

# Computational Exploration of Panchromatic Dye-Sensitized Solar Cells with Broad Visible to Near-Infrared Absorption: A Density Functional Theory Study

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Electronic Supplementary Information:

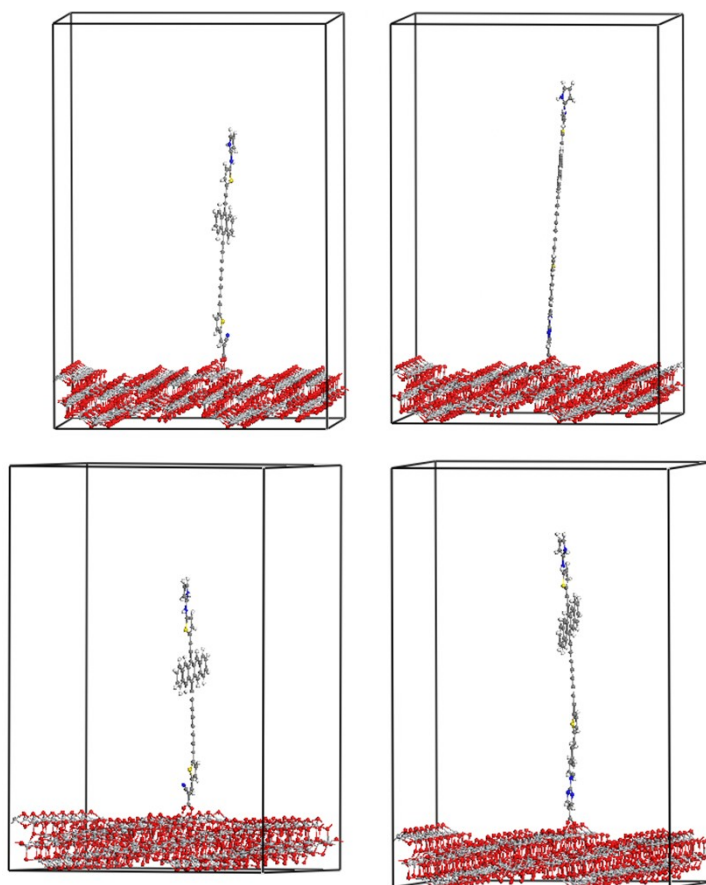


Figure 1: Geometries of bidentate binding mode of investigated dyes on TiO<sub>2</sub>

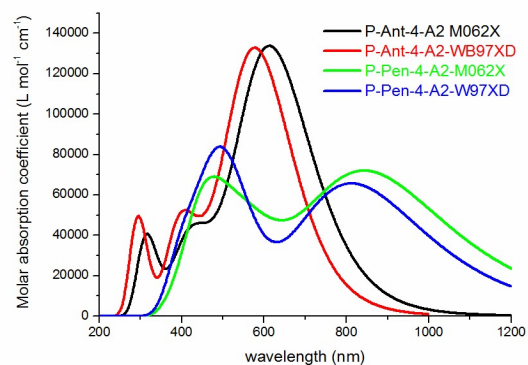


Figure 2: absorption spectra of dyes in acetonitrile at TD-M062X/6-311+G(2d,p)/SMD and level. The spectra are Gaussian broadened with 0.35 eV (half width half maximum).

