657400
C	-6.75942000	1.85863900	-4.23487900
H	-6.37041300	2.14589600	-5.03059600
C	-6.04009000	1.96240800	-3.05078600
H	-5.18070500	2.31673700	-3.06860500
C	-5.97675600	3.41733800	0.28737900
C	-7.25498400	3.94010300	0.24513800
H	-7.96449500	3.40631500	-0.03304000
C	-7.48582500	5.24378800	0.61079000
H	-8.34882400	5.58497000	0.55015200
C	-6.47633600	6.05647600	1.06120100
H	-6.64724000	6.92474300	1.34722700

C	-5.15829300	5.52099700	1.07408100
H	-4.44878100	6.05478500	1.35225900
C	-4.91582900	4.21785900	0.67878000
H	-4.04894200	3.88237800	0.67624400
C	-6.38217500	0.58231000	0.80623100
C	-6.42064800	-0.75680000	0.46039600
H	-5.99855300	-1.03338900	-0.32057000
C	-7.06065300	-1.67914800	1.23003600
H	-7.07823000	-2.57009000	0.96394100
C	-7.68654900	-1.30201900	2.40852600
H	-8.13822300	-1.92872800	2.92589200
C	-7.62658700	0.01917600	2.80329600
H	-8.02345400	0.28294100	3.60072700
C	-6.97175000	0.96047700	2.00850500
H	-6.92994400	1.84759100	2.28291900
C	-4.62983200	-3.11245300	-2.19057700
C	-4.80246600	-1.95960600	-2.96146100
H	-4.11191400	-1.33693900	-2.99403500
C	-5.94249400	-1.70998600	-3.67075600
H	-5.98895100	-0.98022100	-4.24516500
C	-7.04959900	-2.56819000	-3.51886900
H	-7.86220900	-2.36668100	-3.92494900
C	-6.91326900	-3.68793600	-2.77925400
H	-7.62751800	-4.28340300	-2.73254100
C	-5.75022400	-3.98720800	-2.08329000
H	-5.70147800	-4.75005400	-1.55397500
C	-3.67874300	-4.38180500	0.14344300
C	-4.17291800	-3.67389800	1.22276800
H	-4.09590500	-2.74775500	1.25012600
C	-4.77500400	-4.34568700	2.25091400
H	-5.10660600	-3.87139700	2.97870300
C	-4.89526100	-5.74425000	2.21935100
H	-5.33202500	-6.19792700	2.90432800
C	-4.36427600	-6.42361800	1.17543100
H	-4.41791900	-7.35239400	1.15845000
C	-3.72455500	-5.73844700	0.09919100
H	-3.35055800	-6.20712900	-0.61211900
C	-2.05704500	-4.40137500	-2.34963600
C	-2.52574100	-5.51385300	-3.06644100
H	-3.41878400	-5.76254400	-2.98983700
C	-1.68782700	-6.24183700	-3.88138000
H	-2.00437700	-7.00647500	-4.30716000
C	-0.35594600	-5.83169700	-4.07091100
H	0.20123300	-6.29513700	-4.65158900

C	0.11791600	-4.72410000	-3.37760100
H	0.99979500	-4.44840100	-3.48324600
C	-0.73952400	-4.02778000	-2.52091500
H	-0.41257900	-3.29491900	-2.05352000
N	1.45409900	0.24951600	-0.81879900
N	-1.52568400	0.53514700	-0.87307600
P	2.45418100	4.41025800	-0.29713900
P	5.56777000	-1.08704700	-1.17597900
P	1.57745200	-2.97303300	2.03373900
P	-0.66438900	1.00351600	3.33357300
P	-5.60733200	1.74101500	-0.33827900
P	-3.11321500	-3.41183500	-1.27531600
Au	1.87861400	2.23716200	-0.41509500
Au	3.47375700	-0.31043300	-0.99982600
Au	1.31149700	-1.19389100	0.68862100
Au	-0.90106700	0.75789900	1.11241000
Au	-3.44434400	1.24829800	-0.64860200
Au	-2.18181800	-1.41171700	-0.87092600

