

# Exploration on charge transfer and absorption spectra of porphyrin-polyoxometalate hybrids for searching high performance sensitizers

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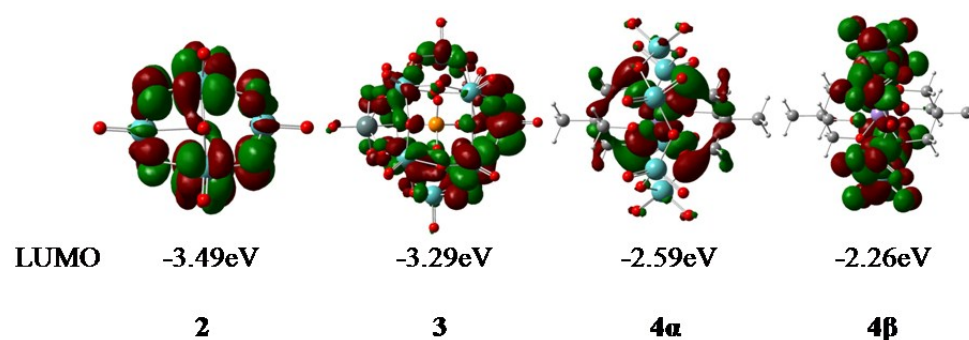
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## Supporting Information

**Fig. S1.** LUMO distributions and energy levels of systems 2-4.

**Table S1.** The orbital composition of LUMO for systems 1-4.

**Table S2.** Optimized Cartesian coordinates for systems 1-4.



**Fig. S1.** LUMO distributions and energy levels of systems 2-4.

**Table S1.** The orbital composition of LUMO for systems 1-4.

System	Orbital composition of LUMO
1	80% p(C)+6% p(N)
2	63% d(Mo)+33% p(O)
3	69% d(Mo)+19% p(O)
4	80% p(C)+6% p(N)

**Table S2.** Optimized Cartesian coordinates for systems **1-4**.

System **1** C<sub>43</sub>H<sub>26</sub>O<sub>2</sub>N<sub>4</sub> (B3LYP/6-31G\*)

Atom	X	Y	Z
N	-0.46697400	-1.50999500	-0.04909300
N	-0.48088000	1.45667400	-0.03802100
C	-0.72028500	-2.86561300	-0.01812000
C	0.55609400	-3.51587100	0.03392200
C	1.52823200	-2.54960400	0.02606800
C	0.88336600	-1.27423100	-0.02077300
C	1.51736400	-0.01009200	-0.01518900
C	0.86388700	1.25240100	-0.01145800
C	1.59339900	2.51106900	0.04055600
C	0.65668800	3.49040400	0.04940300
C	-0.63860100	2.82083000	-0.00705400
C	-1.98685200	-3.47575800	-0.01312800
C	-2.01084000	-4.97369800	-0.00724600
C	-1.54568600	-5.70232000	-1.11383400
C	-2.28685600	7.13245000	1.09622200
C	-1.34436100	7.11008100	-1.12757400
C	-2.49677500	-5.67684400	1.10697100
H	0.69930400	-4.58484900	0.07954800
H	2.59847800	-2.69054500	0.06150600
H	2.66899100	2.61254400	0.07632300

H	0.81511100	4.55785000	0.09895700
H	-1.17450100	-5.17047700	-1.98539200
H	-0.97237700	7.63922900	-2.00059900
H	-2.85151900	-5.12488600	1.97275300
N	-3.38613900	1.54543300	0.02995900
C	-3.13494800	2.90050900	0.00169300
C	-4.41187400	3.55009000	-0.04917700
C	-5.38324900	2.58307100	-0.04424500
C	-4.73703300	1.30778000	-0.00012100
C	-5.36833300	0.04567600	-0.00950400
C	-4.71850000	-1.21462000	-0.01126500
N	-3.37221100	-1.42107200	0.01836600
C	-1.86792700	3.51162000	-0.00283900
C	-1.84542600	5.00971700	-0.00723300
C	-2.30863200	5.73667400	1.10123000
C	-1.36337700	5.71448000	-1.12207000
H	-1.01023900	5.16372100	-1.98927200
H	-2.67704700	5.20356700	1.97320300
C	-3.21680000	-2.78365300	-0.01103900
C	-4.51271900	-3.45283200	-0.06935100
C	-5.44880000	-2.47297700	-0.06367000
H	-6.52450000	-2.57239900	-0.10126700
H	-4.67158000	-4.52026400	-0.11798100
C	-1.56923000	-7.09805800	-1.10757400
C	-2.51746400	-7.07239300	1.11374700
H	-2.89234000	-7.60025500	1.98631000
H	-1.21134300	-7.64565200	-1.97509200
H	-6.45381500	2.72173400	-0.07914300
H	-4.55568300	4.61911400	-0.09195000

