

Supporting Information

Progressive Photocuring Approach: A Macrocyclic Photoinitiator Enabling Exceptional Toughness in *Poly(TMPTA)* Thick Coatings

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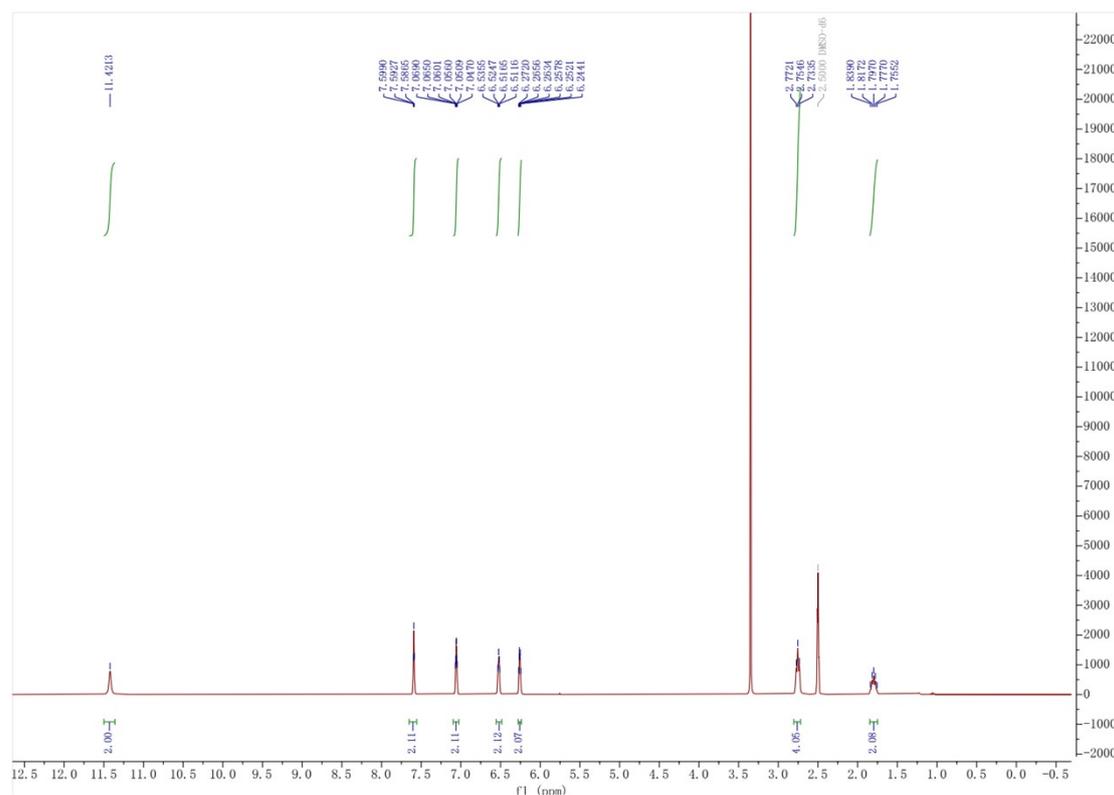


Fig.S1 ¹H-NMR spectrum of BPC dissolved in DMSO-d₆

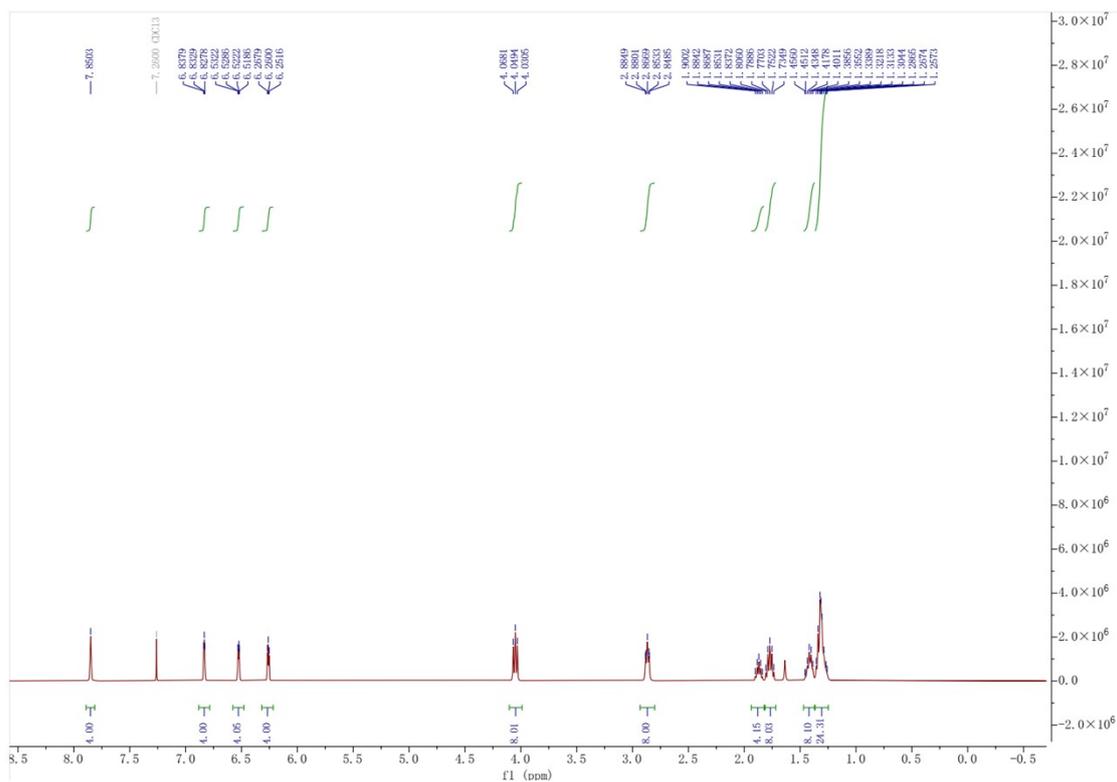


Fig.S2 $^1\text{H-NMR}$ spectrum of $[2](\text{BPC})[2](\text{C}_{12})$ dissolved in CDCl_3