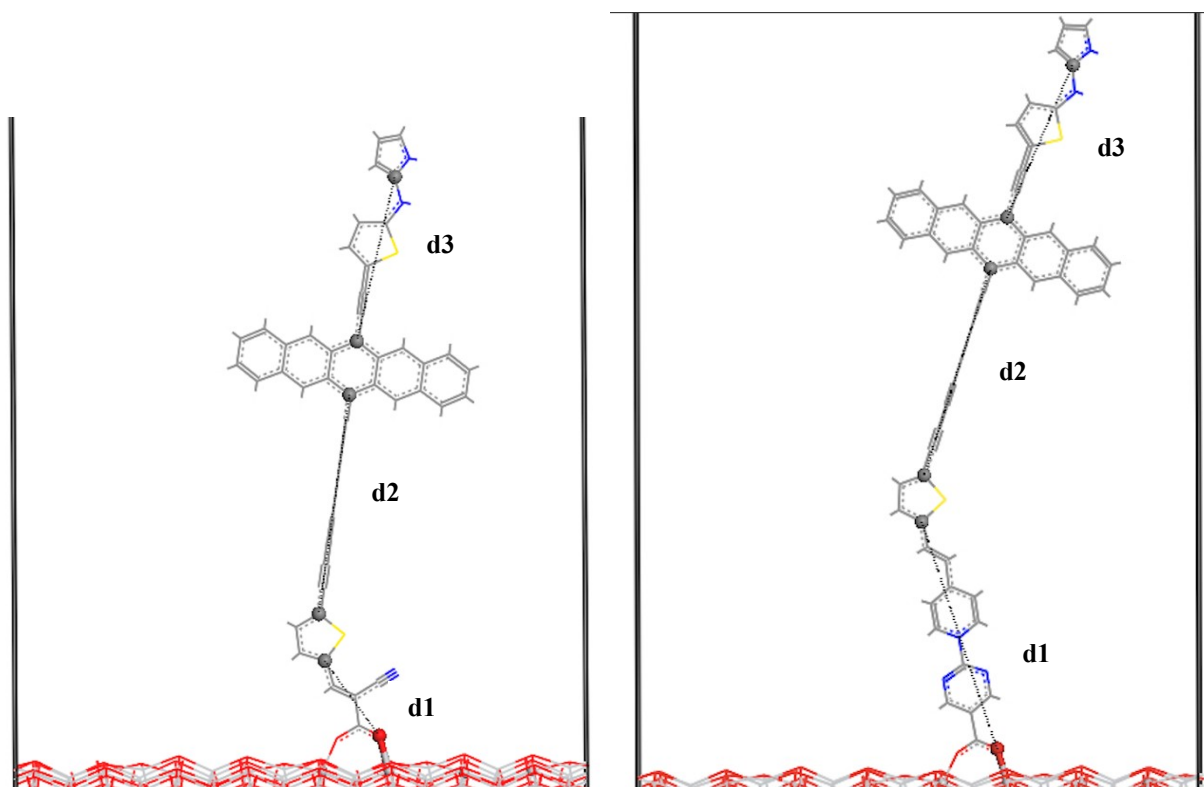


Figure 3: The distances d1, d2, and d3 evaluated during MD simulations are presented above. In brief, d1 represents the distance between the surface and the acceptor (A1 and A2), d2 indicates the distance of the polyynic bridge, and d3 denotes the distance from the acene to the donor.

## Optimized geometries of Dyes

### P-Ant-2-A1

C	1.76861800	-0.76654200	-0.03868100
C	0.33861500	-0.69615300	-0.03655600
C	-0.30899600	0.57217500	-0.04338700
C	0.46100400	1.77082400	-0.05398700
C	1.89091500	1.70002500	-0.05640400
C	2.54053300	0.43148100	-0.04789400
C	2.63421600	2.91305800	-0.06639200
C	2.00842600	4.12947200	-0.07443800
C	0.59505300	4.19913000	-0.07243700
C	-0.15345400	3.05365200	-0.06226900
C	2.38810000	-2.04715900	-0.03107800
C	1.64489000	-3.19558000	-0.02193600
C	0.23138900	-3.12552800	-0.02005200
C	-0.40019000	-1.91162600	-0.02725700
H	3.71525300	2.86092500	-0.06776500
H	-1.23407300	3.11561000	-0.06052900
H	3.46902500	-2.10295700	-0.03281400
H	-1.48181800	-1.86546500	-0.02578500
C	-1.71055200	0.64646900	-0.03750400
C	-2.92774800	0.72992900	-0.03069000
C	-4.27079300	0.83789400	-0.02157000
C	-5.48462800	0.95398600	-0.01286700
C	3.94442700	0.36123900	-0.04810000
C	5.16071800	0.30771800	-0.04690800
C	6.54752500	0.23245600	-0.04339800
C	7.47958400	1.25102500	-0.08639300
S	7.37805800	-1.33274200	0.01971800
C	8.81806800	0.82566300	-0.07649400
H	7.18574800	2.29158300	-0.13064500
C	8.94740600	-0.55269900	-0.03376900
H	9.65911300	1.50000100	-0.11763000
C	11.38683800	-0.87736100	0.09310300
C	11.95290100	0.23320900	0.69016500
C	13.36305100	0.12017300	0.51248800
H	11.42844800	1.01594500	1.21205000
C	13.60933200	-1.04451800	-0.17314300
H	14.10819700	0.81896100	0.86050100
H	14.52930800	-1.50035300	-0.49984900
N	10.07079600	-1.32420400	-0.02639100
H	9.95228200	-2.32659900	-0.09791100
H	12.26667100	-2.50325800	-0.94026500
N	12.39742400	-1.63973500	-0.43186300
C	-6.86942500	1.08969500	-0.00269600
C	-7.60973300	2.26633500	-0.00516800
S	-7.91138600	-0.31478700	0.01526500
C	-8.98485800	2.04149100	0.00710800
H	-7.14594800	3.24242400	-0.01557300

C	-9.34597900	0.69712100	0.01909700
H	-9.72792900	2.82842300	0.00751300
C	-10.69424400	0.26280600	0.03257600
H	-11.40622700	1.08059400	0.03394700
C	-11.23718900	-0.99309600	0.04360100
H	2.59281400	5.04176500	-0.08237300
H	0.10451400	5.16536600	-0.07903000
H	2.13636900	-4.16112500	-0.01613300
H	-0.35191300	-4.03875500	-0.01285700
C	-10.45090600	-2.17686600	0.04131800
N	-9.80124700	-3.13152200	0.03846800
C	-12.69536100	-1.22006800	0.05811100
O	-13.20669900	-2.32064400	0.06812700
O	-13.41611100	-0.08218600	0.05922600
H	-14.35823300	-0.33072300	0.06850300

