

Supporting Information

Photoreactions of Endohedral Metallofullerene with Siliranes: Electronic Properties of Carbosilylated $\text{Lu}_3\text{N}@I_h\text{-C}_{80}$

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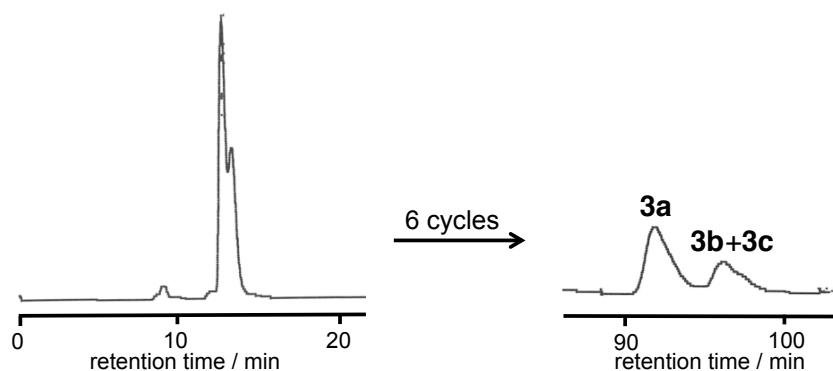
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(a)



(b)

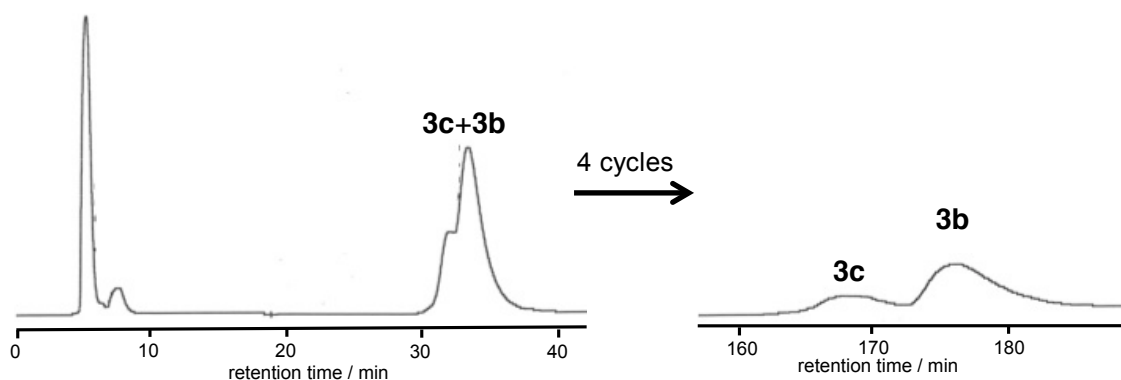


Figure S1. HPLC profiles of the separation of **3a**, **3b**, and **3c**. HPLC conditions: (a) Buckyprep (ϕ 20 $\times$ 250 mm); eluent, toluene; flow rate, 6.5 mL/min; detection wavelength, 282 nm; temperature, room temperature. (b) 5PBB (ϕ 10 $\times$ 250 mm); eluent, toluene; flow rate, 3.0 mL/min; detection wavelength, 282 nm; temperature, room temperature.

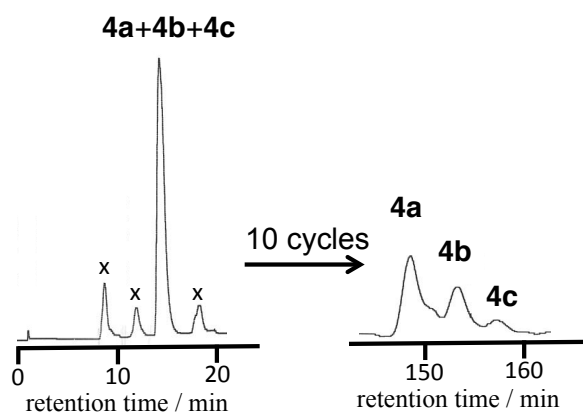


Figure S2. HPLC profiles of the separation of **4a**, **4b**, and **4c**. HPLC conditions: Buckyprep (ϕ 20 $\times$ 250 mm); eluent, toluene; flow rate, 6.5 mL/min; detection wavelength, 330 nm; temperature, room temperature.