**Condition D:** N1-C1-C2-N2 dihedral angle is 61.17°. C1-C2-N2-Au4 dihedral angle is 59.42°.

C	0.62993100	-0.04457600	-2.07772800
H	0.33723300	-0.97752300	-2.03560300
C	-0.66905900	0.83255100	-2.06615700
H	-0.40601500	1.77397900	-2.00135300
C	1.40650300	0.10348600	-3.32786800
C	1.85071100	1.34338700	-3.85237700
H	1.64801600	2.12480800	-3.39086000
C	2.59446000	1.43242000	-5.05713700
H	2.92729000	2.24567400	-5.35984100
C	2.80278600	0.27473400	-5.76015300
H	3.25870800	0.31871800	-6.57112200
C	2.36546800	-0.94860900	-5.31394300
H	2.52734800	-1.71099600	-5.82128600
C	1.68415900	-1.05419000	-4.11259400

H	1.40408000	-1.88920800	-3.81398400
C	-1.49980900	0.64616800	-3.36081100
C	-2.17813800	1.73234600	-3.84717300
H	-2.08407700	2.56022800	-3.43522800
C	-3.00937200	1.60341900	-4.96068200
H	-3.48534700	2.33800000	-5.27149300
C	-3.12692200	0.39374900	-5.59696200
H	-3.67214900	0.31822900	-6.34728200
C	-2.42746600	-0.73283700	-5.12133900
H	-2.50635700	-1.55489200	-5.54864500
C	-1.62261400	-0.58960700	-4.00718500
H	-1.15623900	-1.32596100	-3.68203600
C	0.99249900	5.52672400	-0.32780700
C	-0.29532100	5.07876000	-0.74981600
H	-0.41790900	4.17921800	-0.94651700
C	-1.36175200	5.94403000	-0.87236200
H	-2.16043600	5.65129500	-1.24771900
C	-1.23457700	7.25722300	-0.43150200
H	-1.97378400	7.82076400	-0.40582400
C	0.08075300	7.73932800	-0.00828100
H	0.20984400	8.63262000	0.21480300
C	1.13597700	6.82925900	0.05428800
H	1.96271800	7.11975800	0.36614800
C	3.30861400	4.85076400	-1.81693900
C	4.12169900	3.87401500	-2.44090100
H	4.18892500	3.02276000	-2.07348600
C	4.81016600	4.18497800	-3.58306200
H	5.32997400	3.52175800	-3.97723800
C	4.77598000	5.39307200	-4.16619400
H	5.25499500	5.58223200	-4.93999100

C	3.95784200	6.36688500	-3.52271000
H	3.92126700	7.22580600	-3.87904100
C	3.22986900	6.09363800	-2.41098300
H	2.67434700	6.74592300	-2.04911400
C	3.39077100	4.80409900	1.08255100
C	2.81086500	5.11917800	2.32182900
H	1.88743300	5.21306000	2.38022200
C	3.59326600	5.29624200	3.47851900
H	3.21075300	5.46529000	4.30898900
C	5.02563200	5.20214200	3.30461000
H	5.58814100	5.39305200	4.02203000
C	5.55246900	4.84727300	2.13859600
H	6.47097400	4.70493900	2.10074800
C	4.81361400	4.67532200	0.96205700
H	5.22308500	4.48927800	0.14860600
C	6.67890700	-0.59940900	0.22357100
C	6.25613600	0.43657000	1.06745300
H	5.43820800	0.85101000	0.91157000
C	7.04131900	0.85174600	2.13266800
H	6.76586700	1.54360100	2.68735900
C	8.26745900	0.19642800	2.34689300
H	8.82161200	0.49095700	3.03337300
C	8.66407300	-0.85102300	1.58563400
H	9.46585500	-1.28493400	1.77287900
C	7.86161900	-1.28578100	0.50532100
H	8.11752900	-2.01706200	-0.01082600
C	6.38447300	-0.53133600	-2.66075200
C	5.67870800	0.14866300	-3.58715700
H	4.80575200	0.40893500	-3.39740400
C	6.24851300	0.47524700	-4.84740300