#### P-Ant-4-A1

C	3.80906400	-0.84949100	-0.08649700
C	2.37954300	-0.77822600	-0.08635300
C	1.73255900	0.49200300	-0.08829400
C	2.50359200	1.69099900	-0.09456400
C	3.93308900	1.61859000	-0.09494600
C	4.58173000	0.34873900	-0.08870900
C	4.67765200	2.83045400	-0.10029100
C	4.05308400	4.04769500	-0.10521600
C	2.64006500	4.11871900	-0.10472300
C	1.89020000	2.97374200	-0.09947700
C	4.42827400	-2.12997400	-0.08349600
C	3.68470400	-3.27840200	-0.08086600
C	2.27163000	-3.20727100	-0.08071800
C	1.64042200	-1.99284000	-0.08325100
H	5.75859400	2.77729800	-0.10067600
H	0.80953300	3.03681100	-0.09912700
H	5.50919200	-2.18589700	-0.08366900
H	0.55884600	-1.94690400	-0.08322000
C	0.33373000	0.56301500	-0.08122000
C	-0.88749000	0.62787400	-0.06756000
C	-2.22505800	0.70139700	-0.06345900
C	-3.45049300	0.77057000	-0.04422200
C	5.98445800	0.27828400	-0.08211100
C	7.20115600	0.22740200	-0.06996600
C	8.58702800	0.15578500	-0.05075300
C	9.51653000	1.17863800	-0.06039500
S	9.42209300	-1.40767800	-0.00365900
C	10.85524200	0.75770300	-0.03667000
H	9.21902000	2.21863500	-0.08954400
C	10.98860100	-0.62144200	-0.01707300
H	11.69548600	1.43417500	-0.05049100
C	13.42445500	-0.92995800	0.15677400
C	13.96369600	0.15904600	0.81423100

C	15.37776400	0.07514400	0.65449300
H	13.41803900	0.90990000	1.36075500
C	15.65235000	-1.05302800	-0.08025300
H	16.10682100	0.76775200	1.04615100
H	16.58436800	-1.48036200	-0.41131800
N	12.11564700	-1.38632900	-0.00437100
H	12.00604900	-2.38865200	-0.09166300
H	14.34379000	-2.49420500	-0.93514700
N	14.45418400	-1.65314600	-0.38582000
C	-9.95395300	1.16056800	0.02455300
C	-10.74333200	2.30305800	0.03522500
S	-10.93184800	-0.28891100	0.03267100
C	-12.10829600	2.01689300	0.04957200
H	-10.32297200	3.29870100	0.03241500
C	-12.40682500	0.65822200	0.05010600
H	-12.88545800	2.77000700	0.05946800
C	-13.73692200	0.16110800	0.06291000
H	-14.48590000	0.94506600	0.07460500
C	-14.21761500	-1.11748600	0.06232300
C	-4.78442000	0.84777100	-0.03322900
C	-6.00860500	0.92150000	-0.01959200
C	-7.34707300	1.00209800	-0.00494400
C	-8.56481900	1.08165600	0.00894900
H	4.63865200	4.95919700	-0.10948600
H	2.15033000	5.08533900	-0.10861400
H	4.17576400	-4.24411500	-0.07893600
H	1.68735200	-4.11986800	-0.07870200
C	-13.37545500	-2.26279300	0.04686500
N	-12.68214400	-3.18572300	0.03409000
C	-15.66530400	-1.41495100	0.07726300
O	-16.12133800	-2.53888700	0.07574800
O	-16.43709700	-0.31300200	0.09279500
H	-17.36750200	-0.60280500	0.10086400

### **P-Ant-2-A2**

C	-8.84344600	0.23872300	0.08180900
C	-9.91655400	1.16096500	0.05271600
C	-9.19973600	-1.12946200	0.08782300
C	-11.20872200	0.73137200	0.02554900
H	-9.74571200	2.22766900	0.05012500
C	-10.50508900	-1.52214400	0.06108600
H	-8.43361100	-1.89303900	0.11193700
H	-12.04890600	1.40594600	0.00223000
H	-10.80772700	-2.55632600	0.06311600
N	-11.51324500	-0.60209000	0.02704900
C	-12.88666100	-1.03240300	-0.01277200
C	-15.06904300	-0.47928100	-0.11814700
C	-14.35768800	-2.73814500	-0.04550000
C	-15.41163000	-1.82936500	-0.11464800
H	-15.82348400	0.29655300	-0.16232700