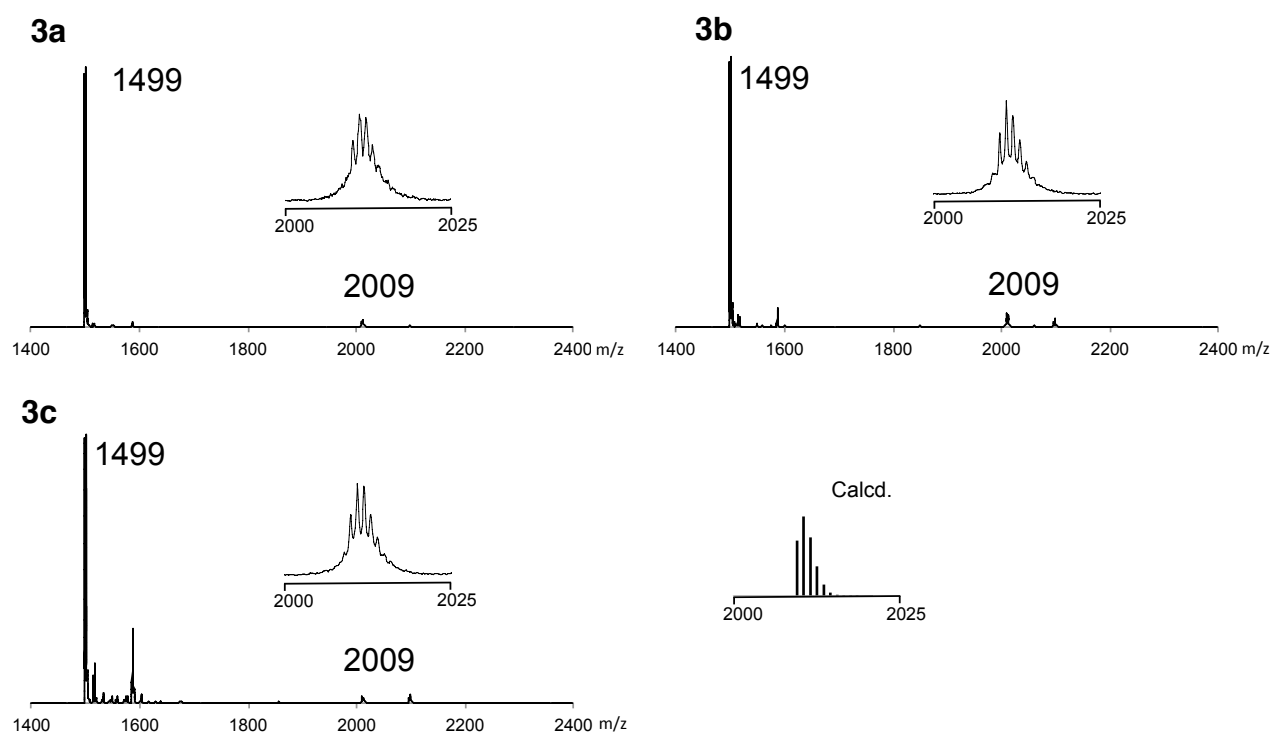


Figure S3. Negative-mode MALDI-TOF mass spectrum of **3a**, **3b**, and **3c**, and the simulated isotope pattern of the parent peak. Matrix: 1,1,4,4-tetraphenyl-1,3-butadiene.