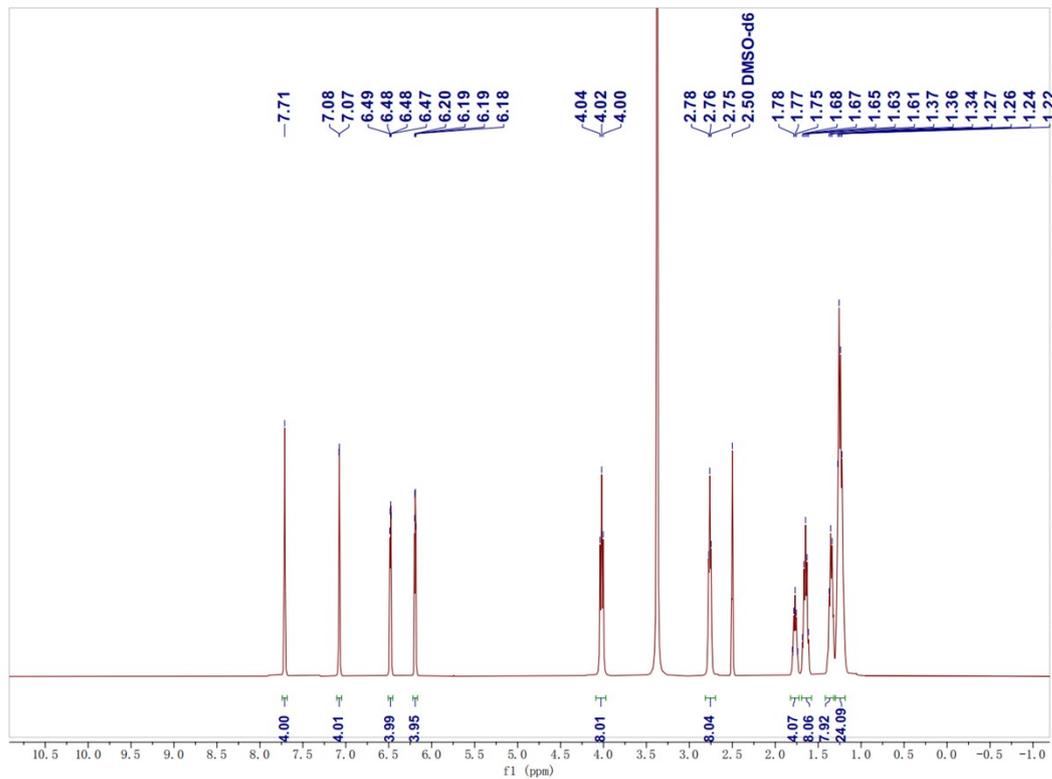


Fig.S3 $^1\text{H-NMR}$ spectrum of $[2](\text{BPC})[2](\text{C}_{12})$ dissolved in DMSO-d_6