H	-14.54341100	-3.80554200	-0.03258700
N	-13.08977300	-2.34131800	0.00320500
N	-13.80047500	-0.07772700	-0.06379600
C	-16.80911800	-2.32284400	-0.17775200
O	-17.11410000	-3.49226500	-0.12669700
C	5.14895800	-0.50474700	0.09261700
C	3.75339200	-0.18677900	0.13707800
C	3.33205400	1.17171500	0.06198900
C	4.29420800	2.21517000	-0.05303300
C	5.68968700	1.89683000	-0.09816900
C	6.11279900	0.53774500	-0.02509200
C	6.62774200	2.95999200	-0.21429800
C	6.21951400	4.26382900	-0.28122400
C	4.84040800	4.57811900	-0.23570500
C	3.90832300	3.58241600	-0.12512000
C	5.54006500	-1.87058600	0.16652500
C	4.61269000	-2.86993300	0.27887000
C	3.23354100	-2.55533700	0.32362700
C	2.81933700	-1.25306500	0.25475300
H	7.68296500	2.72230700	-0.24754000
H	2.85515300	3.83054800	-0.08987200
H	6.59455500	-2.11279200	0.13156900
H	1.76262400	-1.02102000	0.28847900
C	1.96244000	1.47959000	0.09236300
C	0.76980800	1.73627700	0.10979700
C	-0.55068900	2.00579800	0.11951000
C	-1.74604700	2.24824000	0.12213600
C	7.48395500	0.22964300	-0.06433100
C	8.67662300	-0.01322000	-0.09138600
C	10.03858600	-0.28466500	-0.11717900
C	11.09832600	0.59399400	-0.23382300
S	10.65175100	-1.94357700	0.01216200
C	12.36661500	-0.00864800	-0.22961700
H	10.94544900	1.66129800	-0.32600800
C	12.30935100	-1.38760100	-0.11645000
H	13.29112800	0.53993100	-0.32239900
C	14.68430100	-2.02072000	0.00788100
C	15.38945700	-0.99744600	0.61139300
C	16.77225400	-1.27548300	0.40477400
H	14.96988000	-0.16535800	1.15208200
C	16.86446800	-2.44994500	-0.30269600
H	17.60240200	-0.67775900	0.74864100
H	17.71750100	-3.00797400	-0.65181700
N	13.32062300	-2.30072400	-0.08990400
H	13.07129100	-3.28109600	-0.11101200
H	15.34166900	-3.71904500	-1.07175700
N	15.58581200	-2.89084600	-0.54672500
C	-3.11524000	2.49377500	0.11720400
C	-3.77266800	3.71642400	0.10005200
S	-4.26301400	1.16872300	0.12495800
C	-5.16497300	3.59089400	0.09219600

H	-3.24106900	4.65763200	0.09274300
C	-5.61777100	2.27857900	0.10332000
H	-5.84833000	4.43007200	0.07815400
C	-6.98345800	1.87841700	0.09299500
H	-7.68012400	2.71081000	0.07416400
C	-7.45719400	0.60333300	0.10157200
H	-6.76174900	-0.23009700	0.12076200
H	6.95080900	5.05854000	-0.36834200
H	4.52292000	5.61289300	-0.28814200
H	4.93142300	-3.90402300	0.33329000
H	2.50322400	-3.35104800	0.41235000
O	-17.70491800	-1.32991300	-0.30029800
H	-18.59617200	-1.72519600	-0.33077200

**P-Ant-4-A2**

C	-11.61202000	0.15994700	-0.03432800
C	-12.69654900	1.06694500	-0.02181400
C	-11.94613300	-1.21234200	-0.03734200
C	-13.98332500	0.61802600	-0.00859600
H	-12.54073100	2.13600400	-0.02034300
C	-13.24676900	-1.62440300	-0.02393000
H	-11.16827700	-1.96418200	-0.04975800
H	-14.83414800	1.27930600	0.00332700
H	-13.53465200	-2.66286200	-0.02524400
N	-14.26634600	-0.71871100	-0.00766500
C	-15.63545300	-1.16828500	0.01396600
C	-17.82639400	-0.64191400	0.01722100
C	-17.08379800	-2.89083400	0.07822900
C	-18.15110000	-1.99562500	0.06232600
H	-18.59168700	0.12425200	0.00001500
H	-17.25470800	-3.96026900	0.11196300
N	-15.81991200	-2.47828000	0.05391500
N	-16.56174600	-0.22515800	-0.00696000
C	-19.54415000	-2.50519100	0.09737300
O	-19.83200800	-3.67861600	0.15274700
C	7.58599100	-0.77741000	-0.03233100
C	6.17103500	-0.56161500	-0.03575100
C	5.65604700	0.76735000	-0.02190000
C	6.54422400	1.88188200	-0.00357900
C	7.95914000	1.66497700	-0.00033800
C	8.47581800	0.33625600	-0.01519400
C	8.82247900	2.79520600	0.01792100
C	8.32442800	4.06932000	0.03226800
C	6.92587000	4.28319900	0.02912200
C	6.06399200	3.22018000	0.01170700
C	8.07210900	-2.11405400	-0.04658300
C	7.21609600	-3.18112700	-0.06316000
C	5.81750600	-2.96715500	-0.06652000
C	5.31272400	-1.69512100	-0.05326300
H	9.89250500	2.63308200	0.02057300

