Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

A novel acid-controlled second-order nonlinear optical switch based on dimethyldihydropyrene/cyclophanediene photoswitch

Yao Yao[a], Hong-Liang Xu[a,*], Zhong-Min Su[b]

a. Institute of Functional Material Chemistry, National & Local United Engineering Laboratory for Power Batteries, Department of Chemistry, Northeast Normal University, Changchun, 130024, People's Republic of China.

b. School of Chemistry & Environmental Engineering, Changchun University of Science and Technology, Changchun, 130012, People's Republic of China.

Email: hlxu@nenu.edu.cn

Fig. S1. The structure of transient state and the corresponding imaginary frequency for studied compounds.

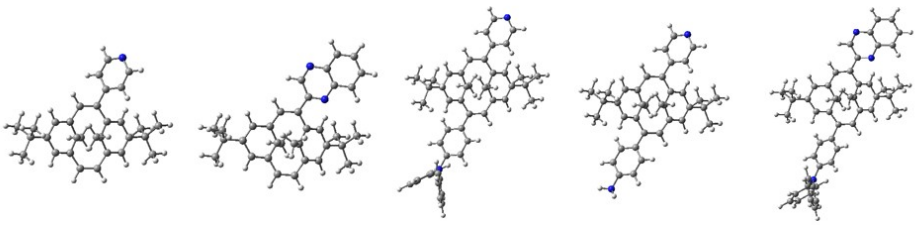
Fig. S2. (a)The comparison of UV-vis absorption spectra of compound **IV-C** and their protonated compounds; (b) Plot of the $-y\rho^{yy\,(2)}$ for compound **IV-C-AH**$^{+}$ and the corresponding β_{yyy} value (Yellow color represents positive value, while blue color represents negative value).

Table S1 The Gibbs free energy (a.u.) and energy barrier of all studied compounds at M062X/6-311+G (d, p) level (at room temperature).

Table S2 The HOMO-LUMO energy (eV) of studied closed-ring compounds in B3LYP and ωB97XD method in acetonitrile solution.

Table S3 The components of the first hyperpolarizabilities (a.u.) of the studied compounds computed at the ωB97XD/6-31+G(d, p) level of theory in acetonitrile solution.

Table S4 The total second hyperpolarizability γ and the γ ratios contrast of some studied compounds calculated at ωB97XD/6-31+G(d, p) in CH_3CN.



Compound	I-TS	II-TS	III-TS	IV-TS	V-TS
imaginary frequency	-890.67	-1551.03	-889.73	-890.69	-1695.68

Fig. S1. The structure of transient state and the corresponding imaginary frequency for studied compounds.

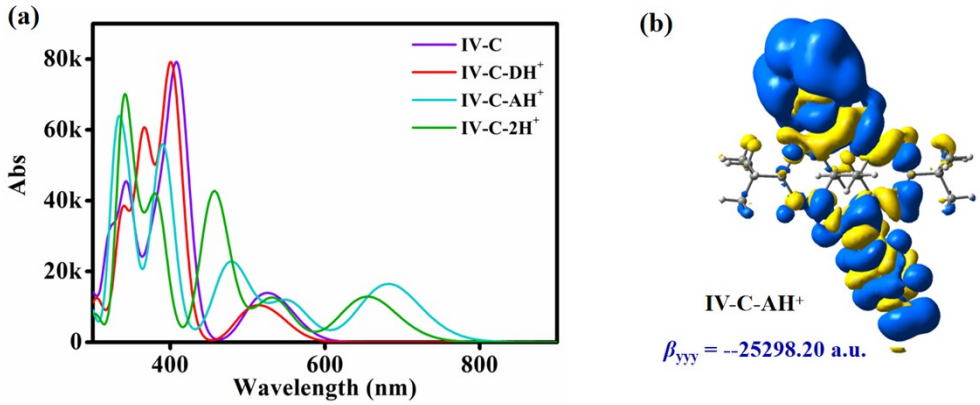


Fig. S2. (a)The comparison of UV-vis absorption spectra of compound **IV-C** and their protonated compounds; (b) Plot of the $-y\rho^{yy\ (2)}$ for compound **IV-C-AH**$^{+}$ and the corresponding β_{yyy} value (Yellow color represents positive value, while blue color represents negative value).