H	-2.07181800	-8.87333800	0.01144300
H	-1.78939100	8.90942100	-0.02241900
C	-1.80528700	7.82310400	-0.01825800
C	-2.05452800	-7.78704800	0.00630000
H	-2.66511200	0.83147700	0.05144900
H	-1.18714700	-0.79517000	-0.07217600
H	-2.64320900	7.67879300	1.96516100
C	-8.00949000	0.08077200	-0.04900800
C	-6.79783200	0.05923700	-0.03169400
C	2.93849800	-0.02269400	-0.00056400
C	4.15732300	-0.04300800	0.00887900
C	5.57796200	-0.06323000	0.01957800
C	6.31258500	1.14269300	0.03481200
C	6.27851600	-1.29008200	0.01518400
C	7.70104300	1.12130500	0.04581500
H	5.78239600	2.08947500	0.03787800
C	7.66552300	-1.30361500	0.02651100
H	5.72238600	-2.22179800	0.00260700
C	8.39022100	-0.10186300	0.04201200
H	8.25473300	2.05322000	0.05757400
H	8.20693600	-2.24359100	0.02345800
C	9.87285300	-0.17595800	0.05392400
O	10.51524200	-1.21239000	0.05249300
O	10.46524900	1.03964000	0.06674800
H	11.42884100	0.88468700	0.07361400
H	-9.07715500	0.09571500	-0.06392700

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System 2 [C<sub>43</sub>H<sub>25</sub>O<sub>2</sub>N<sub>4</sub>(Mo<sub>6</sub>O<sub>18</sub>N)]<sup>2-</sup> (B3LYP/6-31G\*/LanL2DZ)

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Atom	X	Y	Z
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Mo	8.31290500	-0.12956500	0.06208200
Mo	5.91355300	-1.79126100	-1.57272700
Mo	3.73743400	0.12982600	-0.02301600
Mo	5.84418900	-1.59103500	1.80681200
Mo	6.09661600	1.58646800	-1.77228400
Mo	6.02947300	1.79201500	1.60625700
O	5.91743600	0.00113600	0.01613500
O	7.78119600	-1.41972400	1.33742700
O	5.95582300	-2.73157200	-0.01372400
O	7.89445100	1.34485200	-1.20769900
O	7.83202700	-1.30819900	-1.34434400
O	7.84107900	1.23568100	1.42219800
O	5.93558700	-0.03859500	2.74939400
O	4.11134400	-1.28258600	-1.42694200
O	4.12952600	1.34936000	1.41705300
O	6.02013000	2.73642700	0.05153700
O	6.03530800	0.03123400	-2.71501700
O	5.84275600	-2.86592800	2.95119200
O	4.18237200	1.45907100	-1.33824300
O	4.05332200	-1.38900900	1.28403800
O	6.05448600	2.93581300	2.88124300
O	5.96513500	-2.94062700	-2.84199700
O	10.02182200	-0.14756000	0.09018500
O	6.17149800	2.85897000	-2.91654600
N	1.93588900	0.14914600	-0.04848800
N	-6.88924500	-1.50665300	0.01511400
N	-6.88755400	1.45898100	0.00484500
C	-6.63203300	-2.85973000	-0.02030700
C	-7.90397000	-3.51650600	-0.06010400