H	4.99539100	3.39307600	0.00957500
H	9.14167200	-2.27978100	-0.04410600
H	4.24138400	-1.53986100	-0.05600100
C	4.27083200	0.97776600	-0.02644500
C	3.06153000	1.15941800	-0.03495900
C	1.73620000	1.35683600	-0.03082900
C	0.52203400	1.53699500	-0.04079100
C	9.86449500	0.12413200	-0.01351500
C	11.06965900	-0.05049500	-0.01375300
C	12.44110600	-0.26454300	-0.01457200
C	13.47092400	0.65702700	-0.02652400
S	13.11093200	-1.90625300	-0.00754500
C	14.75950400	0.10012100	-0.03836900
H	13.28169100	1.72246900	-0.03415400
C	14.74932000	-1.28529600	-0.04551600
H	15.66455900	0.68687700	-0.06109600
C	17.14102900	-1.85987000	0.07672100
C	17.80608700	-0.84940800	0.74441900
C	19.20001300	-1.08844600	0.56482900
H	17.35425600	-0.05224300	1.31070900
C	19.33822300	-2.22726500	-0.19141600
H	20.00649900	-0.48873700	0.95795000
H	20.21271400	-2.75045000	-0.54134500
N	15.78828800	-2.16546100	-0.07356900
H	15.56776900	-3.14645500	-0.18829100
H	17.86686500	-3.49731000	-1.05320300
N	18.07677000	-2.68438900	-0.49073100
C	-5.91943000	2.51691100	-0.03903600
C	-6.60006100	3.72579700	-0.03154100
S	-7.03935000	1.16819800	-0.04520700
C	-7.99012100	3.57171500	-0.03033400
H	-6.08708500	4.67724600	-0.02680300
C	-8.41364900	2.25067300	-0.03708700
H	-8.68999400	4.39714100	-0.02448200
C	-9.77527600	1.82538200	-0.03538100
H	-10.48458600	2.64696200	-0.02691800
C	-10.22777900	0.54533400	-0.04169500
H	-9.52128300	-0.27879500	-0.05035700
C	-0.79992200	1.73348000	-0.03975100
C	-2.01287000	1.91624300	-0.04129700
C	-3.33875200	2.11698900	-0.04101000
C	-4.54468100	2.30780100	-0.04063100
H	8.99923200	4.91684300	0.04607900
H	6.53669300	5.29445800	0.04068700
H	7.60673000	-4.19160900	-0.07376600
H	5.14386700	-3.81590000	-0.07960100
O	-20.45636400	-1.52061200	0.06263500
H	-21.34347500	-1.92561100	0.08850100

**P-Pen-2-A1**



C	1.57370200	-0.83762500	-0.07456700
C	0.13294000	-0.72777800	-0.06614500
C	-0.48169900	0.56455100	-0.06006300
C	0.32249200	1.74830100	-0.06640400
C	1.76314900	1.63712200	-0.07468300
C	2.37939100	0.34508500	-0.07586400
C	2.53537100	2.80933400	-0.08022700
C	1.96028800	4.07430700	-0.07822400
C	0.52247100	4.18688500	-0.06963400
C	-0.24942000	3.02963100	-0.06394400
C	-0.06109800	5.49218200	-0.06745900
C	0.72585800	6.60631700	-0.07334600
C	2.14887600	6.49442000	-0.08194500
C	2.74640300	5.26871400	-0.08432500
C	2.15807400	-2.11403000	-0.08010700
C	1.39649300	-3.27635100	-0.07785800
C	-0.04177800	-3.16805500	-0.06896400
C	-0.62795800	-1.90655300	-0.06330900
C	-0.81801000	-4.36877800	-0.06648200
C	-0.21059500	-5.59007100	-0.07237600
C	1.21282000	-5.69692800	-0.08127900
C	1.99073200	-4.57699000	-0.08392000
H	3.61519600	2.72877700	-0.08669100
H	-1.32817200	3.12655400	-0.05765400
H	-1.14205200	5.57749900	-0.06098700
H	0.27336900	7.59118700	-0.07157300
H	2.75112500	7.39530900	-0.08648100
H	3.82693500	5.17788600	-0.09079700
H	3.23767500	-2.19976100	-0.08668100
H	-1.70888800	-1.83713200	-0.05690700
H	-1.89928000	-4.28774200	-0.05976700
H	-0.80845700	-6.49409100	-0.07038600
H	1.67016500	-6.67935200	-0.08583200
H	3.07247600	-4.65250600	-0.09058000
C	-1.87308700	0.67213200	-0.04618400
C	-3.09218800	0.77140900	-0.03194300
C	-4.43142900	0.88407100	-0.01456400
C	-5.64778900	0.99630400	0.00196000
C	3.77336700	0.23948000	-0.07488300
C	4.99051600	0.16088000	-0.06639000
C	6.37088900	0.06341000	-0.05030400
C	7.31851100	1.07356200	-0.05565100
S	7.18168700	-1.51382600	-0.01281800
C	8.64734100	0.63255600	-0.03538400
H	7.03647200	2.11791700	-0.07957500
C	8.75932500	-0.75089700	-0.02294500
H	9.49868600	1.29504400	-0.04701200
C	11.18917300	-1.08986600	0.15234200
C	11.74054700	-0.01754800	0.82693300
C	13.15283900	-0.11449300	0.66484800
H	11.20302500	0.73029100	1.38560600