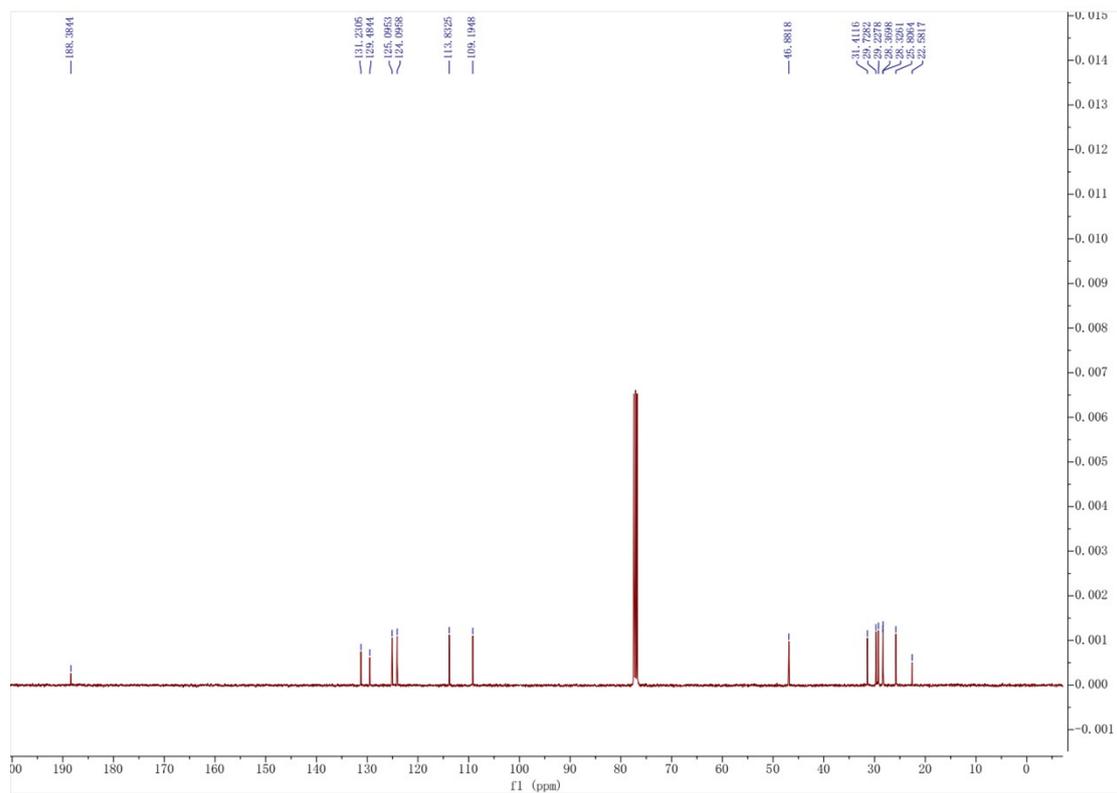


Fig.S4 ¹³C-NMR spectrum of [2](BPC)[2](C₁₂) dissolved in CDCl₃

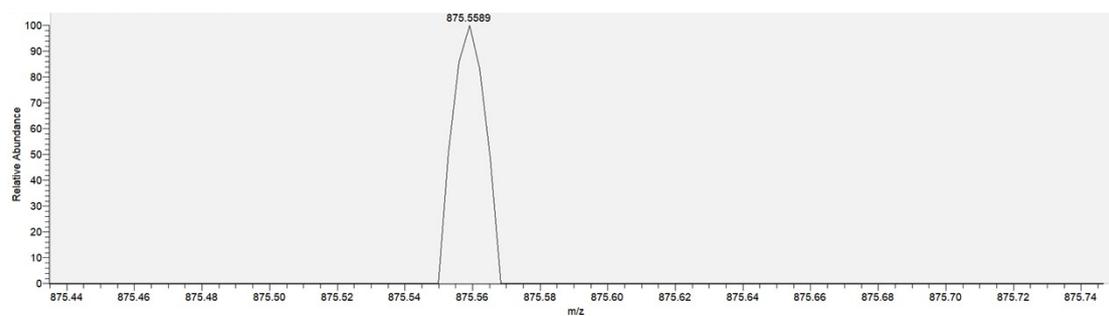
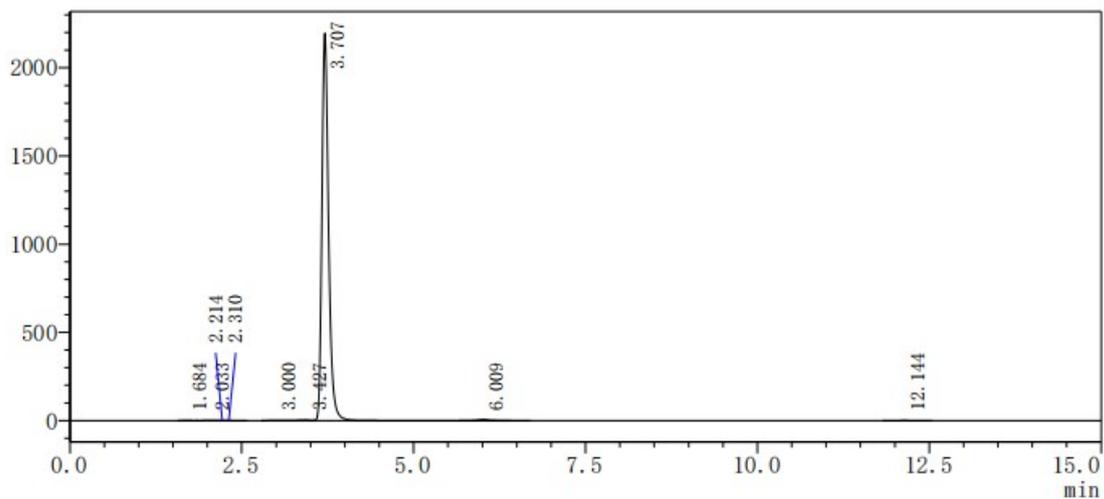


Fig.S5 HRMS spectrum of [2](BPC)[2](C₁₂)



254nm

No.	tR	Area	Height	Area (%)	Tailing Factor	Resolution (USP)
1	1.684	6295	764	0.042	--	--
2	2.033	11277	1370	0.076	--	1.703
3	2.214	3129	679	0.021	--	0.964
4	2.310	3439	488	0.023	--	0.423
5	3.000	6564	577	0.044	--	2.141
6	3.427	41628	3600	0.279	--	1.299
7	3.707	14791621	2196673	99.095	1.315	1.214
8	6.009	57253	6009	0.384	1.179	10.461
9	12.144	5493	312	0.037	1.119	16.740
总计		14926697	2210472	100.000		

Fig.S6 HPLC spectrum of [2](BPC)[2](C₁₂)

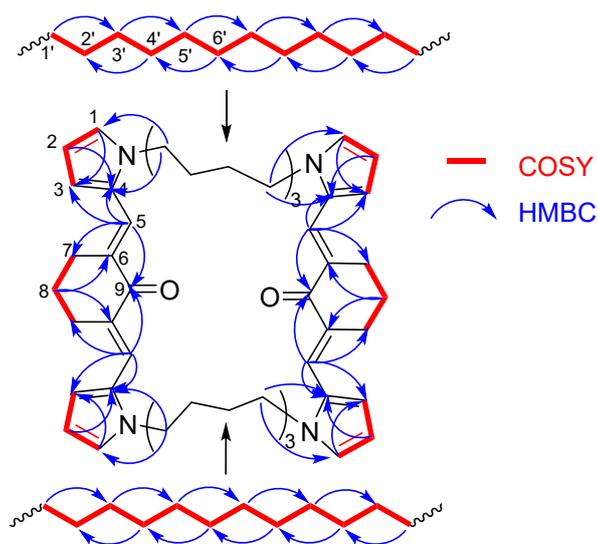


Fig.S7 Two-dimensional NMR correlation spectrum related to [2](BPC)[2](C₁₂)