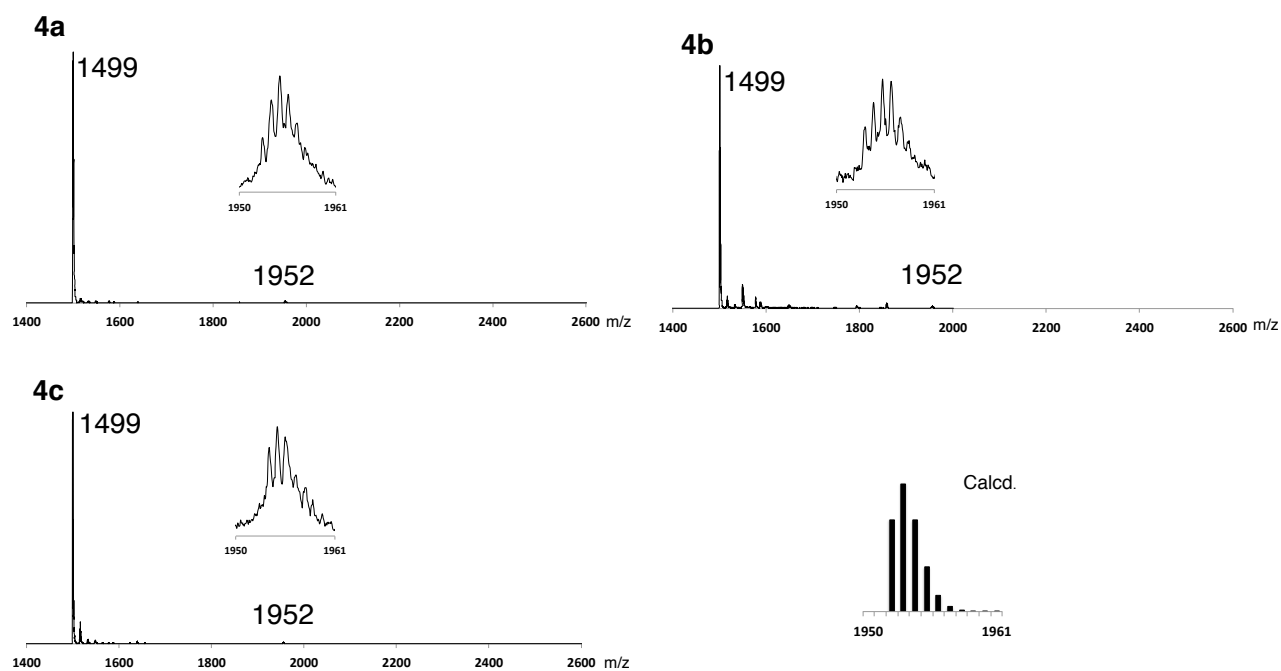


Figure S4. Negative-mode MALDI-TOF mass spectrum of **4a**, **4b**, and **4c**, and the simulated isotope pattern of the parent peak. Matrix: 1,1,4,4-tetraphenyl-1,3-butadiene.

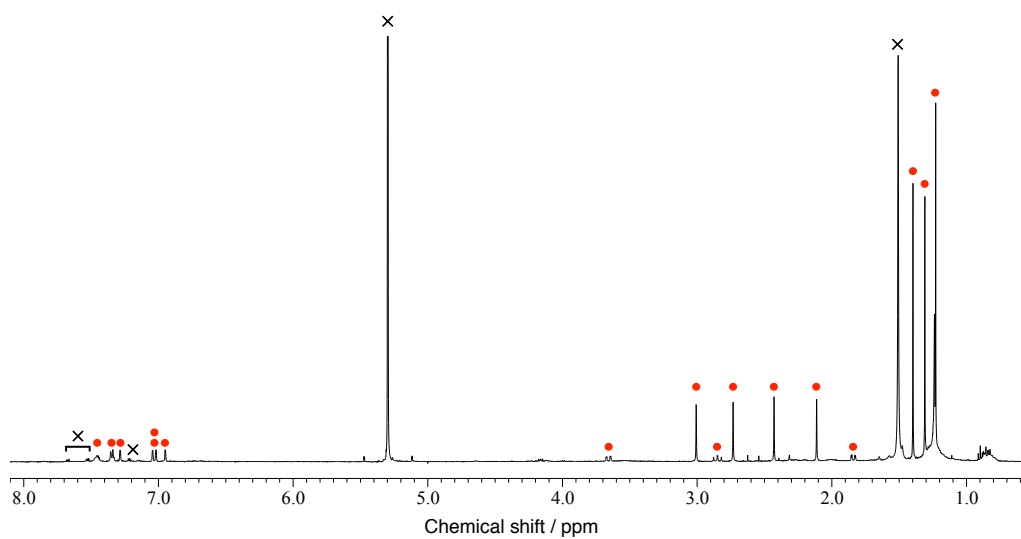


Figure S5. 500 MHz ^1H NMR of **3a** recorded at 293 K in CD_2Cl_2 .