C	13.41435300	-1.23425500	-0.08810500
H	13.88988200	0.56335900	1.06711400
H	14.34149900	-1.66632200	-0.42661500
N	9.87469900	-1.52854700	-0.01430700
H	9.75257300	-2.52934100	-0.10575900
H	12.09022700	-2.64684700	-0.96519100
N	12.21020000	-1.81633900	-0.40190000
C	-7.03082700	1.11581800	0.02117400
C	-7.79034900	2.28295100	0.03119900
S	-8.05532200	-0.30355700	0.03640100
C	-9.16035600	2.03907500	0.05057000
H	-7.34056500	3.26569000	0.02441700
C	-9.50569100	0.68862700	0.05588200
H	-9.91367600	2.81630400	0.06089500
C	-10.84478800	0.23546100	0.07482500
H	-11.56886800	1.04249600	0.08700900
C	-11.37135700	-1.03038000	0.08008600
C	-10.56921400	-2.20245100	0.06329200
N	-9.90779100	-3.14931100	0.04868500
C	-12.82411500	-1.27748300	0.10256500
O	-13.32242400	-2.38490900	0.10815300
O	-13.56208800	-0.14967200	0.11676900
H	-14.49989000	-0.41338500	0.13022400

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C	-3.36974100	-0.93056700	0.08221000
C	-1.92786500	-0.84527800	0.08200600
C	-1.29088300	0.43823600	0.07864100
C	-2.07624700	1.63659000	0.08083300
C	-3.51803100	1.54892200	0.08093700
C	-4.15596700	0.26642900	0.07861100
C	-4.27149900	2.73269700	0.08206100
C	-3.67609000	3.98867900	0.08342400
C	-2.23698000	4.07770900	0.08315700
C	-1.48364800	2.90738100	0.08178100
C	-1.63238300	5.37292300	0.08443600
C	-2.40143700	6.49985500	0.08587600
C	-3.82573300	6.41127800	0.08620300
C	-4.44302000	5.19518900	0.08505900
C	-3.97625500	-2.19606000	0.08487800
C	-3.23471200	-3.37181900	0.08748100
C	-1.79522700	-3.28792300	0.08691600
C	-1.18747300	-2.03588200	0.08410700
C	-1.03955000	-4.50122100	0.08947400
C	-1.66786700	-5.71223000	0.09239600
C	-3.09251700	-5.79501400	0.09303200
C	-3.85123200	-4.66174800	0.09068200
H	-5.35250700	2.66942000	0.08230600
H	-0.40336400	2.98691000	0.08167100
H	-0.55020100	5.44086300	0.08420500

H	-1.93280100	7.47713500	0.08678500
H	-4.41337300	7.32174600	0.08735100
H	-5.52488500	5.12168100	0.08528600
H	-5.05719300	-2.26303400	0.08524300
H	-0.10543900	-1.98522100	0.08396300
H	0.04295600	-4.43864900	0.08901300
H	-1.08528500	-6.62616500	0.09425100
H	-3.56663400	-6.76943200	0.09537000
H	-4.93411900	-4.71876300	0.09110100
C	1.32282600	0.59588100	0.05682700
C	2.65607600	0.67767300	0.05373900
C	3.88395900	0.75346900	0.03421500
C	5.21491100	0.83611400	0.02415000
C	6.44083300	0.91387100	0.01138900
C	7.77742700	0.99790800	-0.00262200
C	8.99624100	1.08004200	-0.01602100
C	0.09846400	0.52152300	0.07081700
C	-5.54983000	0.18341600	0.06986400
C	-6.76840700	0.12208800	0.05493100
C	-8.14828500	0.04078600	0.03228400
C	-9.08500100	1.06246000	0.03459300
S	-8.97678400	-1.52722300	-0.00926100
C	-10.41749400	0.63700000	0.00893400
H	-8.79072400	2.10335400	0.06062800
C	-10.54519800	-0.74610700	-0.00476700
H	-11.26157500	1.30871300	0.01797800
C	-12.97834500	-1.05632300	-0.18525500
C	-13.51700200	0.02384500	-0.85756100
C	-14.93030800	-0.05860300	-0.69813300
H	-12.97065300	0.76722100	-1.41360100
C	-15.20495400	-1.17787100	0.05107000
H	-15.65947400	0.62810300	-1.09969400
H	-16.13728600	-1.60082400	0.38683500
N	-11.66888700	-1.50973900	-0.01788300
H	-11.55889500	-2.51212900	0.07365400
H	-13.89777400	-2.60729300	0.92597900
N	-14.00790500	-1.77392400	0.36484400
C	10.38378000	1.16108400	-0.03119400
C	11.17307200	2.30519000	-0.03841200
S	11.36505700	-0.28715000	-0.04375200
C	12.53752000	2.02130800	-0.05366500
H	10.75132400	3.30023900	-0.03256300
C	12.83978700	0.66259700	-0.05837400
H	13.31337700	2.77587300	-0.06131900
C	14.16913200	0.16846500	-0.07298900
H	14.91685700	0.95365500	-0.08272400
C	14.65357100	-1.11023500	-0.07632800
C	13.81438700	-2.25728000	-0.06346500
N	13.12350200	-3.18228900	-0.05272500
C	16.10084900	-1.40377900	-0.09302900
O	16.56109000	-2.52644200	-0.09489800