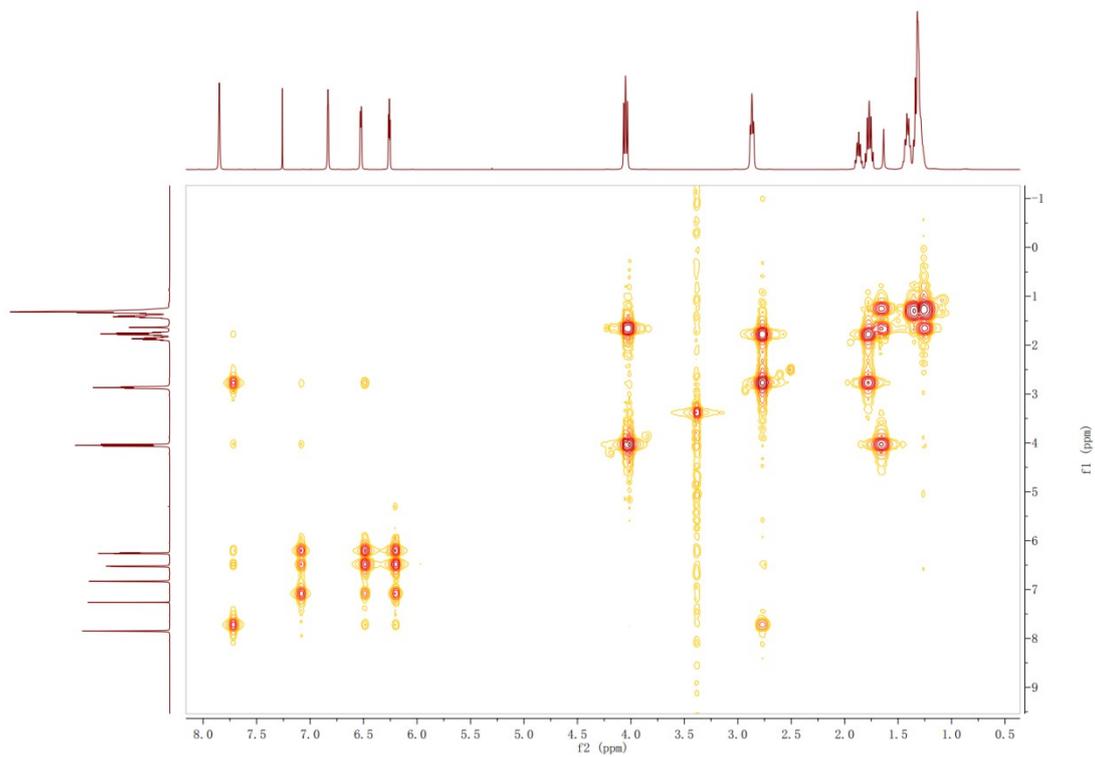


Fig.S8 ^1H - ^1H COSY spectrum of $[2](\text{BPC})[2](\text{C}_{12})$

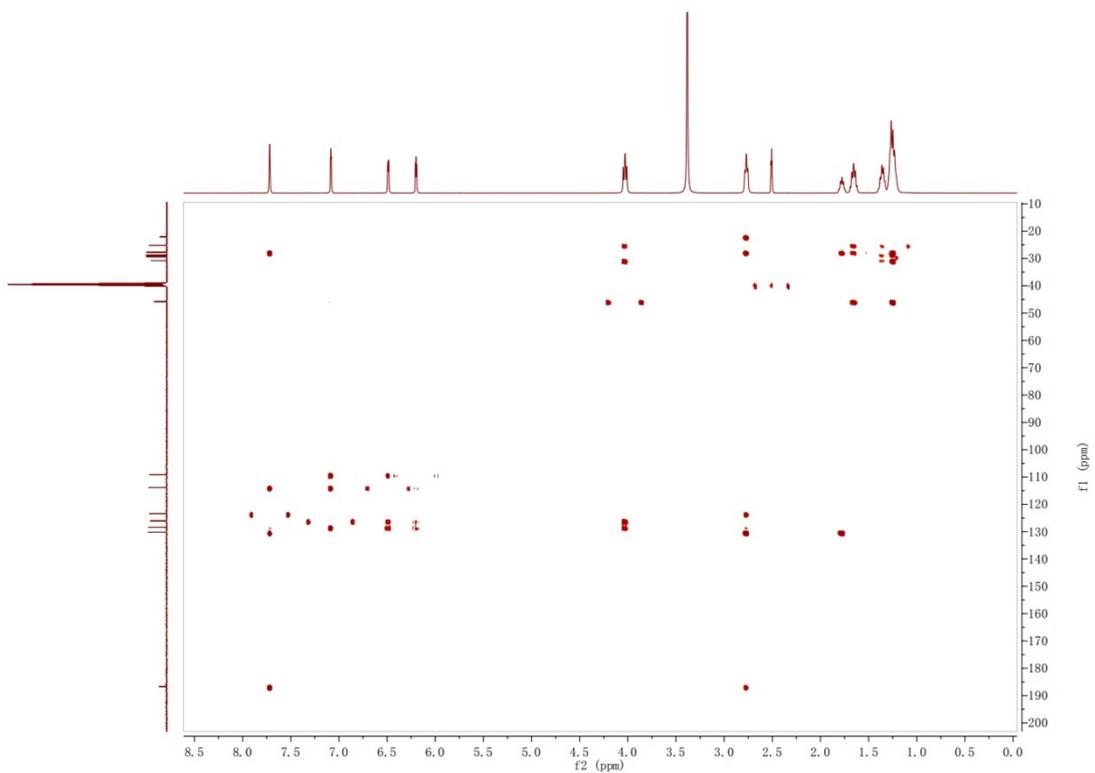


Fig.S9 ^1H - ^{13}C HMBC spectrum of $[2](\text{BPC})[2](\text{C}_{12})$

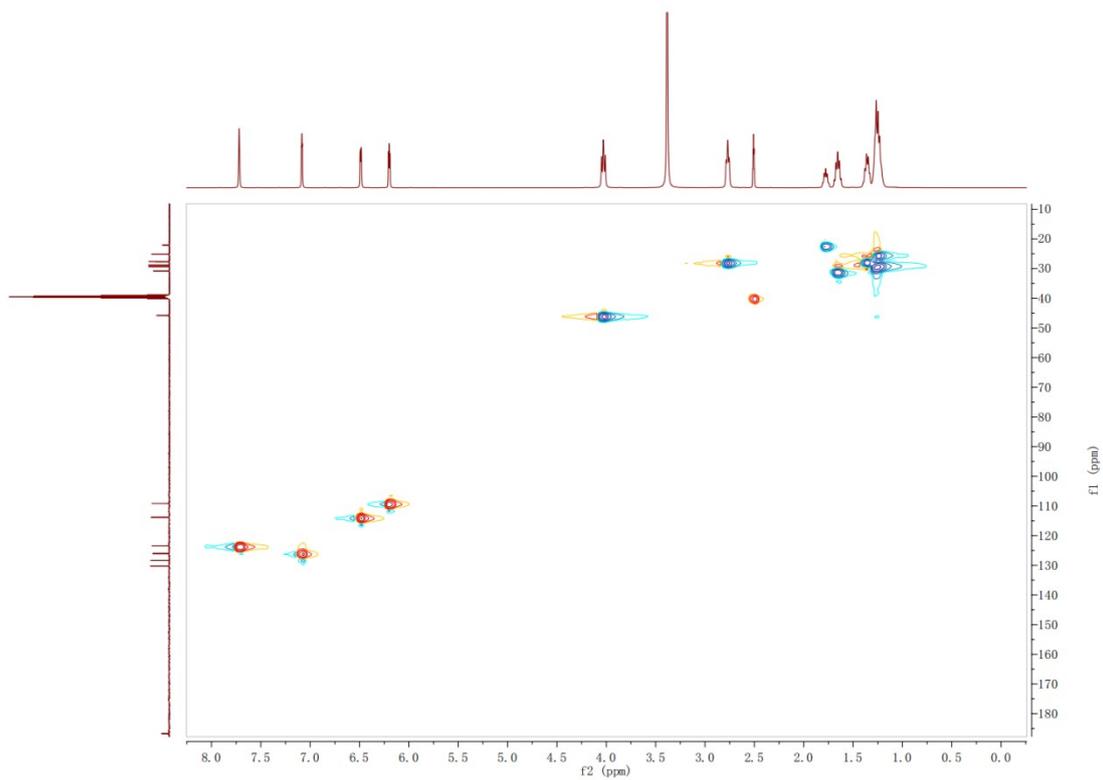


Fig.S10 ^1H - ^{13}C HSQC spectrum of $[2](\text{BPC})[2](\text{C}_{12})$

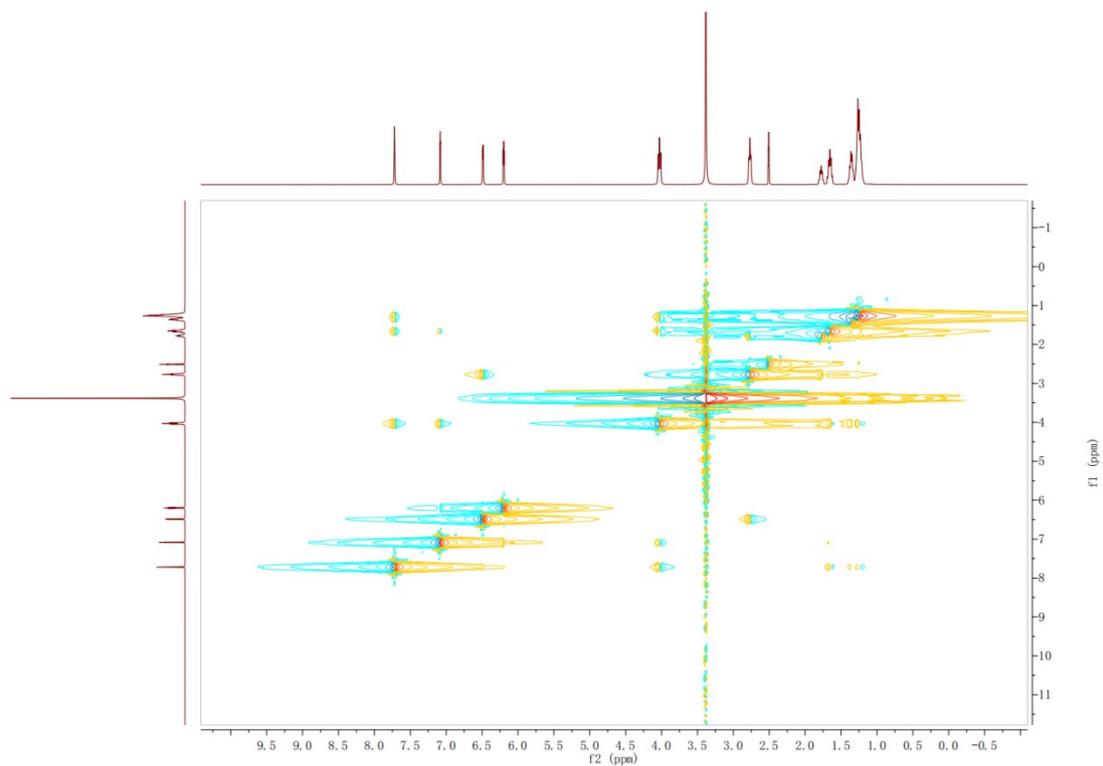


Fig.S11 ^1H - ^1H NOESY spectrum of $[2](\text{BPC})[2](\text{C}_{12})$

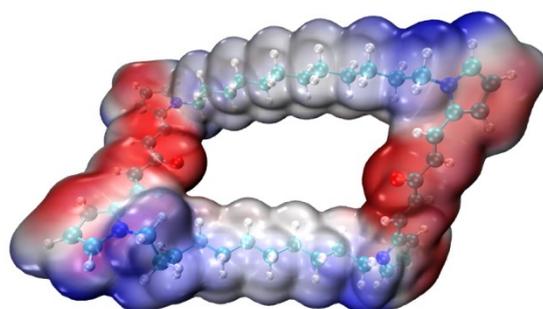


Fig.S12 Calculated molecular electrostatic potential map of the optimized macrocyclic photoinitiator [2](BPC)[2](C₁₂)

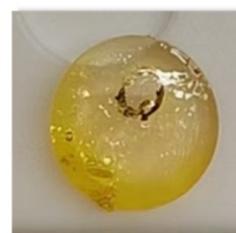
Ø 10 mm × 1 mm deep



TMPTA: 3g
PI: 60mg
Uncured(x)



TMPTA: 3g
PI: 10mg
Uncured(x)



TMPTA: 3g
PI: 1mg
Cured(✓)

Fig.S13 Effective curing achieved at an extremely low loading(1mg) of the macrocyclic photoinitiator [2](BPC)[2](C₁₂)

Table S1. Optimized Cartesian Coordinates (Å) for E,E,E,E-[2](BPC)[2](C₁₂) in
at the TD-B3LYP/6-31G(d,p) Level of Theory.