Table S1 The Gibbs free energy (a.u.) and energy barrier of all studied compounds at M062X/6-311+G (d, p) level (at room temperature).

Compounds	Gibbs free energy (a.u.)	Energy barrier (Kcal/mol))
I-C	-1256.36967	39.40
I-TS	-1256.30688	
I-O	-1256.35164	28.09
II-C	-1425.99816	46.53
II-TS	-1425.92401	
II-O	-1425.98054	35.47
III-C	-2004.53322	38.25
III-TS	-2004.47227	
III-O	-2004.51707	28.11
IV-C	-1542.66216	38.47
IV-TS	-1542.60085	
IV-O	-1542.64665	28.74
V-C	-2174.12942	46.79
V-TS	-2174.05485	
V-O	-2174.11349	36.80

Table S2 The HOMO-LUMO energy (eV) of studied closed-ring compounds in B3LYP and ωB97XD method in acetonitrile solution.

	B3LYP	ωB97XD
I-C	3.00	6.20
I-C-H$^+$	2.32	5.53
II-C	2.75	6.00
II-C-H$^+$	1.38	4.26
III-C	2.85	6.02
III-C-H	2.18	5.38
IV-C	2.86	6.02
IV-C-DH$^+$	2.91	6.08
IV-C-AH$^+$	2.20	5.36
IV-C-2H$^+$	2.34	5.53
V-C	2.62	5.83
V-C-2H$^+$	1.17	4.08

Table S3 The components of the first hyperpolarizabilities (a.u.) of the studied compounds computed at the ωB97XD/6-31+G (d, p) level of theory in acetonitrile solution.

	1-C	**1-C-H$^+$**	**II-C**	**II-C-2H$^+$**	**III-C**	**III-C-H$^+$**
XXX	13.22	12.56	-231.144	6645.09	448.41	-286.272
XXY	-889.90	-3395.19	-1018.33	-10016.3	-1640.43	-3820.02
XYY	735.16	5029.99	1093.75	35684.7	2755.34	9174.2
YYY	-2658.56	-6937.15	-3873.1	-44830.2	-6592.04	-24507.1
XXZ	-30.54	-14.00	10.4953	-1788.00	15.0722	167.826
XYZ	25.52	150.83	-55.4731	8025.18	87.0428	-471.993
YYZ	131.57	149.70	-312.871	-12496.9	-493.165	1242.02
XZZ	-82.70	-152.31	-14.6745	1751.15	-708.623	-667.248
YZZ	268.26	381.14	264.547	-2659.19	1539.76	1696
ZZZ	-13.51	19.13	6.48481	-549.327	241.997	-52.3827
	IV-C	**IV-C-DH$^+$**	**IV-C-AH$^+$**	**IV-C-2H$^+$**		
XXX	202.159	-188.476	77.08	-1040.09		
XXY	-1183.34	-893.241	-4295.54	-2377.30		
XYY	2370.12	645.308	10044.40	4885.02		
YYY	-7741.14	-1650.59	-25298.20	-14061.60		
XXZ	-94.1475	-59.3261	41.09	-31.02		
XYZ	185.008	-10.9747	-226.57	-110.48		
YYZ	-312.641	153.705	1097.63	665.48		
XZZ	-36.5304	-43.0256	-126.13	-82.48		
YZZ	262.658	170.954	392.50	302.59		
ZZZ	16.8192	-24.2069	-53.30	-30.06		

Table S4 The total second hyperpolarizability γ_{tot} and the γ ratios contrast of some studied compounds calculated at ωB97XD/6-31+G(d, p) in CH_3CN.