O	16.87077900	-0.29972700	-0.10619300
H	17.80143300	-0.58842300	-0.11561300

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C	9.40851800	0.26269000	-0.00706300
C	10.47180300	1.19592000	0.06780500
C	9.78238300	-1.10210600	-0.02889900
C	11.76718100	0.78070800	0.11463700
H	10.28908000	2.26046600	0.08937500
C	11.09039800	-1.48048800	0.01838400
H	9.02590300	-1.87360700	-0.08473900
H	12.59838500	1.46426700	0.17101500
H	11.40439800	-2.51102200	0.00227600
N	12.08874700	-0.54990900	0.09070000
C	13.46389500	-0.96501900	0.14094300
C	15.64005300	-0.38914200	0.26755900
C	14.95374900	-2.65508600	0.18119600
C	15.99744500	-1.73547200	0.26342300
H	16.38576200	0.39456500	0.32105400
H	15.15137500	-3.72035800	0.16625200
N	13.68225700	-2.27229700	0.12246700
N	14.36816900	-0.00083900	0.20254300
C	17.39888500	-2.21442600	0.33878700
O	17.71642700	-3.38093000	0.29432800
C	-4.56990400	-0.65033100	-0.23728700
C	-3.16668000	-0.31248500	-0.30698800
C	-2.76155800	1.05906800	-0.25537800
C	-3.73962400	2.09841300	-0.15477100
C	-5.14268900	1.75946200	-0.08583400
C	-5.54845500	0.38731900	-0.12163200
C	-6.08677300	2.79278400	0.01974100
C	-5.71709200	4.13175800	0.05775400
C	-4.31729000	4.47162200	-0.01438400
C	-3.37559100	3.45293200	-0.11741500
C	-3.94621800	5.85189400	0.02341600
C	-4.89619300	6.82530700	0.12700200
C	-6.28141600	6.48840800	0.19902700
C	-6.67866900	5.18443100	0.16566600
C	-4.94664800	-2.00183800	-0.28247300
C	-4.01443700	-3.02630200	-0.39579200
C	-2.61369500	-2.69012500	-0.46847200
C	-2.23272400	-1.35318700	-0.42112300
C	-1.66090500	-3.74947900	-0.58698200
C	-2.06841500	-5.05044500	-0.62936800
C	-3.45470900	-5.38297000	-0.55729500
C	-4.39662500	-4.40338300	-0.44414200
H	-7.13896900	2.54227600	0.07170400
H	-2.32717200	3.71993700	-0.17117900
H	-2.89398400	6.10821700	-0.03119200
H	-4.60413300	7.86869600	0.15512500

H	-7.01602700	7.28098600	0.28013800
H	-7.72962800	4.92281500	0.21932500
H	-5.99757600	-2.25833000	-0.22914200
H	-1.17793400	-1.11299700	-0.47477000
H	-0.60788000	-3.49659900	-0.64142800
H	-1.33786800	-5.84616600	-0.71842200
H	-3.75206300	-6.42444300	-0.59334700
H	-5.45102400	-4.65087900	-0.38955100
C	-1.40350400	1.38062200	-0.28354700
C	-0.21062400	1.65140000	-0.28821600
C	1.10325700	1.93503100	-0.27030900
C	2.29760600	2.19175500	-0.24270000
C	-6.90601100	0.06227300	-0.04365600
C	-8.09413900	-0.20369500	0.02799900
C	-9.44180800	-0.50744000	0.11264400
C	-10.52424300	0.35063300	0.21226200
S	-10.01118500	-2.18724900	0.11686000
C	-11.77057700	-0.28228800	0.29719700
H	-10.39819700	1.42516300	0.22900600
C	-11.67752600	-1.66706200	0.27747400
H	-12.70412800	0.24924900	0.39372400
C	-14.03444000	-2.38273900	0.34460000
C	-14.81719200	-1.39162800	-0.21620900
C	-16.17234700	-1.73626100	0.05915900
H	-14.46814000	-0.54117200	-0.77716300
C	-16.17225200	-2.91638500	0.76302200
H	-17.04628900	-1.17707800	-0.23759000
H	-16.97859800	-3.51421400	1.15454700
N	-12.65740500	-2.60538900	0.36446600
H	-12.37390100	-3.57460800	0.43727300
H	-14.55520800	-4.11646800	1.44393500
N	-14.86376000	-3.29857200	0.93672800
C	3.65990900	2.45194500	-0.19501100
C	4.30430300	3.68374200	-0.14730800
S	4.82517300	1.14022100	-0.17442100
C	5.69476000	3.57482500	-0.09373400
H	3.76134900	4.61850000	-0.15065700
C	6.16628900	2.26706000	-0.09937800
H	6.36682900	4.42220800	-0.05120600
C	7.53248400	1.88404000	-0.04966400
H	8.21899100	2.72356300	-0.00031200
C	8.02244300	0.61220000	-0.05908400
H	7.33585800	-0.22732900	-0.10955600
O	18.28429000	-1.21229100	0.46456200
H	19.17883400	-1.59913800	0.50355100