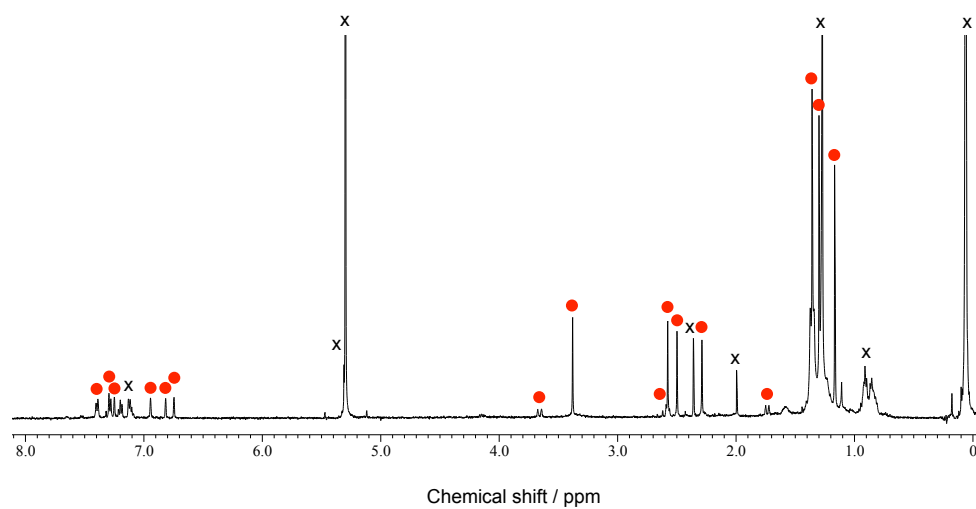


Figure S6. 500 MHz ^1H NMR of **3b** recorded at 293 K in $\text{CD}_2\text{Cl}_2 / \text{CS}_2(1:1)$.

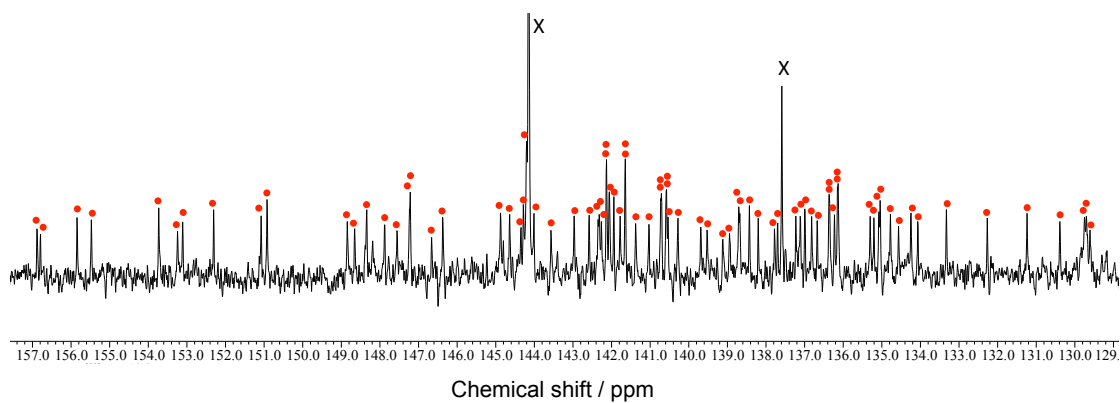
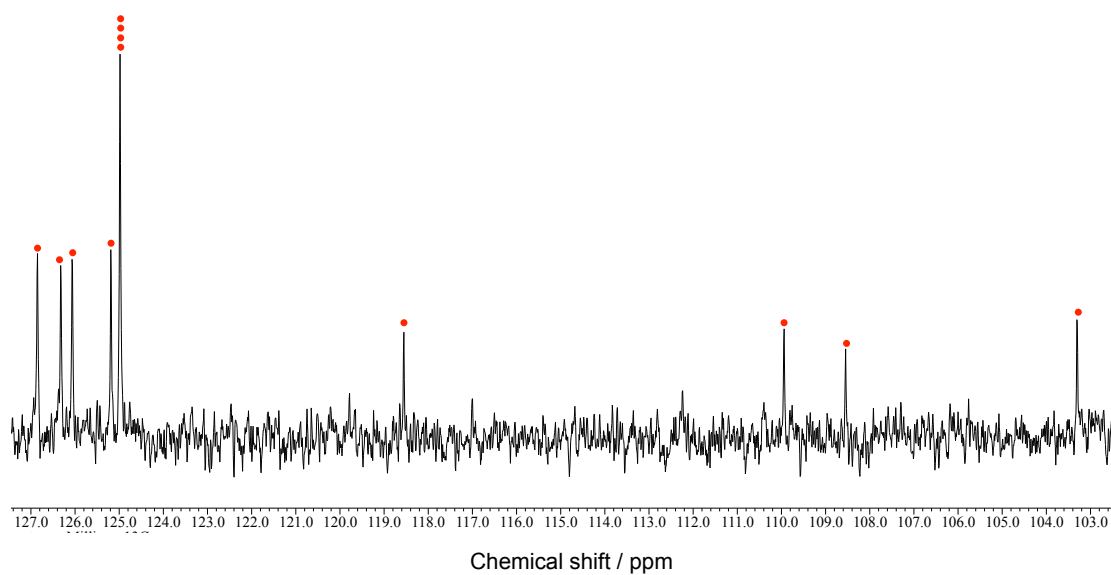
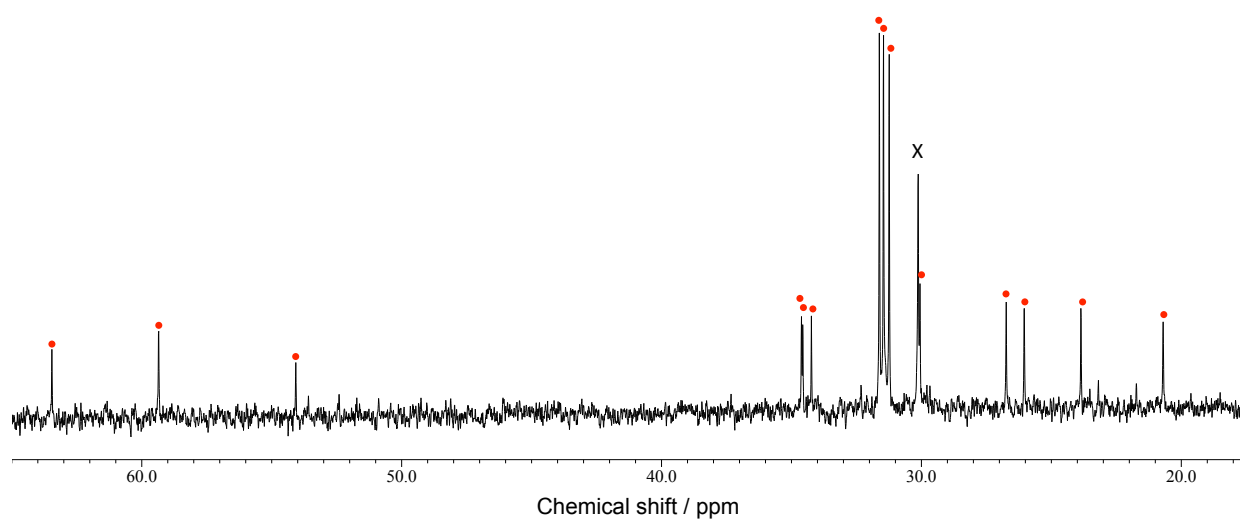