Compound	γ_{tot}	γ_{tot}(protonated)/$_{\gamma tot}$(neutral)
I-C	4.18×10^5 a.u.	2.0
I-C-H$^+$	8.33×10^5 a.u.	
I-O	2.17×10^5 a.u.	1.6
I-O-H$^+$	3.54×10^5 a.u.	
II-C	5.58×10^5 a.u.	7.5
II-C-2H$^+$	4.16×10^6 a.u.	
V-C	1.28×10^6 a.u.	15.6
V-C-2H$^+$	2.00×10^7 a.u.	

Coordinates of the optimal structure (in acetonitrile)

I-C

C	-1.81453600	-3.03571000	0.09422800
C	-0.42445100	-3.36279200	0.05473700
C	-2.24238800	-1.73988600	-0.02189700
C	-3.61283300	-1.35274600	0.00798400
C	-4.00705800	-0.03896600	0.01137600
C	-3.00233700	0.99294600	0.03820900
C	-1.67093000	0.72430500	-0.04752200
C	-0.66088300	1.73339600	0.01352000
C	0.68057200	1.44896400	0.01166500
C	1.14202000	0.07658200	0.04821500
C	2.43756100	-0.30212400	-0.11382200
C	2.87206600	-1.67553400	-0.06047000
C	1.93660200	-2.67016600	0.03801500
C	0.54154900	-2.39324800	0.11399000
C	0.10065300	-0.96968300	0.40338500
C	-0.07857600	-0.88464100	1.94960700
C	-1.20673500	-0.68150700	-0.35093900
C	-1.01048100	-0.74053700	-1.89770400
H	-0.66391200	-1.72864000	-2.20824500
H	-0.29060000	0.00937400	-2.23462800
H	-1.96991300	-0.53931600	-2.38100500
H	-0.37820400	0.11882200	2.26089700
H	0.87594600	-1.12273500	2.42632900
H	-0.82770000	-1.60096300	2.29421600
C	4.37472700	-1.94862300	-0.16669800
C	5.10048500	-1.21118300	0.97650300
H	4.74603400	-1.56319800	1.95055800
H	6.17841700	-1.39476200	0.91754000
H	4.94463700	-0.12920000	0.93042400
C	4.89667200	-1.43419000	-1.52303600
H	4.39152100	-1.94300400	-2.35001700
H	5.97135100	-1.62671200	-1.60763800
H	4.74329200	-0.35782500	-1.64237800
C	4.70465800	-3.44287400	-0.06006600
H	4.35769600	-3.86582900	0.88807300
H	5.78872700	-3.58192100	-0.11137700
H	4.25857300	-4.01638000	-0.87870900
C	-5.47739300	0.38777000	0.04707700
C	-5.75337300	1.17555400	1.34311600

H	-5.54928400	0.55693700	2.22269500
H	-5.14100900	2.07892500	1.41422600
H	-6.80361200	1.48372200	1.37737300
C	-6.43531100	-0.80966100	0.00076200
H	-6.31225300	-1.46221000	0.87088000
H	-6.29015300	-1.40816400	-0.90418700
H	-7.46864700	-0.44988300	0.00092300
C	-5.76880200	1.28500800	-1.17214200
H	-5.14760500	2.18530600	-1.17497100
H	-6.81671200	1.60285300	-1.16324200
H	-5.58350900	0.74267500	-2.10482300
H	-4.34977100	-2.14690900	0.07172900
H	-2.54524000	-3.83489900	0.18846700
H	2.23576600	-3.71298900	0.00556600
H	3.18336800	0.45961800	-0.31444800
H	-3.31358200	2.02689700	0.16319700
H	-0.98192600	2.77098100	0.06752600
H	-0.12814800	-4.40664900	-0.01005900
C	1.64695900	2.57593800	0.02996400
C	2.67997400	2.65317600	0.97031300
C	1.53353200	3.63477300	-0.87430000
C	3.52755800	3.75323500	0.95886600
H	2.81457100	1.87105600	1.70952600
C	2.43352400	4.69196300	-0.80172300
H	0.75969000	3.62907100	-1.63451800
N	3.42415900	4.76807800	0.09261400
H	4.33042300	3.82392600	1.68900000
H	2.35449600	5.51822700	-1.50449100