C	-8.88149500	-2.55376300	-0.04015800
C	-8.24143500	-1.27719100	0.00168300
C	-8.88076500	-0.01457700	0.00402600
C	-8.23287400	1.25023200	-0.00791600
C	-8.96694900	2.50571600	-0.05482600
C	-8.03274800	3.48814500	-0.07510100
C	-6.73573600	2.82171100	-0.02961600
C	-5.35975200	-3.46714700	-0.03763300
C	-5.33396300	-4.96499200	-0.04545200
C	-5.78750400	-5.69506000	1.06531900
C	-5.10967400	7.13870200	-1.15022200
C	-6.04274100	7.11386800	1.07840100
C	-4.85773400	-5.66539900	-1.16576500
H	-8.04247200	-4.58596100	-0.10587100
H	-9.95134400	-2.69940800	-0.06425300
H	-10.04303700	2.60376500	-0.08026200
H	-8.19456000	4.55490300	-0.12549700
H	-6.15075900	-5.16486900	1.94116400
H	-6.41280900	7.64214900	1.95269900
H	-4.51222800	-5.11167200	-2.03406300
N	-3.97745900	1.55810000	-0.09340100
C	-4.23805200	2.91397000	-0.06150700
C	-2.96473300	3.57104900	-0.02007900
C	-1.98741400	2.60957000	-0.03435600
C	-2.62781500	1.33211900	-0.07488100
C	-1.98577900	0.06658400	-0.07273000
C	-2.63970600	-1.20237800	-0.06457000
N	-3.97989900	-1.40692000	-0.08179600
C	-5.50639500	3.51771400	-0.04559400

C	-5.53635600	5.01523900	-0.04252100
C	-5.08077500	5.74278000	-1.15410100
C	-6.01781800	5.71817500	1.07412800
H	-6.36439000	5.16659100	1.94337100
H	-4.71330800	5.21053600	-2.02689300
C	-4.13497000	-2.77501900	-0.05108500
C	-2.83697800	-3.44071000	-0.00479000
C	-1.90367400	-2.45824800	-0.01886900
H	-0.82733700	-2.55767800	0.00943100
H	-2.67486600	-4.50752700	0.04276100
C	-5.76115100	-7.09095100	1.05713800
C	-4.83496400	-7.06123600	-1.17427400
H	-4.46750800	-7.58744100	-2.05090900
H	-6.10882600	-7.64024100	1.92767800
H	-0.91764000	2.75772200	-0.00741300
H	-2.82635100	4.64061400	0.02388700
H	-5.26626800	-8.86407200	-0.06914100
H	-5.61049500	8.91422900	-0.03055700
C	-5.58978700	7.82802700	-0.03395100
C	-5.28567200	-7.77785500	-0.06274400
H	-4.69248900	0.83798100	-0.10932100
H	-6.17268000	-0.78809700	0.03210600
H	-4.75940900	7.68591100	-2.02100700
C	0.65680200	0.11295100	-0.05771200
C	-0.57860000	0.08314100	-0.06480100
C	-10.30130300	-0.03278500	0.00773200
C	-11.52006100	-0.05721700	0.01572800
C	-12.94061800	-0.08069400	0.02700700
C	-13.67719200	1.12443600	0.02454600

C	-13.63811400	-1.30949400	0.04175200
C	-15.06595000	1.10029200	0.03661000
H	-13.14873000	2.07208800	0.01342200
C	-15.02546600	-1.32553000	0.05364100
H	-13.07988700	-2.23999800	0.04419100
C	-15.75212600	-0.12466200	0.05124100
H	-15.62179700	2.03096200	0.03474400
H	-15.56539300	-2.26625200	0.06511300
C	-17.23520700	-0.20153100	0.06481600
O	-17.87476500	-1.23979200	0.07763900
O	-17.82976500	1.01229700	0.06168400
H	-18.79339900	0.85586900	0.07116700

System 3 [C<sub>43</sub>H<sub>25</sub>O<sub>2</sub>N<sub>4</sub>(PSnMo<sub>11</sub>O<sub>39</sub>)]<sup>4+</sup> (B3LYP/6-31G\*/ LanL2DZ)

Atom	X	Y	Z
P	-3.76256000	-0.00887000	0.04393800
Mo	-2.15770700	1.75376300	-2.76112400
Mo	-5.22329400	-1.88551900	2.75967600
Mo	-5.85903400	2.00413800	-2.10412000
Mo	-7.33549500	-0.14565500	0.23458600
Mo	-4.03225100	-3.64048200	-0.04628000
Mo	-2.08440000	-1.77316000	-2.68727300
Mo	-5.32471900	1.91953400	2.69831400
Mo	-1.79299400	-2.16392000	2.18559900
Mo	-3.54046400	3.66456800	0.29089800
Mo	-5.83729700	-1.47397500	-2.60033800
Mo	-1.84300900	1.56752800	2.58924100
O	-1.60970900	-2.73457300	-4.01761700
O	-3.67381400	1.23046100	0.97734100