Atom	X	Y	Z
C	9.40449300	3.84678600	3.48458500
C	10.61676000	3.52630200	2.89441000
C	10.38189000	2.42970600	2.03907100
C	9.02505200	2.08991600	2.12600900
N	8.44934100	2.97693400	3.04049200
C	8.25162600	1.03446900	1.52639600
C	8.48922600	0.34220000	0.37805000
C	7.53013900	-0.75325300	0.05026500
C	7.69604500	-1.47921900	-1.24030800
C	6.91358700	-2.58507800	-1.40957900
C	6.87211800	-3.52249800	-2.49394000
C	7.65864800	-3.68082800	-3.64828400
C	7.18249700	-4.79802300	-4.35920800
C	6.11788000	-5.31418600	-3.63666800
N	5.93125100	-4.56112900	-2.51496800
O	6.62747300	-1.06496900	0.84801900
C	7.02353900	3.09113800	3.35566800
C	6.20155000	3.68991000	2.20692600
C	4.70639700	3.79286800	2.53401100
C	3.86873600	4.18782000	1.31073500
C	2.36320300	4.28788900	1.58827800
C	1.53508700	4.46757300	0.30944200
C	0.02303500	4.56846800	0.54898600
C	-0.79003400	4.52649100	-0.75126000
C	-2.30602900	4.63836000	-0.54457700
C	-3.10170200	4.37782500	-1.83010100
C	-4.61916400	4.51503600	-1.65143700
C	-5.37771300	4.04166600	-2.89899000
C	4.86572200	-4.82552200	-1.54487000
C	3.57619100	-4.02974600	-1.79135600
C	2.45855700	-4.47898900	-0.84077700
C	1.11703300	-3.76582000	-1.06126300
C	0.00416100	-4.33753200	-0.17253600
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C	-2.45824000	-4.36930000	0.47894000
C	-3.85635900	-3.74614500	0.34879900
C	-4.95798900	-4.55155100	1.06533300
C	-4.86402700	-4.55893000	2.60224700
C	-7.58326100	-4.00083000	4.23121700
C	-8.93590700	-3.78100000	4.02789900

C	-9.04711600	-2.85095900	2.97770500
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N	-6.86637700	-3.23871700	3.35432000
C	-7.28834700	-1.56788800	1.57065600
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C	-7.22945500	0.14232500	-0.14531300
C	-7.99606500	1.14363300	-0.94139900
C	-7.27560500	2.17444400	-1.46805100
C	-7.73241400	3.34410300	-2.16495000
C	-9.00489000	3.91640900	-2.32546000
C	-8.86312400	5.10956900	-3.06017500
C	-7.51379700	5.25204700	-3.34508600
N	-6.83100000	4.20011900	-2.80759800
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C	-5.39991200	-3.29522400	3.29802500
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H	7.34608000	0.74015000	2.05326000
H	6.23071500	-2.77494500	-0.58550900
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H	7.57262300	-5.19644300	-5.28599200
H	5.48274800	-6.16646600	-3.83517700
H	6.94544600	3.71356800	4.25188300
H	6.63975700	2.10051800	3.62239100
H	6.60366600	4.68109500	1.95942700
H	6.33512400	3.06488800	1.31494500
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H	4.55155100	4.51787000	3.34587400
H	4.23130800	5.14568100	0.90992400
H	4.03631700	3.44384800	0.51791300
H	2.02846800	3.37560800	2.10414500
H	2.16869100	5.12001900	2.28072500
H	1.87922600	5.36245100	-0.23002600
H	1.73408400	3.61625000	-0.35871200
H	-0.29785800	3.73870400	1.19630400
H	-0.20304500	5.49229100	1.10157400
H	-0.45390200	5.33038000	-1.42276800
H	-0.56877500	3.58336500	-1.27296700
H	-2.62310100	3.91648700	0.22233300
H	-2.55262600	5.63438200	-0.14901400
H	-2.76413400	5.06442300	-2.61992900
H	-2.86975900	3.36368000	-2.18739500
H	-4.94408100	3.93033900	-0.78142800

H	-4.88432000	5.55993100	-1.44453800
H	-5.05112500	4.61210200	-3.77370700
H	-5.15486400	2.99048700	-3.10598600
H	4.65333100	-5.89756800	-1.60226000
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H	3.77355600	-2.95674500	-1.67047000
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H	2.30737400	-5.56205800	-0.96020000
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H	1.23384300	-2.68956900	-0.86860400
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H	-6.20345000	2.09507300	-1.30931100
H	-9.92516200	3.52433100	-1.91999900
H	-9.64898600	5.79161500	-3.35542100
H	-6.99020000	6.01920100	-3.89866700
H	-5.04376600	-3.26562400	4.33242800
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H	10.48163200	-0.00166300	-0.38756900
C	9.15622600	0.44495100	-2.03259200
C	8.69705800	-0.99586900	-2.26745600
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H	9.57872400	-1.65733900	-2.26905200
H	8.25867900	-1.08072500	-3.26944500
H	8.33097400	1.13671100	-2.24898300
C	-9.49112600	0.98703800	-1.10041600
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H	-9.79390300	1.36494800	-2.08410200
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H	-9.75052200	-2.08609200	0.48605000
H	-10.05036500	-0.51531000	1.20867300

Table S2. Optimized Cartesian Coordinates (Å) for E,Z,E,Z-[2](BPC)[2](C₁₂) in
at the TD-B3LYP/6-31G(d,p) Level of Theory.