I-O

C	1.56663100	-3.10387100	-0.18585500
C	0.43961600	-3.17888000	-0.92362600
C	2.08790500	-1.85251200	0.43626100
C	3.37742900	-1.44513300	0.06639700
C	3.82418800	-0.13969600	0.26261700
C	2.85936800	0.78977600	0.66625800
C	1.56219900	0.40874000	1.02189000
C	0.52730400	1.47110100	0.92988000
C	-0.59635800	1.42627700	0.16982400
C	-1.12684400	0.15203800	-0.42247300
C	-2.40475400	-0.24602100	-0.02351200
C	-2.85612100	-1.56103800	-0.17085200
C	-1.90306500	-2.49923400	-0.56226100
C	-0.61388200	-2.12360600	-0.96240100

C	-0.29864100	-0.76086400	-1.10304700
C	0.86876300	-0.30447600	-1.93773600
C	1.25138900	-0.96251500	1.12993000
C	0.09000600	-1.44373800	1.95681500
H	-0.21522700	-2.45396800	1.68596800
H	-0.77777000	-0.78682300	1.90146100
H	0.41574100	-1.46639600	3.00342900
H	1.45295200	0.48867300	-1.47153500
H	0.47331600	0.09122300	-2.88040400
H	1.53572200	-1.13186000	-2.18041900
C	-4.28946200	-1.92962700	0.22446100
C	-5.27400200	-1.06569800	-0.58593400
H	-5.15686900	-1.24663000	-1.65922200
H	-6.30592600	-1.30640600	-0.30904600
H	-5.11889200	0.00198000	-0.40460500
C	-4.49071600	-1.66354400	1.72860900
H	-3.78672000	-2.25479100	2.32311700
H	-5.50786500	-1.93669700	2.02943500
H	-4.34081300	-0.60873500	1.97695800
C	-4.60217700	-3.40627800	-0.05247500
H	-4.44298800	-3.66059900	-1.10534400
H	-5.65010100	-3.61015400	0.18793600
H	-3.98862400	-4.07432100	0.56024700
C	5.24548200	0.32257900	-0.07524800
C	5.19675300	1.30924700	-1.25769600
H	4.75033900	0.83555000	-2.13798200
H	4.60872500	2.20006600	-1.01805700
H	6.20835800	1.63703000	-1.52034300
C	6.15675900	-0.85031500	-0.46149700
H	5.82117300	-1.34130500	-1.38044800
H	6.20452800	-1.60158400	0.33336800
H	7.17214700	-0.48233500	-0.63780700
C	5.85434600	1.02399200	1.15324000
H	5.26399200	1.89397600	1.45557200
H	6.86894700	1.36953400	0.92801100
H	5.90783100	0.33872100	2.00524900
H	4.01502700	-2.17367300	-0.42390500
H	2.22013500	-3.97419200	-0.17552500
H	-2.12826100	-3.55989200	-0.51508500
H	-3.04007500	0.48966000	0.46254200
H	3.08888200	1.85220100	0.63984800
H	0.81437000	2.44260000	1.32851500
H	0.20804400	-4.13272300	-1.39392400
C	-1.42118700	2.64962200	0.00810400

C	-2.11374900	2.88291500	-1.18511400
C	-1.55041100	3.61698200	1.00988300
C	-2.85450500	4.04850500	-1.32797400
H	-2.07143100	2.16293500	-1.99543700
C	-2.31839200	4.74930200	0.76795100
H	-1.07981300	3.48440800	1.97789500
N	-2.96725500	4.98381300	-0.37772400
H	-3.38680100	4.23975300	-2.25686900
H	-2.42451600	5.50390600	1.54395800