O	-3.71441800	-1.32585500	0.87213000
O	-2.51160500	0.01088400	-0.92003200
O	-6.30553000	2.44355600	3.99821900
O	-4.02534500	-5.30795600	-0.42764500
O	-0.68334300	-2.85673200	3.28634800
O	-5.20723700	3.12531100	-0.82559900
O	-2.60224100	3.07055800	-1.15121800
O	-3.47196900	-2.32064600	3.27804400
O	-5.00578900	3.45746500	1.75227800
O	-8.98791400	-0.14796600	0.66916200
O	-4.03939600	-1.52654900	-3.08038900
O	-6.21270200	0.20286100	-3.19300100
O	-6.17821200	-2.64122400	3.96132700
O	-2.36820200	-3.59747800	1.18282700
O	-0.75915100	1.36227100	1.10074900
O	-6.63418300	3.04974000	-3.21529000
O	-4.10102000	1.80198200	-2.84137100
O	-0.71549800	-1.39727500	0.91157200
O	-3.58031100	1.93804800	3.46543700
O	-1.73156500	2.87275000	-3.98113200
O	-1.90254600	-0.22006600	2.95843400
O	-7.31517500	1.35159800	-1.07047100
O	-6.59454600	-2.49449000	-3.74563900
O	-7.30223700	-1.29630500	-1.25760800
O	-0.78753700	2.21771700	3.77091500
O	-3.59636500	5.36415000	0.09286400
O	-2.34126700	3.41906500	1.63935200
O	-6.58667100	1.19193100	1.47634600
O	-5.02108100	-3.55266500	1.49119000

O	-2.60935200	-2.96870800	-1.40054100
O	-6.58524900	-1.42169000	1.38838100
O	-0.47831500	-1.27497700	-1.92946600
O	-5.06419700	0.04466000	-0.79599800
O	-2.06872600	0.11369500	-3.58615800
O	-5.23259900	-2.91949400	-1.21189100
O	-0.56507300	1.54435100	-1.81945700
O	-5.21190900	-0.13983300	3.23467400
N	9.30257100	1.53455700	0.01357000
N	9.22383400	-1.43035300	-0.00047800
C	9.07912800	2.89565100	-0.01858500
C	10.37013400	3.51866900	-0.03446200
C	11.32118800	2.53134300	-0.00583900
C	10.64800900	1.26995500	0.01916900
C	11.25453100	-0.00788800	0.02625400
C	10.57294200	-1.25574500	0.00740200
C	11.27562600	-2.53043400	-0.02269700
C	10.31767600	-3.48916600	-0.05296000
C	9.03645800	-2.79079000	-0.03226700
C	7.82638200	3.53319500	-0.05613800
C	7.83562300	5.03128400	-0.05622400
C	8.28913500	5.74515900	1.06513300
C	7.32421500	-7.07089500	-1.16683700
C	8.20657600	-7.05928000	1.08216500
C	7.39409400	5.74966400	-1.17955400
H	10.53692600	4.58449100	-0.07174900
H	12.39476700	2.64902600	-0.01249500
H	12.34925100	-2.65548100	-0.03006400
H	10.45351400	-4.55999100	-0.09554900

H	8.62527400	5.20163100	1.94364700
H	8.54219800	-7.59253200	1.96735700
H	7.04824000	5.20924200	-2.05609100
N	6.31914400	-1.45610000	-0.15317200
C	6.53980900	-2.81639900	-0.11517500
C	5.24808100	-3.43860200	-0.10908100
C	4.29819400	-2.45060600	-0.15190300
C	4.97340600	-1.18966800	-0.17337900
C	4.36874500	0.08654500	-0.18853300
C	5.04777200	1.33222000	-0.15815200
N	6.39836500	1.50903100	-0.13912900
C	7.79282200	-3.45479800	-0.06990400
C	7.78282000	-4.95298300	-0.05995400
C	7.33391500	-5.67471600	-1.17806500
C	8.21886700	-5.66332200	1.07056900
H	8.55992600	-5.11643600	1.94500300
H	7.00062900	-5.13761800	-2.06160100
C	6.58224900	2.86796700	-0.09860000
C	5.29985700	3.56540800	-0.08098400
C	4.34321800	2.60612400	-0.12567000
H	3.26917700	2.72851500	-0.12666800
H	5.16226700	4.63569700	-0.03197900
C	8.29773000	7.14138500	1.06424100
C	7.40538400	7.14564200	-1.18084400
H	7.06417300	7.68507600	-2.06010300
H	8.64533700	7.67740700	1.94310200
H	3.22420400	-2.56607200	-0.15832900
H	5.07964900	-4.50409500	-0.07027200
H	7.86364200	8.93203100	-0.05961400