Atom	X	Y	Z
C	-6.21496500	-3.46116000	3.18970900
C	-6.81412600	-3.39047400	4.43504900
C	-8.15026300	-2.98937800	4.21933500
C	-8.32712800	-2.77837900	2.85055600
N	-7.11384900	-3.07304200	2.22864300
C	-9.59398000	-2.45473100	2.21493400
C	-9.95942400	-1.60408600	1.21466200
C	-9.06347300	-0.52804000	0.70312900
C	-9.59375000	0.41031700	-0.33023400
C	-8.72698100	1.37083200	-0.76221500
C	-8.89961100	2.35685800	-1.79113200
C	-9.80639700	2.46279300	-2.85775100
C	-9.47724300	3.61112200	-3.60374000
C	-8.38373800	4.19700100	-2.98401900
N	-8.02887500	3.44600000	-1.90160000
O	-7.92169900	-0.38251300	1.16850700
C	8.22341100	4.78228200	0.92897700
C	9.32506900	5.28378400	1.60174800
C	9.90878100	4.19889300	2.28730400
C	9.18028000	3.04476800	1.97752500
N	8.12889700	3.43407600	1.15485600
C	9.52911400	1.72450400	2.46579800
C	9.55419200	0.46651400	1.93806500
C	9.29290800	0.15783200	0.50578600
C	9.29264700	-1.27188600	0.07004200
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C	8.76739200	-2.77109400	-1.88694400
C	9.62871700	-3.87447400	-1.85223400
C	9.21150000	-4.78965000	-2.84198400
C	8.09712100	-4.24132200	-3.45526400
N	7.83720900	-3.01884900	-2.89998600
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C	10.04067500	-0.66391000	2.83880700
C	9.42314100	-2.01287700	2.47118800
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C	-6.91280900	-3.28500700	0.78783600
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C	0.55849000	3.10824500	0.57058500
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H	-9.97599500	3.97924100	-4.49009700
H	-7.83979200	5.09953000	-3.22638200
H	7.48848200	5.29289900	0.32394200
H	9.65759900	6.31330300	1.59489000
H	10.79674700	4.21618700	2.90654700
H	9.93146700	1.78581000	3.47876600
H	8.40622100	-0.64985300	-1.69958200
H	10.50305800	-3.96030800	-1.22244700
H	9.67510300	-5.73356100	-3.09548200
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H	9.30823800	-3.31253000	0.72843800
H	10.84783700	-2.49353600	0.93255300
H	9.83444000	-0.41696500	3.88588900
H	11.13559700	-0.75487000	2.75269000
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H -7.86665200	-3.06503300	0.30851700
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H -0.88621000	-0.88641000	-1.05222900
H 0.60220100	-3.56235600	-0.84894900
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H 1.36477500	-2.15264200	-2.80357700
H 1.67259900	-0.81513500	-1.70219800
H 2.99441100	-3.57838800	-1.51746300
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H 3.83231400	-2.22624100	-3.48079400
H 4.23992600	-0.91065900	-2.38389100
H 5.36699000	-3.76394100	-2.20102600
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H 6.80899800	-1.20326500	-3.07777700
H 6.29323600	-2.48322100	-4.17023600
H 7.01367600	2.47358600	-0.33329500
H 7.09576200	1.64037700	1.20958600
H 5.55990700	4.26294300	0.79244600
H 5.58401700	3.29559900	2.26204000
H 4.53770300	2.34893100	-0.46911000
H 4.46541700	1.40875300	1.01607400
H 3.12128400	4.14280000	0.65278100
H 2.94134400	3.08538400	2.04520600
H 2.06102900	2.40961800	-0.81661400
H 1.83593100	1.35756500	0.57498300
H 0.65451300	4.18036400	0.34241200
H 0.34703600	3.04475900	1.64826000
H -0.40849600	2.60914700	-1.29474100
H -0.73492900	1.46591100	0.00134300

H	-1.82041300	4.33491700	-0.08496900
H	-2.20446600	3.13212500	1.13820900
H	-2.87439300	2.90390900	-1.84884400
H	-3.25544400	1.67999500	-0.64430600
H	-4.29457400	4.56649400	-0.56926200
H	-4.71424200	3.29860100	0.57498600
H	-5.35578200	3.26908400	-2.43155400
H	-5.74618400	1.96424000	-1.31531500
H	-6.76015300	4.85359600	-1.07445300
H	-7.19693300	3.54340400	0.01112500

Table S3. Optimized Cartesian Coordinates (Å) for E,E,E,E-[2](BPC-OH)[2](C₁₂) in
at the TD-B3LYP/6-31G(d,p) Level of Theory.

Atom	X	Y	Z
C	9.20864200	-5.01262100	-2.48179900
C	10.53512000	-4.85021800	-2.13593100
C	10.71231700	-3.48350600	-1.80535300
C	9.48510500	-2.83500900	-1.95126000
N	8.57508700	-3.79772700	-2.38406100
C	9.09470100	-1.43697600	-1.80913100
C	9.64021800	-0.49469100	-1.01261300
C	9.17593000	0.95898400	-1.09833200
C	8.87686300	1.50181000	0.29768400
C	7.66187600	1.98342600	0.62267900
C	7.22425000	2.46729000	1.93136300
C	7.46492600	1.98981800	3.21660200
C	6.77783400	2.82741500	4.13053500
C	6.13293600	3.79672100	3.38783100
N	6.38833800	3.57374300	2.05407100
O	8.09345600	1.07897500	-2.01115000
C	7.14509300	-3.61333600	-2.62665700
C	6.29742500	-3.52629400	-1.35020300
C	4.79664400	-3.54663500	-1.66731200
C	3.90067800	-3.37238300	-0.43382800
C	2.41222700	-3.57520700	-0.74645400
C	1.48002200	-3.29494100	0.43948500
C	0.01621100	-3.65305500	0.15001800
C	-0.95608700	-3.25272500	1.26721100
C	-2.39094800	-3.73728100	1.02004400
C	-3.40420000	-3.21061000	2.04465400
C	-4.80943600	-3.79660400	1.85368500
C	-5.84573800	-3.13277900	2.77131800
C	-9.22909300	4.82593100	-1.74541900
C	-10.46389700	4.44104600	-1.26220400
C	-10.42450700	3.03498600	-1.09340800
C	-9.15790100	2.58312200	-1.47564600
N	-8.43965000	3.71078100	-1.87721000
C	-8.54768500	1.26490800	-1.50407600
C	-9.14521300	0.06271600	-1.36875300
C	-8.32174200	-1.21963800	-1.41796800
C	-8.78035900	-2.17488300	-0.31561100
C	-7.91072500	-2.60644800	0.62122800
C	-8.14346600	-3.53389900	1.71423700
C	-9.21883500	-4.36818300	2.03463600
C	-8.89153800	-5.08090000	3.21400700