I-TS

C	1.71771600	-3.07640500	-0.17448100
C	0.46026200	-3.29970000	-0.62928800
C	2.19430100	-1.75474200	0.24294800
C	3.50936200	-1.37699700	0.01733600
C	3.94744300	-0.04686400	0.15552100
C	2.95976800	0.93148200	0.38888400
C	1.63178600	0.61215500	0.62106400
C	0.61266300	1.65355100	0.55233700
C	-0.65665000	1.45792200	0.09529600
C	-1.14187500	0.10132000	-0.25907100
C	-2.42573200	-0.29438200	0.06113300
C	-2.86721300	-1.63135300	-0.05112600
C	-1.89600900	-2.60027400	-0.34430800
C	-0.58069100	-2.26660400	-0.63936800
C	-0.18360000	-0.87293700	-0.75087600
C	0.63589900	-0.48311500	-1.97381000
C	1.22624700	-0.78071900	0.72240300
C	0.40747600	-1.16600300	1.94669500
H	-0.01826800	-2.16594400	1.84944900
H	-0.40186300	-0.45660900	2.12825100
H	1.06623700	-1.15958000	2.82135700
H	1.05405100	0.52006100	-1.87743100
H	-0.02096900	-0.49372300	-2.84984300
H	1.45099500	-1.18584000	-2.15273300
C	-4.33157600	-1.96688300	0.23634600
C	-5.23125000	-1.14677000	-0.70944500
H	-5.02121900	-1.39345500	-1.75508800
H	-6.28618100	-1.36476600	-0.51150100
H	-5.08248100	-0.07056400	-0.57989900
C	-4.66630600	-1.60870900	1.69785600
H	-4.03162100	-2.17186500	2.38944900
H	-5.71173700	-1.85141800	1.91674300

H	-4.52269800	-0.54277900	1.89767500
C	-4.63764900	-3.45519400	0.02128200
H	-4.40282000	-3.77144500	-1.00017100
H	-5.70289700	-3.63819500	0.19205800
H	-4.07885100	-4.08992500	0.71634100
C	5.40494100	0.37609400	-0.04282400
C	5.51475000	1.27796800	-1.28826200
H	5.17416300	0.74612900	-2.18237000
H	4.91415600	2.18648100	-1.18518900
H	6.55554900	1.58111400	-1.44534000
C	6.33725000	-0.82793200	-0.23571200
H	6.10064300	-1.38450400	-1.14804500
H	6.28593900	-1.51771900	0.61286300
H	7.37089600	-0.47935700	-0.32217700
C	5.87950500	1.15807100	1.19751800
H	5.27628600	2.05455200	1.36789500
H	6.91986000	1.47528600	1.06861700
H	5.82069000	0.53469600	2.09540500
H	4.20471500	-2.14391100	-0.30948400
H	2.43868700	-3.89015400	-0.19577500
H	-2.15178600	-3.65469100	-0.30463400
H	-3.11545300	0.45820800	0.43268900
H	3.22960000	1.98428600	0.34732400
H	0.94117100	2.67212700	0.74645300
H	0.17512100	-4.30874100	-0.91745900
C	-1.57760300	2.60961800	-0.02669800
C	-2.48701800	2.70501700	-1.08745700
C	-1.57449800	3.66314300	0.89420600
C	-3.30942200	3.81941100	-1.18283000
H	-2.54811900	1.92047300	-1.83363500
C	-2.43826000	4.73505600	0.70778300
H	-0.92172800	3.64096200	1.76008100
N	-3.30150100	4.83319700	-0.30910100
H	-4.01236100	3.90185400	-2.00862200
H	-2.44130700	5.55522800	1.42214600

IV-C

C	-2.07515700	-1.09936500	-0.07045400
C	-1.05777600	-2.11269700	-0.09666900
C	-1.70980900	0.23310700	-0.11659500
C	-2.62346500	1.31915500	-0.01917800
C	-2.22804300	2.63356400	0.01909400
C	-0.82646900	2.94212400	0.02767300