Figure S7. 125 MHz ^{13}C NMR spectra of **3a** recorded at 293 K in $\text{CDCl}_3/\text{CS}_2(1:1)$.

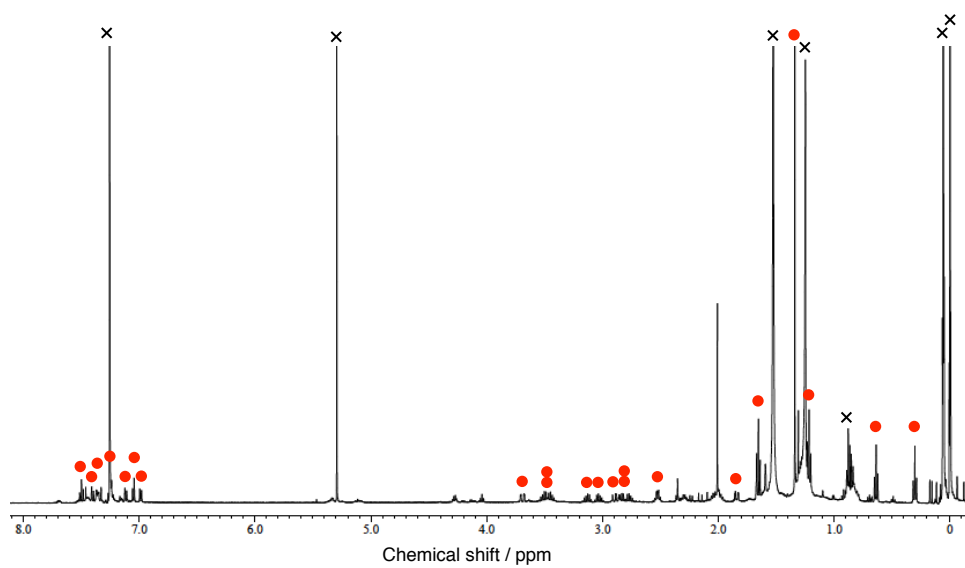


Figure S8. 500 MHz ^1H NMR of **4a** recorded at 293 K in $\text{CDCl}_3/\text{CS}_2(1:1)$.