C	-7.62899600	-4.67326200	3.59641100
N	-7.17462400	-3.74072800	2.69765600
O	-6.93464000	-0.91165200	-1.37589500
C	-10.25025900	-2.53461300	-0.38055500
C	-10.63281000	-0.15696600	-1.17701800
C	-11.03361600	-1.62945100	-1.34952900
C	10.75517500	-0.72774700	-0.01574400
C	10.07047700	1.39372600	1.21112900
C	10.47987900	-0.08253200	1.35763800
C	-7.04314600	3.76009000	-2.31035900
C	-6.04580300	3.84997300	-1.14706500
C	-4.59173800	3.93944200	-1.62731000
C	-3.58865200	4.08064700	-0.47496200
C	-2.12989500	4.18975100	-0.93787100
C	-1.14244200	4.38869400	0.21932500
C	0.31842600	4.53178200	-0.22781800
C	1.28047600	4.80170300	0.93633500
C	2.74155600	4.99150200	0.50699200
C	3.65980300	5.35534800	1.68305800
C	5.12385400	5.62966200	1.28847700
C	5.96998300	4.40741300	0.91613300
H	8.65986700	-5.89058500	-2.79342400
H	11.29195400	-5.62368300	-2.13698500
H	11.64519900	-3.00457400	-1.54310100
H	8.27696500	-1.11176200	-2.44711100
H	10.03837500	1.53777700	-1.48262500
H	6.91594600	2.00705500	-0.17059700
H	8.04190700	1.10613400	3.45445800
H	6.74626200	2.73259000	5.20813000
H	5.52044600	4.62235400	3.71291600
H	7.96824600	2.02557400	-2.18293700
H	6.81965500	-4.46557100	-3.23159600
H	6.99896000	-2.71801700	-3.24056000
H	6.55029100	-4.37303400	-0.69845100
H	6.55855200	-2.61283000	-0.80050000
H	4.56299800	-2.75608100	-2.39553200
H	4.55096500	-4.49816500	-2.16160900
H	4.20611100	-4.08635500	0.34511800
H	4.05768500	-2.37010300	-0.00921800
H	2.12476200	-2.92839200	-1.58875500
H	2.25945400	-4.60852200	-1.09215800
H	1.82290900	-3.86046600	1.31865800
H	1.55216200	-2.23191600	0.71343700
H	-0.29842600	-3.17012400	-0.78720900

H	-0.05825700	-4.73632700	-0.02756100
H	-0.59956700	-3.65377700	2.22753400
H	-0.95183000	-2.15774400	1.37349400
H	-2.71083500	-3.43135000	0.01298100
H	-2.40507600	-4.83712500	1.02288200
H	-3.05244500	-3.43604900	3.06189700
H	-3.44972100	-2.11399400	1.97233900
H	-5.12118800	-3.68002500	0.80757500
H	-4.79494300	-4.87539400	2.05730600
H	-5.52121800	-3.20715900	3.81399500
H	-5.93137100	-2.06533100	2.54355300
H	-8.84625500	5.80067500	-2.01479100
H	-11.30044800	5.09729100	-1.06070500
H	-11.22500000	2.41834600	-0.71372800
H	-7.47316300	1.24485400	-1.65315100
H	-8.54100900	-1.71332900	-2.38343900
H	-6.90345100	-2.20651600	0.55069600
H	-10.13215600	-4.46480700	1.46756300
H	-9.50921700	-5.80466700	3.72940700
H	-7.01607300	-4.96326500	4.43860800
H	-6.45557800	-1.71934300	-1.62122500
H	-10.68131200	-2.44898500	0.62695600
H	-10.38096500	-3.58785300	-0.67065100
H	-11.19620500	0.47707200	-1.87420600
H	-10.93000200	0.17324400	-0.16870300
H	-10.85497400	-1.94009400	-2.38679400
H	-12.10846900	-1.74709400	-1.17410500
H	10.92367500	-1.79953900	0.11175700
H	11.69351300	-0.30839400	-0.41418900
H	9.86857500	1.84692100	2.18431900
H	10.91391100	1.94381800	0.76318500
H	11.37312900	-0.16935500	1.98814600
H	9.67343200	-0.63127700	1.86164900
H	-6.93934500	4.63627100	-2.95835900
H	-6.83578800	2.88327300	-2.93112900
H	-6.29318900	4.73224800	-0.54167400
H	-6.16897300	2.97667900	-0.49318900
H	-4.34579800	3.04617000	-2.21989400
H	-4.48487700	4.79764700	-2.30700900
H	-3.84616900	4.97106700	0.11741600
H	-3.69203700	3.22199800	0.20462900
H	-1.85666100	3.28635100	-1.50300700
H	-2.03559500	5.03037400	-1.64140200
H	-1.43278200	5.28553700	0.78683400

H	-1.22748300	3.54511300	0.92040800
H	0.63047600	3.62118700	-0.76038700
H	0.39459500	5.35294700	-0.95614300
H	0.94670100	5.70227500	1.47323700
H	1.21830900	3.97606900	1.66066700
H	3.09678000	4.07513800	0.01435600
H	2.79635800	5.78801600	-0.24991300
H	3.26324300	6.25936900	2.16512300
H	3.61012100	4.56188100	2.43991500
H	5.13104700	6.29113000	0.41247400
H	5.63335200	6.18725200	2.08369700
H	5.42050200	3.77547500	0.20842900
H	6.87636600	4.74363200	0.39997300