C	0.13308200	1.98170700	-0.07779000
C	1.52817700	2.27094000	0.00831200
C	2.49695100	1.30001300	0.01261500
C	2.12869400	-0.09849100	0.02300700
C	3.00911000	-1.12372800	-0.13092700
C	2.61942200	-2.51006800	-0.10863700
C	1.28925200	-2.82920400	-0.05008100
C	0.27554000	-1.83170700	0.01733600
C	0.67573100	-0.40759500	0.34153400
C	0.53611100	-0.26584300	1.88749300
C	-0.25173600	0.55767400	-0.41321100
C	-0.09362100	0.43034400	-1.95960600
H	-0.34554800	-0.57825900	-2.29470500
H	0.92586900	0.66485000	-2.27609100
H	-0.77490700	1.13717300	-2.44024700
H	0.82576100	0.73289800	2.22252900
H	1.19256700	-0.99574900	2.36841000
H	-0.49170200	-0.46120400	2.20249500
C	3.72795700	-3.56148000	-0.20396500
C	4.71224200	-3.35981400	0.96561400
H	4.20009100	-3.47308500	1.92646300
H	5.51360600	-4.10433900	0.91482500
H	5.17679000	-2.36946100	0.94430200
C	4.47781400	-3.39791800	-1.54091800
H	3.79595700	-3.53489000	-2.38606300
H	5.27335400	-4.14648100	-1.61774900
H	4.94127100	-2.41169500	-1.63523700
C	3.18154600	-4.99293300	-0.13065300
H	2.63648000	-5.16917000	0.80212700
H	4.01262100	-5.70343000	-0.17176700
H	2.51405900	-5.21602100	-0.96894200
C	-3.22613100	3.79059300	0.12377700
C	-2.99687700	4.55325700	1.44360500
H	-3.14154100	3.89089700	2.30291200
H	-1.98916600	4.97392800	1.50553000
H	-3.70776900	5.38213900	1.52654600
C	-4.68350000	3.31108900	0.09346800
H	-4.91873700	2.67019200	0.94909200
H	-4.90818200	2.75774500	-0.82409000
H	-5.35246900	4.17598000	0.13476900
C	-3.00958900	4.74635200	-1.06621600
H	-1.99677400	5.15940200	-1.07909500
H	-3.71114800	5.58523700	-1.00810600
H	-3.17543400	4.22640100	-2.01518200

H	-3.67393200	1.07822000	0.07753300
H	0.96663500	-3.86373100	-0.10989900
H	4.05484400	-0.89184400	-0.30205400
H	-0.51217900	3.97250700	0.17433200
H	1.82471200	3.31433600	0.08568300
H	-1.37110500	-3.14772200	-0.21111200
C	3.92128800	1.71433200	0.06799400
C	4.80837800	1.19863500	1.01927200
C	4.42466600	2.67823000	-0.80918200
C	6.11948400	1.65581200	1.04362600
H	4.47764500	0.45869000	1.73992400
C	5.75424000	3.06981200	-0.70113600
H	3.79002100	3.10967800	-1.57591600
N	6.60629900	2.57643400	0.20313200
H	6.81447600	1.26341800	1.78235700
H	6.15469000	3.81668100	-1.38281600
C	-3.49010700	-1.55051400	-0.02551100
C	-4.43891500	-1.11566800	-0.95906100
C	-3.91161800	-2.47306000	0.93928100
C	-5.75286500	-1.56096700	-0.92091300
H	-4.13869500	-0.42095500	-1.73829300
C	-5.22279200	-2.92575900	0.98936000
H	-3.19885100	-2.83392900	1.67592100
C	-6.17032600	-2.47289500	0.05972100
H	-6.46421200	-1.20870300	-1.66272800
H	-5.52144300	-3.63540400	1.75588800
N	-7.47144800	-2.96503400	0.06928300
H	-8.15812500	-2.35840700	-0.35569900
H	-7.78881500	-3.30788600	0.96479000

IV-O

C	2.07954300	-1.00952000	-0.20749300
C	1.21537900	-1.77247000	-0.92468200
C	1.66291800	0.30305100	0.39494200
C	2.37551100	1.44315800	-0.00507200
C	1.88271300	2.72986400	0.18986800
C	0.55635700	2.82433500	0.62499700
C	-0.18372700	1.70146600	1.00239000
C	-1.66057300	1.85978900	0.94480300
C	-2.51073700	1.11867600	0.19044500
C	-2.11410400	-0.19442800	-0.41946900
C	-2.84308100	-1.31808500	-0.02363500