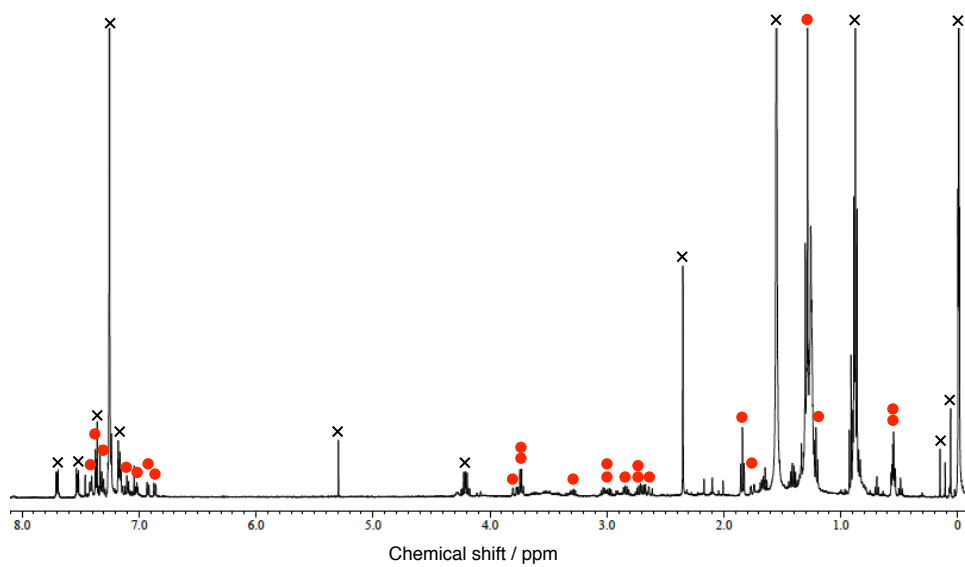


Figure S9. 500 MHz ^1H NMR of **4b** recorded at 293 K in $\text{CDCl}_3/\text{CS}_2(1:1)$.

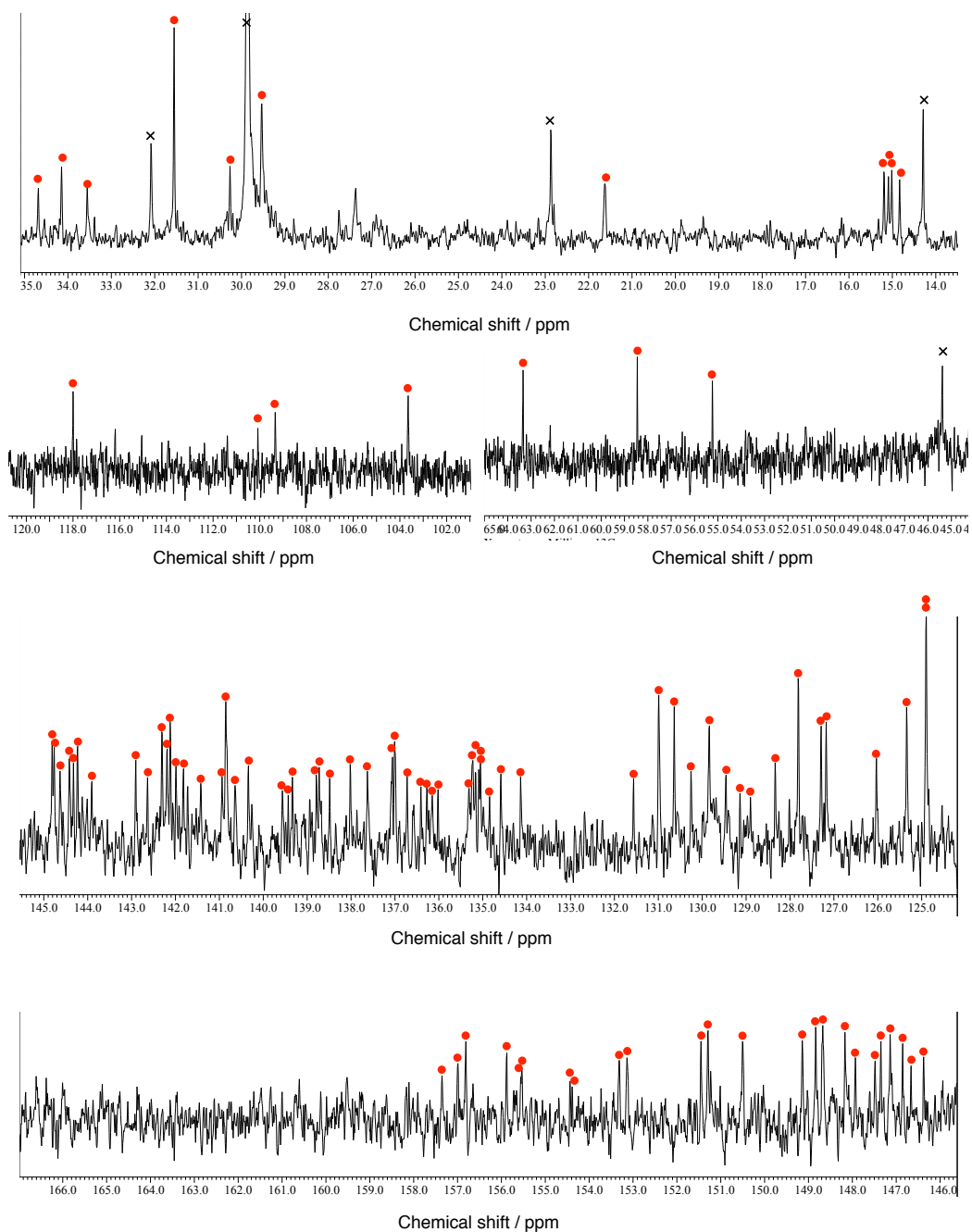
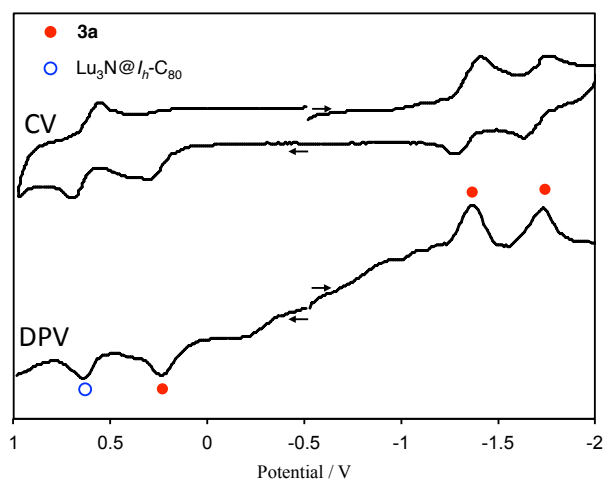