H	7.75069400	-8.85352500	-0.02749600
C	7.75988700	-7.76715900	-0.03665200
C	7.85653000	7.84561300	-0.05883400
H	7.05500100	-0.75729800	-0.15042700
H	8.56722700	0.83504100	0.01373600
H	6.97875900	-7.61305300	-2.04275300
C	1.71914400	0.10921800	-0.27652800
C	2.94159600	0.10437800	-0.23151100
C	12.67551600	-0.02676300	0.04239100
C	13.89462100	-0.03396500	0.05676900
C	15.31519100	-0.04453500	0.07282000
C	16.02458700	-1.26616400	0.06952900
C	16.04224700	1.16725300	0.09206600
C	17.41344800	-1.27438500	0.08517000
H	15.47472300	-2.20156800	0.05450000
C	17.42943700	1.15110500	0.10749300
H	15.50623700	2.11078200	0.09481400
C	18.12873700	-0.06610300	0.10426400
H	17.94712400	-2.21799300	0.08249600
H	17.99060800	2.07930200	0.12228600
C	19.61233800	-0.02371300	0.12152300
O	20.27681200	0.99904300	0.13844800
O	20.17947300	-1.25113000	0.11684100
H	21.14621700	-1.11577100	0.12899400
Sn	-0.36796700	0.10479400	-0.41551100

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System 4 [C<sub>47</sub>H<sub>31</sub>O<sub>2</sub>N<sub>4</sub>[MnMo<sub>6</sub>O<sub>24</sub>[C(CH<sub>2</sub>)<sub>3</sub>]CH<sub>3</sub>]]<sup>3-</sup> (B3LYP/6-31G\*/ LanL2DZ)

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Atom	X	Y	Z
Mo	4.56332100	-1.96102200	2.89030900

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Mo	4.37734900	1.46916500	3.12720200
Mo	4.47724400	3.45956500	0.31782900
Mo	4.79100800	2.00622500	-2.74658300
Mo	4.97289800	-1.42059700	-2.98222500
Mo	4.87179700	-3.41326000	-0.16689200
Mn	4.67518000	0.02338300	0.07212100
O	3.17680200	-2.04570300	3.91970800
O	5.73496100	-3.00603600	3.60623100
O	3.84253000	-3.00854100	1.42616300
O	5.27902100	-0.23021100	3.37644800
O	5.82534600	-1.57435400	0.94852200
O	3.44439500	-0.11519500	1.56899700
O	3.04386200	1.32554100	4.21305300
O	5.51839600	2.49441400	3.91850700
O	3.57301900	2.67769000	1.83683600
O	5.64743500	1.35990200	1.08593300
O	5.67062900	4.43749400	1.09791700
O	3.27104000	4.56013600	-0.24039600
O	5.50197300	3.05085800	-1.27705500
O	3.51104900	1.61801600	-0.80282700
O	6.17512100	2.09713200	-3.77815800
O	3.61623900	3.05107900	-3.45778100
O	4.07041400	0.27907900	-3.23528800
O	5.89780600	0.16260000	-1.42539600
O	6.30352200	-1.28420800	-4.07234200
O	3.82614500	-2.44329800	-3.76871400
O	5.76954600	-2.62801100	-1.68868700
O	3.68630100	-1.30925300	-0.94206200
O	3.67374900	-4.38498600	-0.94841900

O	6.07518000	-4.51919200	0.38627400
C	2.11225400	1.37286500	-0.83096500
H	1.76021800	1.39627000	-1.86934700
H	1.59482300	2.16741400	-0.27934800
C	2.04265600	-0.10672900	1.30045800
H	1.59101200	0.74023000	1.82637900
H	1.61297300	-1.03543500	1.69142100
C	2.26243300	-1.20998000	-0.99654400
H	1.83797100	-2.13028800	-0.58018900
H	1.95783000	-1.12544800	-2.04456800
C	7.23051900	-1.31099900	0.97158100
H	7.74536800	-2.11237300	0.42578000
H	7.57493800	-1.34158900	2.01334800
C	7.07801300	1.24856600	1.13329400
H	7.37657200	1.17284100	2.18474400
H	7.49673900	2.17363400	0.71927100
C	7.30469500	0.15091000	-1.13943600
H	7.73150000	1.07782900	-1.54083600
H	7.75061700	-0.69684500	-1.67119400
C	7.65788400	0.04675100	0.35871000
N	-7.34695700	-1.56474600	-0.15770000
N	-7.29104700	1.39923000	-0.14435600
C	-7.11385700	-2.92341500	-0.22124900
C	-8.40061000	-3.55596700	-0.22114700
C	-9.35792100	-2.57720700	-0.14780500
C	-8.69375100	-1.31108300	-0.11412000
C	-9.30950600	-0.03855900	-0.07153100
C	-8.63793000	1.21460600	-0.10475200
C	-9.35096900	2.48395100	-0.12060800