C	-2.35032800	-2.61716300	-0.18026000
C	-1.01836400	-2.72598400	-0.57246900
C	-0.26262600	-1.61108200	-0.96438200
C	-0.89571500	-0.36367600	-1.10531600
C	-0.30079300	0.73093100	-1.94997100
C	0.46154300	0.44977700	1.10383000
C	-0.10888700	-0.66584400	1.93723200
H	0.35805900	-1.62250400	1.70280200
H	-1.18951500	-0.77019200	1.83794700
H	0.10297300	-0.44038200	2.98874700
H	-0.43506500	1.72543600	-1.52537400
H	-0.81110600	0.71784300	-2.92024400
H	0.76107700	0.56921500	-2.13450100
C	-3.21559000	-3.81965300	0.20928000
C	-4.52483400	-3.78191200	-0.60109000
H	-4.31897800	-3.84065900	-1.67468700
H	-5.16399500	-4.62848400	-0.32847300
H	-5.08863400	-2.86292700	-0.41520400
C	-3.54105700	-3.75138900	1.71368900
H	-2.62187900	-3.75740200	2.30839200
H	-4.14736700	-4.61405100	2.01023800
H	-4.10166000	-2.84653900	1.96613300
C	-2.51055300	-5.15297400	-0.07366200
H	-2.22633000	-5.24218600	-1.12712400
H	-3.18463400	-5.98158700	0.16413900
H	-1.61085100	-5.27551800	0.53769200
C	2.66759100	3.99246300	-0.17936800
C	1.97566200	4.69841500	-1.36116500
H	1.92367600	4.03480600	-2.23038000
H	0.95649800	5.00568200	-1.10872900
H	2.53453300	5.59588900	-1.64749700
C	4.11291200	3.67256400	-0.58492700
H	4.15577600	3.06920000	-1.49720300
H	4.64385000	3.13590300	0.20800400
H	4.65296900	4.60385700	-0.78134400
C	2.70381600	4.93916500	1.03466500
H	1.69772500	5.22978600	1.35107100
H	3.25360000	5.85317600	0.78603100
H	3.20117200	4.46159100	1.88493800
H	3.32515800	1.29139700	-0.50594600
H	-0.51410800	-3.68616100	-0.53026100
H	-3.79971500	-1.15980000	0.46699200
H	0.04837100	3.78552100	0.60379300
H	-2.05114200	2.78573900	1.36329700

H	1.60206900	-2.70337600	-1.33547800
C	-3.92887700	1.53567300	0.05716100
C	-4.63058200	1.28518400	-1.12712900
C	-4.62877400	2.18802600	1.07719200
C	-5.94708700	1.71048100	-1.24376300
H	-4.15187300	0.76606600	-1.95060400
C	-5.94663300	2.57154900	0.86105100
H	-4.16542600	2.37712100	2.03929300
N	-6.61497000	2.34881100	-0.27577800
H	-6.49437700	1.52685300	-2.16545500
H	-6.49684900	3.07711200	1.65133600
C	3.51241100	-1.38262600	-0.11136200
C	4.23767200	-1.10441900	1.05489400
C	4.19368900	-2.02164100	-1.15487300
C	5.56775600	-1.47200100	1.19011400
H	3.74507200	-0.59052500	1.87550000
C	5.52535700	-2.39177200	-1.03372900
H	3.67967600	-2.21266000	-2.09232400
C	6.23730600	-2.12772500	0.14575600
H	6.09944000	-1.25051500	2.11127300
H	6.02830600	-2.87790600	-1.86504300
N	7.55426500	-2.54536800	0.29387900
H	8.06300700	-2.66930900	-0.56965700
H	8.09415700	-2.02483800	0.97023600