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C	-12.42678500	0.19084800	-0.02740400
C	-13.50774600	1.10331600	-0.01612300
C	-12.76901600	-1.18027000	-0.02927600

C	-14.79640900	0.66127900	-0.00356300
H	-13.34667700	2.17159100	-0.01534600
C	-14.07126000	-1.58548800	-0.01650800
H	-11.99513200	-1.93624400	-0.04035200
H	-15.64367300	1.32708800	0.00712900
H	-14.36440300	-2.62243700	-0.01705700
N	-15.08714600	-0.67447200	-0.00201000
C	-16.45740700	-1.11653800	0.01819800
C	-18.64608100	-0.57907800	0.02241900
C	-17.91514900	-2.83185300	0.07785400
C	-18.97798600	-1.93120000	0.06425000
H	-19.40744200	0.19105300	0.00704500
H	-18.09165700	-3.90048100	0.10870700
N	-16.64924300	-2.42598300	0.05463700
N	-17.37946900	-0.16865400	-0.00051800
C	-20.37338600	-2.43369000	0.09824900
O	-20.66728900	-3.60579400	0.15165400
C	6.76195000	-0.90045200	-0.02710700
C	5.33557700	-0.67318800	-0.03108000
C	4.82889100	0.66673700	-0.02750900
C	5.72870300	1.78139200	-0.01906600
C	7.15485400	1.55179400	-0.01528400
C	7.66263600	0.21281900	-0.01961800
C	8.02133800	2.65565400	-0.00726000
C	7.55265200	3.96423500	-0.00267200
C	6.12940500	4.19481400	-0.00621300
C	5.26453700	3.10455700	-0.01424500
C	5.65511200	5.54327300	-0.00130800
C	6.53127100	6.58899600	0.00661900
C	7.93995700	6.36044200	0.01012100
C	8.43451700	5.08954300	0.00561200
C	7.24026000	-2.21968300	-0.03093000
C	6.38654600	-3.31645800	-0.03817600
C	4.96244700	-3.09097500	-0.04205800
C	4.48120900	-1.78511900	-0.03846700
C	4.09114800	-4.22415600	-0.04953500
C	4.59717900	-5.49109200	-0.05290600
C	6.00679800	-5.71383900	-0.04904300
C	6.87328600	-4.66074600	-0.04188800
H	9.09095500	2.48655300	-0.00437800
H	4.19753000	3.29098300	-0.01674100
H	4.58481400	5.71720800	-0.00395400
H	6.16123900	7.60768300	0.01034200
H	8.61432900	7.20869200	0.01639400
H	9.50388500	4.90973500	0.00825200
H	8.30915200	-2.39356200	-0.02815000
H	3.40939600	-1.62818600	-0.04149300
H	3.02007600	-4.05517900	-0.05241400
H	3.92756400	-6.34335300	-0.05851300
H	6.38261300	-6.73021300	-0.05180600
H	7.94534200	-4.82384900	-0.03886600

C	3.45385500	0.88625400	-0.03224500
C	2.24262800	1.07898300	-0.04066600
C	0.92292700	1.28841700	-0.03495000
C	-0.29206300	1.48118400	-0.04461700
C	9.04165300	-0.00855100	-0.01662200
C	10.24758200	-0.19410600	-0.01500100
C	11.61174100	-0.41972400	-0.01306300
C	12.65082900	0.49714400	-0.03207900
S	12.27068300	-2.06662700	0.00835800
C	13.93150600	-0.06680000	-0.03761400
H	12.46738800	1.56337900	-0.04985700
C	13.91194600	-1.45543500	-0.03246600
H	14.84134200	0.51227000	-0.06480000
C	16.30001400	-2.03553300	0.09676000
C	16.96856000	-1.02831500	0.76586600
C	18.36063700	-1.27053400	0.58332500
H	16.51927700	-0.23189800	1.33535300
C	18.49423000	-2.40854300	-0.17596700
H	19.16955700	-0.67443600	0.97677000
H	19.36694900	-2.93289300	-0.52858200
N	14.94557800	-2.33687100	-0.05083100
H	14.72191900	-3.31871700	-0.15600500
H	17.01914900	-3.67297500	-1.03800900
N	17.23210600	-2.86213400	-0.47352000
C	-6.72243200	2.51619300	-0.03693400
C	-7.39734200	3.72964400	-0.03023300
S	-7.85118000	1.17395400	-0.04093800
C	-8.78735900	3.58383700	-0.02793000
H	-6.87877700	4.67806800	-0.02685800
C	-9.22013200	2.26490800	-0.03298100
H	-9.48228300	4.41350600	-0.02250200
C	-10.58236800	1.84776000	-0.03020100
H	-11.28773300	2.67280600	-0.02245300
C	-11.04233300	0.56888900	-0.03501400
H	-10.33946500	-0.25837900	-0.04292700
C	-1.60945700	1.69059400	-0.04214400
C	-2.82245800	1.88507000	-0.04219300
C	-4.14492300	2.09765900	-0.04082600
C	-5.35036100	2.29846400	-0.03947500
O	-21.28092900	-1.44455600	0.06520000
H	-22.16989400	-1.84544800	0.09033000