Figure S10. 125 MHz ^{13}C NMR spectra of **4a** recorded at 293 K in $\text{CDCl}_3/\text{CS}_2(1:1)$.

(a)



(b)

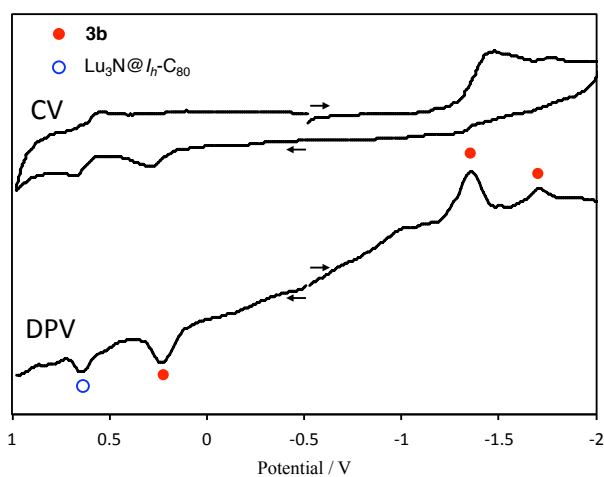
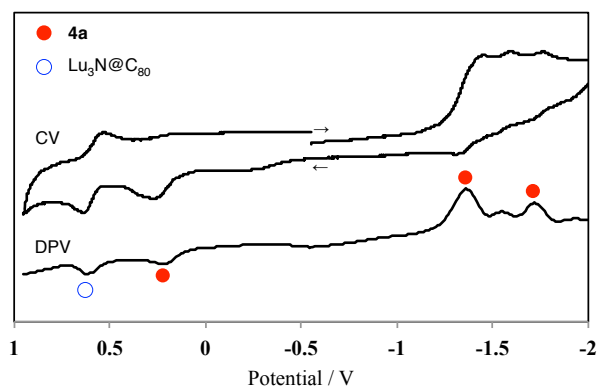


Figure S11. Cyclic voltammograms (CV) and differential pulse voltammograms (DPV) of (a) **3a** and (b) **3b** in ODCB containing 0.1 M $(n\text{-Bu})_4\text{NPF}_6$. Conditions: working electrode, a glassy carbon electrode; counter-electrode, Pt wire; reference electrode, SCE; CV scan rates, 20 mV/s; DPV scan rate, 50 mV/s.