H	5.72051100	0.84982400	-5.51583300
C	7.57921500	0.23437100	-5.07098500
H	8.00348300	0.52024500	-5.84851000
C	8.25184400	-0.44832300	-4.09578100
H	9.14594200	-0.65917800	-4.24479600
C	7.69881400	-0.83381300	-2.93700200
H	8.20509900	-1.30735400	-2.31708500
C	5.53816700	-2.88480500	-1.19803400
C	4.93197400	-3.42228000	-2.33789400
H	4.64611000	-2.86152700	-3.02288800
C	4.75848700	-4.80266400	-2.44738700
H	4.37902100	-5.15955000	-3.21638900
C	5.15194800	-5.65675600	-1.40590200
H	5.00464400	-6.57337400	-1.46343800
C	5.74092100	-5.12539800	-0.32672700
H	6.07121300	-5.69664900	0.32803000
C	5.88358300	-3.72028900	-0.14300100
H	6.19785600	-3.37300000	0.66087000
C	3.24130700	-3.20852500	2.56947600
C	4.07915600	-2.10276000	2.76849300
H	3.77141600	-1.25850700	2.52617300
C	5.33447600	-2.21553600	3.30573600
H	5.85179500	-1.45858000	3.45733800
C	5.82320900	-3.48233800	3.62095000
H	6.68866500	-3.58017900	3.94564800
C	5.00609500	-4.60429600	3.44634700
H	5.30172900	-5.44216700	3.72175500
C	3.75192300	-4.46786300	2.86038900
H	3.25070600	-5.22631700	2.66099100
C	0.57838500	-3.06087800	3.56263700



C	-0.76662000	-2.65343500	3.54767400
H	-1.12691100	-2.31153600	2.76227500
C	-1.56894800	-2.75096600	4.67585300
H	-2.46488900	-2.50346000	4.64612200
C	-0.99725100	-3.23284200	5.86600100
H	-1.51240600	-3.29253600	6.63875600
C	0.32332300	-3.61544800	5.88724900
H	0.69335400	-3.93474400	6.67912400
C	1.10956100	-3.53599600	4.76021000
H	2.00077700	-3.79931600	4.79827200
C	1.12968200	-4.57103100	1.17921200
C	0.03869100	-5.33502200	1.55228400
H	-0.52333300	-5.05330400	2.23800000
C	-0.20596400	-6.54684600	0.87831500
H	-0.94481300	-7.06586600	1.10043600
C	0.66221600	-6.96212900	-0.11856900
H	0.49640600	-7.75820700	-0.57199800
C	1.71255700	-6.24643900	-0.43074400
H	2.30174900	-6.55756400	-1.08029900
C	1.96917000	-5.00596200	0.20089800
H	2.70359400	-4.49314600	-0.04828600
C	-1.84904537	0.26876229	4.22801592
C	-1.73069562	0.10471692	5.59116616
H	-0.93334842	0.32825066	6.01416846
C	-2.77967777	-0.38780791	6.33286070
H	-2.69069279	-0.49560638	7.25245048
C	-3.99590557	-0.72924495	5.69364610
H	-4.70278101	-1.09400278	6.17626373
C	-4.10903670	-0.50078458	4.29431388
H	-4.92172076	-0.65458674	3.86822410

C	-3.02952486	-0.05290378	3.55981534
H	-3.08933770	0.03297939	2.63568511
C	-0.40776862	2.72190025	3.72228760
C	0.11052120	3.08067290	4.98068421
H	0.45295635	2.43755710	5.55829280
C	0.09506584	4.44002712	5.33979145
H	0.44197184	4.69427430	6.16527678
C	-0.41146040	5.39344174	4.51517289
H	-0.43104397	6.28029921	4.79046719
C	-0.90929290	5.04200083	3.23532089
H	-1.22895760	5.69471350	2.65596038
C	-0.91079657	3.68128683	2.85954182
H	-1.24956754	3.42809138	2.03092216
C	1.07547016	0.29518758	3.91054637
C	1.18319583	-0.80278333	4.75475167
H	0.41827153	-1.28339915	4.97880201
C	2.38704565	-1.18955318	5.26515926
H	2.42912733	-1.89617266	5.86851594
C	3.58199659	-0.52038507	4.87724687
H	4.41315194	-0.80264294	5.18759517
C	3.47316937	0.53299563	4.05161665
H	4.24100572	1.00601937	3.82268594
C	2.24687204	0.94472787	3.52174653
H	2.21114284	1.64829106	2.91447006
C	-6.52328226	1.79245639	-1.75987271
C	-7.86965871	1.38291944	-1.66666942
H	-8.24180777	1.19185605	-0.83668277
C	-8.63827835	1.26453843	-2.82074922
H	-9.50985943	0.94403185	-2.77135573
C	-8.08030982	1.64078491	-4.08329837