IV-TS

C	2.06850300	-1.12126400	-0.12844100
C	1.12971300	-2.00829100	-0.57349500
C	1.68025800	0.26177700	0.23870600
C	2.51055400	1.32968900	-0.06633300
C	2.10522500	2.67048300	0.05809000
C	0.74795400	2.90266400	0.34994400
C	-0.13864400	1.87619200	0.63101700
C	-1.57314500	2.14190300	0.59250800
C	-2.50346900	1.25641300	0.13866600
C	-2.12309200	-0.12830100	-0.23153900
C	-2.95160200	-1.18975300	0.06672400
C	-2.54905700	-2.53927600	-0.06817800
C	-1.19907300	-2.77420800	-0.35199100
C	-0.30209600	-1.74232900	-0.61750400
C	-0.77625300	-0.37240500	-0.72436300
C	-0.33943700	0.40961400	-1.95534300
C	0.33669200	0.50502900	0.73484700

C	-0.10202200	-0.27723400	1.96511300
H	0.13449800	-1.33839600	1.87315700
H	-1.17269200	-0.17136000	2.14912100
H	0.43243200	0.11625900	2.83602900
H	-0.56210400	1.47374600	-1.85988900
H	-0.88549400	0.02515800	-2.82314500
H	0.72826800	0.29076000	-2.14704000
C	-3.56312200	-3.65485100	0.18915500
C	-4.75847200	-3.47793600	-0.76816700
H	-4.43287800	-3.54477000	-1.81117800
H	-5.50416000	-4.26045300	-0.59142100
H	-5.24990800	-2.51023700	-0.62932500
C	-4.05976500	-3.57629700	1.64633000
H	-3.22554400	-3.68912600	2.34605600
H	-4.78282500	-4.37521100	1.84296900
H	-4.55197000	-2.62223700	1.85680300
C	-2.96273800	-5.04793100	-0.04234900
H	-2.57700900	-5.15630500	-1.06116800
H	-3.73504300	-5.80879500	0.10623100
H	-2.15008900	-5.26208100	0.65907000
C	3.04523000	3.84906800	-0.20397600
C	2.55711100	4.63533300	-1.43662300
H	2.53778700	3.99282700	-2.32268000
H	1.55073400	5.03770700	-1.28796700
H	3.22754900	5.47770800	-1.63849400
C	4.48791300	3.39231200	-0.46235900
H	4.56738400	2.78972000	-1.37272100
H	4.88185000	2.80591400	0.37417900
H	5.13108100	4.26830900	-0.59042100
C	3.04688500	4.77711900	1.02638200
H	2.04780500	5.16718300	1.24166900
H	3.70935800	5.63213800	0.85413400
H	3.40063100	4.24359900	1.91437100
H	3.50646000	1.10387800	-0.42948700
H	-0.80716200	-3.78644900	-0.32578900
H	-3.94918700	-0.97252400	0.43791700
H	0.35558900	3.91627700	0.30867500
H	-1.88720400	3.16252300	0.79932800
H	1.44270700	-3.03133100	-0.77007300
C	-3.92036900	1.67036000	0.03450400
C	-4.72643600	1.24416800	-1.02844400
C	-4.51675700	2.51833800	0.97409900
C	-6.04041100	1.68497000	-1.10741700
H	-4.33041300	0.57980100	-1.78860700

C	-5.84099000	2.90232700	0.80309000
H	-3.96351700	2.86043900	1.84204600
N	-6.61056600	2.50405900	-0.21560300
H	-6.66857800	1.36279600	-1.93472600
H	-6.30992700	3.55944700	1.53196500
C	3.49214300	-1.51785900	-0.05298100
C	4.30685700	-1.09566400	1.00783000
C	4.07590500	-2.34726600	-1.01980100
C	5.63085600	-1.49329200	1.11099400
H	3.88985300	-0.44559200	1.77135000
C	5.39999100	-2.75123600	-0.92833400
H	3.48633700	-2.66555800	-1.87467900
C	6.20321600	-2.33281500	0.14275100
H	6.23300200	-1.15596000	1.95001400
H	5.82525400	-3.38760500	-1.69936800
N	7.51309100	-2.77816500	0.26994500
H	8.11618100	-2.18129900	0.81751400
H	7.95492700	-3.05945100	-0.59350300