C	-8.40146200	3.44978600	-0.17705000
C	-7.11466500	2.76131800	-0.18176900
C	-5.85749700	-3.55006000	-0.28977900
C	-5.85453200	-5.04777000	-0.32452100
C	-6.28934300	-5.79254000	0.78408000
C	-5.43814500	7.04909800	-1.34791400
C	-6.30288700	7.04043400	0.90792000
C	-5.41826500	-5.73495500	-1.46923200
H	-8.56063100	-4.62201700	-0.27689200
H	-10.43048600	-2.70319100	-0.13116900
H	-10.42540200	2.60088400	-0.10372100
H	-8.54655100	4.51937000	-0.21992700
H	-6.62082200	-5.27348200	1.67900100
H	-6.63434000	7.57490700	1.79395000
H	-5.08632200	-5.17042400	-2.33593200
N	-4.38609400	1.44712200	-0.32613600
C	-4.61896800	2.80511600	-0.28594500
C	-3.33333900	3.43871000	-0.26957600
C	-2.37449600	2.45907600	-0.30132300
C	-3.03737500	1.19221800	-0.33178000
C	-2.42147400	-0.07906800	-0.34269400
C	-3.09157800	-1.32936900	-0.34145700
N	-4.44186800	-1.51517700	-0.33896600
C	-5.87713100	3.43417400	-0.23609900
C	-5.87676500	4.93247300	-0.23035200
C	-5.44020700	5.65285800	-1.35422300
C	-6.30759100	5.64438800	0.90119800
H	-6.63852900	5.09875100	1.78027900
H	-5.11036700	5.11446900	-2.23828400

C	-4.61751400	-2.87512400	-0.32483900
C	-3.33114200	-3.56508200	-0.31305500
C	-2.38008400	-2.59920300	-0.32669800
H	-1.30542200	-2.71600800	-0.31864600
H	-3.18745300	-4.63535100	-0.28525200
C	-6.28549800	-7.18837600	0.74954600
C	-5.41716500	-7.13055100	-1.50417800
H	-5.08049200	-7.64557900	-2.39967100
H	-6.61883300	-7.74855500	1.61882800
H	-1.30198900	2.58573900	-0.29487300
H	-3.17457900	4.50560800	-0.22866400
H	-5.84767600	-8.94748100	-0.42164600
H	-5.86559300	8.83331200	-0.21138000
C	-5.86889500	7.74688600	-0.21677500
C	-5.85015800	-7.86137600	-0.39475600
H	-5.11520100	0.74133000	-0.32541500
H	-6.61737600	-0.85927800	-0.15737600
H	-5.10240000	7.59014800	-2.22828700
C	9.19488600	0.12812000	0.47311200
H	9.51285900	0.06380700	1.51977100
H	9.67216300	-0.69263500	-0.07409000
H	9.57221400	1.07151600	0.06305000
C	1.68559900	0.00198400	-0.21144800
C	0.22189800	-0.06117300	-0.29927100
C	-0.99288500	-0.08202900	-0.32787000
C	-10.72876100	-0.02983400	0.00113100
C	-11.94579900	-0.02765600	0.07395200
C	-13.36345300	-0.01876600	0.16583600
C	-14.07167600	1.20271800	0.21231000



C	-14.08856600	-1.23081000	0.21558200
C	-15.45739300	1.21057100	0.30642900
H	-13.52312000	2.13826700	0.17464000
C	-15.47269600	-1.21503100	0.30977700
H	-13.55335800	-2.17416000	0.18047700
C	-16.17074100	0.00202800	0.35616200
H	-15.99017700	2.15403200	0.34216100
H	-16.03239900	-2.14341800	0.34915000
C	-17.65092300	-0.04046300	0.45778200
O	-18.31382700	-1.06323200	0.50594700
O	-18.21687300	1.18704300	0.49280200
H	-19.18149700	1.05180700	0.55835600

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