H	-8.58218844	1.58293661	-4.86295961
C	-6.78866900	2.08622237	-4.10996614
H	-6.41439850	2.34664552	-4.92182327
C	-6.02205889	2.16027869	-2.95363370
H	-5.14640336	2.46837053	-3.00573995
C	-5.76005650	3.63401466	0.36655245
C	-7.00961135	4.22354399	0.36570808
H	-7.75599240	3.72614644	0.11825880
C	-7.15782623	5.54026302	0.72746364
H	-8.00326029	5.92630553	0.69490617
C	-6.09107439	6.30149472	1.13362783
H	-6.20535902	7.17966136	1.41764791
C	-4.80353034	5.69694102	1.10380900
H	-4.05714926	6.19433853	1.35125928
C	-4.64477218	4.37993641	0.71200182
H	-3.79746599	3.99892152	0.68123618
C	-6.29524946	0.82833545	0.92574367
C	-6.41693770	-0.50932508	0.59384592
H	-6.03885788	-0.81358602	-0.19928290
C	-7.07615010	-1.39079808	1.39454621
H	-7.15042509	-2.28146118	1.13746025
C	-7.63777392	-0.97243747	2.59136024
H	-8.10266879	-1.57052203	3.13044165
C	-7.49379698	0.34654777	2.97154788
H	-7.84677659	0.63678636	3.78033588
C	-6.81970294	1.24597764	2.14500411
H	-6.72114699	2.13159395	2.40956464
C	-4.85101503	-2.97587889	-2.09832469
C	-4.99065058	-1.82112704	-2.87303109
H	-4.26986029	-1.23623047	-2.93624845

C	-6.14108796	-1.51652926	-3.54294821
H	-6.16994494	-0.78951912	-4.12198592
C	-7.28563632	-2.31365479	-3.34328755
H	-8.10078451	-2.07226883	-3.72158322
C	-7.18162681	-3.43365315	-2.59881958
H	-7.92411339	-3.99002889	-2.52086632
C	-6.01132654	-3.78915043	-1.94260075
H	-5.98357829	-4.54964225	-1.40840357
C	-3.88353218	-4.27691526	0.21138470
C	-4.29988007	-3.53596133	1.30130340
H	-4.17316239	-2.61503524	1.31735007
C	-4.89858166	-4.16736960	2.35665895
H	-5.17786917	-3.67087800	3.09156106
C	-5.09353404	-5.55777318	2.34231566
H	-5.52829121	-5.98264893	3.04676245
C	-4.63765151	-6.27192491	1.28618417
H	-4.74080654	-7.19664551	1.27968790
C	-4.00244500	-5.62950088	0.18128644
H	-3.67995066	-6.12252234	-0.53873152
C	-2.35735251	-4.40061883	-2.33836201
C	-2.90998213	-5.49183902	-3.02751393
H	-3.81150505	-5.69223145	-2.91641829
C	-2.14199680	-6.26915807	-3.86546298
H	-2.51380386	-7.01899713	-4.27248527
C	-0.79815338	-5.93165303	-4.10674235
H	-0.28780210	-6.42821181	-4.70288450
C	-0.24148415	-4.84575149	-3.44120955
H	0.64925924	-4.61800802	-3.58117167
C	-1.02909950	-4.09871168	-2.56054759
H	-0.64707498	-3.38085382	-2.11202173

N	1.42793800	0.20598200	-0.85820300
N	-1.51265300	0.51135400	-0.92739000
P	2.36148700	4.38255700	-0.33976900
P	5.56564400	-1.07755500	-1.11932900
P	1.53255000	-2.99859000	2.01526000
P	-0.47463708	0.96391363	3.24091900
P	-5.50271074	1.93594838	-0.25660868
P	-3.31986091	-3.34865228	-1.23573133
Au	1.81736600	2.20134800	-0.45721800
Au	3.45824600	-0.32797500	-0.99263600
Au	1.27206800	-1.23072500	0.65429600
Au	-0.80498698	0.71507022	1.03210611
Au	-3.38152444	1.32691671	-0.64031930
Au	-2.27007337	-1.39788656	-0.88364846

**Condition E:** N1-C1-C2-N2 dihedral angle is 64.92°. C1-C2-N2-Au4 dihedral angle is 59.42°.

C	0.62688800	0.01671800	-2.02227900
H	0.32273700	-0.91251000	-1.97910500
C	-0.65973700	0.91085700	-1.97787800
H	-0.38462200	1.84274700	-1.85309000
C	1.37841800	0.16186500	-3.28797000
C	1.82779800	1.39885300	-3.81494300
H	1.64547600	2.18015300	-3.34480300
C	2.54669800	1.48514400	-5.03489100
H	2.88379100	2.29569600	-5.34011300
C	2.72445700	0.32896600	-5.74870100
H	3.16345500	0.37169700	-6.56902100

C	2.28051000	-0.89109700	-5.30006200
H	2.42130200	-1.65255400	-5.81503300
C	1.62373600	-0.99473700	-4.08496000
H	1.33899900	-1.82772500	-3.78508500
C	-1.47238300	0.81414500	-3.29365400
C	-2.12767100	1.93729200	-3.72446600
H	-2.02859100	2.73773400	-3.26250200
C	-2.94286900	1.88716900	-4.85601900
H	-3.40354500	2.64593200	-5.12955400
C	-3.06721300	0.71933900	-5.56502200
H	-3.60147800	0.69667700	-6.32660000
C	-2.39119600	-0.44381600	-5.14702200
H	-2.47478400	-1.23775500	-5.62374400
C	-1.60218500	-0.37906200	-4.01436700
H	-1.15135900	-1.14030400	-3.72677000
C	1.10115200	5.57233300	-0.24934500
C	-0.20127300	5.14392600	-0.64608600
H	-0.34003600	4.24725800	-0.84514700
C	-1.25844300	6.02392400	-0.74083200
H	-2.06881700	5.74399100	-1.10057300
C	-1.10434600	7.33270200	-0.29545100
H	-1.83524900	7.90580500	-0.25073400
C	0.22606000	7.79487400	0.10210200
H	0.37180700	8.68505300	0.32736500
C	1.27014500	6.87058300	0.13687600
H	2.10717800	7.14828500	0.43252100
C	3.37562200	4.87459800	-1.79167400
C	4.16205400	3.89087900	-2.43843100
H	4.22576800	3.03665900	-2.07732500
C	4.82999200	4.19943700	-3.59336200

H	5.33234500	3.53173700	-4.00233000
C	4.79945000	5.41129200	-4.16884300
H	5.26426600	5.59865900	-4.95168200
C	4.00834500	6.39202800	-3.50247500
H	3.97561200	7.25344200	-3.85311700
C	3.30076400	6.12188300	-2.37691000
H	2.76187200	6.77931200	-1.99953500
C	3.51922000	4.80976900	1.10507400
C	2.97024000	5.12518000	2.35827500
H	2.04960400	5.23091500	2.43702500
C	3.77952300	5.28506800	3.49885800
H	3.41717100	5.45426100	4.33829200
C	5.20645400	5.17306800	3.29368400
H	5.78669400	5.35229300	3.99990800
C	5.70341900	4.81814000	2.11464500
H	6.61892200	4.66390200	2.05626900
C	4.93731100	4.66290700	0.95331100
H	5.32674900	4.47626100	0.13021800
C	6.71581600	-0.63157900	0.14534700
C	6.32507200	0.40490700	1.00391500
H	5.50959700	0.83103600	0.86797100
C	7.13835600	0.80338400	2.05432100
H	6.88410100	1.49554100	2.61867400
C	8.35994900	0.13066400	2.23846900
H	8.93255500	0.41379200	2.91452200
C	8.72615900	-0.91743600	1.46300100
H	9.52590600	-1.36300300	1.63053700
C	7.89502600	-1.33517400	0.39776300
H	8.13004500	-2.06672200	-0.12785700
C	6.36061900	-0.54262900	-2.73155600

C	5.64431500	0.15208800	-3.63875300
H	4.77917100	0.42275500	-3.42882700
C	6.19130800	0.47853000	-4.90910100
H	5.65415800	0.86398500	-5.56392000
C	7.51358400	0.22140500	-5.16257500
H	7.92488200	0.50622200	-5.94742400
C	8.19777400	-0.47585500	-4.20589500
H	9.08558200	-0.69763000	-4.37527000
C	7.66459000	-0.86082100	-3.03767900
H	8.17767000	-1.34465700	-2.43145000
C	5.51450200	-2.89328000	-1.26420600
C	4.87692200	-3.41597000	-2.39377100
H	4.58396300	-2.84746100	-3.06931000
C	4.68272700	-4.79327100	-2.50724700
H	4.28215400	-5.14057200	-3.26990700
C	5.08697000	-5.65861100	-1.47926400
H	4.92625000	-6.57284600	-1.53876000
C	5.70595400	-5.14145300	-0.41003400
H	6.04254000	-5.72086800	0.23426100
C	5.87125300	-3.73946000	-0.22154100
H	6.20727400	-3.40109800	0.57732500
C	3.29473200	-3.20880000	2.54992000
C	4.15133000	-2.11540000	2.73708200
H	3.84976400	-1.26573900	2.50616800
C	5.41625000	-2.24792400	3.24658300
H	5.94675100	-1.49877900	3.39127400
C	5.89467500	-3.52291100	3.54411400
H	6.76550300	-3.63409600	3.84958400
C	5.05911100	-4.63292000	3.38082300
H	5.34936900	-5.47623500	3.64511200



C	3.79461100	-4.47647100	2.82272700
H	3.27916400	-5.22704500	2.62989700
C	0.65589500	-3.03181800	3.60089100
C	-0.68356500	-2.60654800	3.61712000
H	-1.05599900	-2.25529500	2.84157500
C	-1.46278100	-2.70010900	4.76171600
H	-2.35577100	-2.44061000	4.75263500
C	-0.87221000	-3.19650500	5.93658300
H	-1.37145000	-3.25393500	6.71988400
C	0.44329400	-3.59665300	5.92730100
H	0.82590400	-3.92547300	6.70923800
C	1.20620700	-3.52096300	4.78409000
H	2.09444000	-3.79626200	4.80151300
C	1.13582800	-4.53505800	1.19773800
C	0.04297900	-5.28674400	1.58988100
H	-0.50042300	-5.00166600	2.28908600
C	-0.23220000	-6.49123600	0.91454200
H	-0.97298300	-7.00174400	1.14957600
C	0.60881600	-6.91207900	-0.10308200
H	0.42272700	-7.70321000	-0.55729900
C	1.66168700	-6.20850900	-0.43374100
H	2.23263100	-6.52356500	-1.09754100
C	1.94829600	-4.97527700	0.19918700
H	2.68399300	-4.47075500	-0.06284400
C	-1.94711595	-0.00838604	4.25305178
C	-1.85269407	-0.25490317	5.60560978
H	-1.05910706	-0.06880715	6.05309921
C	-2.92008247	-0.77496113	6.30079003
H	-2.84720216	-0.93853821	7.21354085
C	-4.13067810	-1.05964994	5.62418331

H	-4.85014301	-1.44187894	6.07352907
C	-4.21840765	-0.74676567	4.23943394
H	-5.02630506	-0.86284978	3.79279128
C	-3.12123503	-0.27215086	3.54922967
H	-3.16518392	-0.13061353	2.63107593
C	-0.46386112	2.44873326	3.91623572
C	0.03937800	2.72432043	5.20142331
H	0.36359335	2.04298206	5.74470505
C	0.03723218	4.06000678	5.64071361
H	0.37452717	4.25954750	6.48500403
C	-0.44278586	5.06818581	4.86694080
H	-0.45433505	5.93730635	5.19432685
C	-0.92512980	4.80088629	3.56108383
H	-1.22641653	5.49156788	3.01696585
C	-0.93969223	3.46508645	3.10481799
H	-1.26879134	3.26666057	2.25758202
C	0.98214716	-0.00670223	3.98160425
C	1.06112272	-1.15438734	4.76032481
H	0.28610135	-1.63602416	4.94381047
C	2.25120810	-1.58869810	5.26473903
H	2.27384017	-2.33047652	5.82543041
C	3.46139333	-0.91553045	4.93539724
H	4.28349731	-1.22808206	5.24077956
C	3.38039929	0.18656266	4.17254012
H	4.15830412	0.66086801	3.98377371
C	2.16852939	0.64727890	3.64985208
H	2.15226675	1.38614586	3.08516235
C	-6.50409233	1.93795207	-1.70267324
C	-7.85736938	1.54369825	-1.65426407
H	-8.24526190	1.30920705	-0.84282633

C	-8.60917658	1.50558019	-2.82474357
H	-9.48582642	1.19572071	-2.80763097
C	-8.02605964	1.94784706	-4.05409123
H	-8.51627709	1.94392170	-4.84325170
C	-6.72806103	2.37479427	-4.03477083
H	-6.33736458	2.67740512	-4.82394225
C	-5.97891818	2.36856677	-2.86471694
H	-5.09832612	2.66613445	-2.88521661
C	-5.74901025	3.63829801	0.54102864
C	-6.99003385	4.24538252	0.55662310
H	-7.73927622	3.77474454	0.26877896
C	-7.12554812	5.54033466	0.99402268
H	-7.96488330	5.94017917	0.97188181
C	-6.05483531	6.26010641	1.46082305
H	-6.16132427	7.12144533	1.79498171
C	-4.77555535	5.63928501	1.41429807
H	-4.02631198	6.10992292	1.70214219
C	-4.62902703	4.34567664	0.94704315
H	-3.78674695	3.95458588	0.90630897
C	-6.33215780	0.81262777	0.92375879
C	-6.46725238	-0.50097987	0.51086410
H	-6.08093511	-0.76316314	-0.29324563
C	-7.15132921	-1.41856785	1.24757921
H	-7.23395977	-2.29117243	0.93673105
C	-7.72595376	-1.06376027	2.45866508
H	-8.20764822	-1.68583690	2.95407629
C	-7.56960217	0.22800648	2.91897785
H	-7.93126800	0.47488692	3.73825770
C	-6.86998614	1.16483113	2.15776252
H	-6.76326881	2.03159172	2.47613262

C	-4.89347288	-2.82621598	-2.29987887
C	-5.00465795	-1.62551016	-3.00632367
H	-4.27485331	-1.04869149	-3.02372298
C	-6.13996184	-1.26453324	-3.67404675
H	-6.14947379	-0.50404541	-4.20905020
C	-7.29855993	-2.05498059	-3.53947818
H	-8.10415556	-1.77942273	-3.91487850
C	-7.22202769	-3.21867119	-2.86167708
H	-7.97335863	-3.76757501	-2.82819427
C	-6.06735993	-3.62993314	-2.21036360
H	-6.05871447	-4.42115904	-1.72213067
C	-3.98100238	-4.27649435	-0.05765578
C	-4.40418039	-3.59550984	1.06816133
H	-4.26487465	-2.67915486	1.14101594
C	-5.02830192	-4.27953845	2.07487349
H	-5.31223863	-3.82349787	2.83381661
C	-5.24241418	-5.66357421	1.97468675
H	-5.69418008	-6.12304318	2.64593554
C	-4.77987189	-6.32040397	0.88478573
H	-4.89582505	-7.24146418	0.82158976
C	-4.11831398	-5.62297877	-0.17017115
H	-3.79136848	-6.07708385	-0.91340308
C	-2.41647358	-4.27115425	-2.58707299
C	-2.97330506	-5.31113410	-3.34830439
H	-3.87918733	-5.50432545	-3.26289008
C	-2.20307181	-6.04862941	-4.21952627
H	-2.57882138	-6.76732972	-4.67608503
C	-0.85098565	-5.71743436	-4.42006721
H	-0.33823878	-6.18522933	-5.03705224
C	-0.28981607	-4.68141962	-3.68266826

H	0.60613073	-4.45905292	-3.79542359
C	-1.08077537	-3.97639292	-2.77091361
H	-0.69591458	-3.29223199	-2.27468548
N	1.45409900	0.24951600	-0.81879900
N	-1.52568400	0.53514700	-0.87307600
P	2.45418100	4.41025800	-0.29713900
P	5.56777000	-1.08704700	-1.17597900
P	1.57745200	-2.97303300	2.03373900
P	-0.54765130	0.72365617	3.32990041
P	-5.50557456	1.97662789	-0.17839635
P	-3.38154453	-3.27236289	-1.43820318
Au	1.87861400	2.23716200	-0.41509500
Au	3.47375700	-0.31043300	-0.99982600
Au	1.31149700	-1.19389100	0.68862100
Au	-0.84639065	0.61147870	1.10547234
Au	-3.38729036	1.35995119	-0.56591329
Au	-2.31031042	-1.36182411	-0.95467166