(a)



(b)

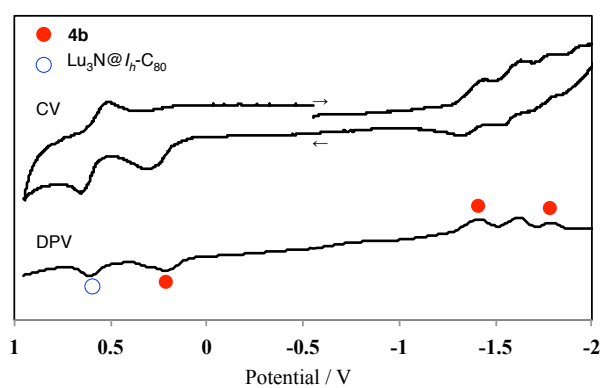


Figure S12. Cyclic voltammograms (CV) and differential pulse voltammograms (DPV) of (a) **4a** and (b) **4b** in ODCB containing 0.1 M $(n\text{-Bu})_4\text{NPF}_6$. Conditions: working electrode, a glassy carbon electrode; counter-electrode, Pt wire; reference electrode, SCE; CV scan rates, 20 mV/s; DPV scan rate, 50 mV/s.

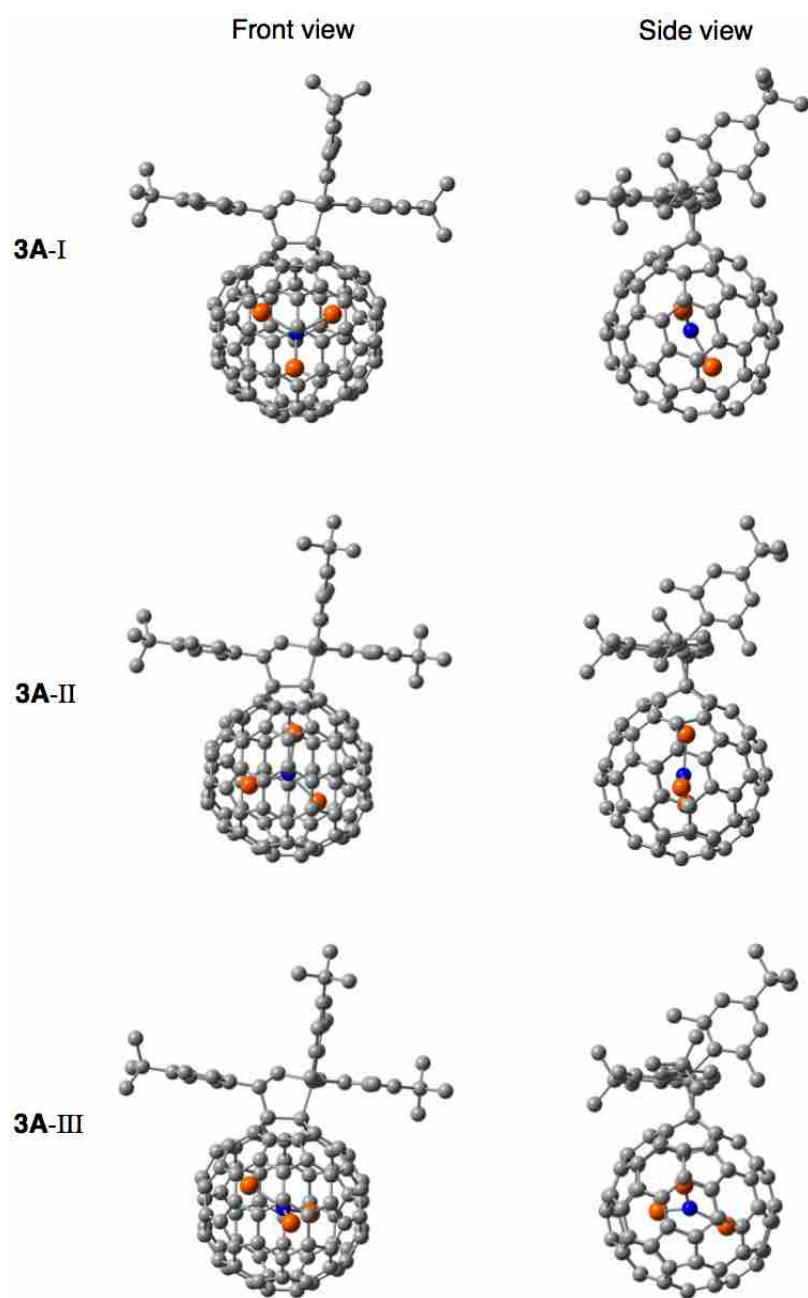


Figure S13. Optimized structures of **3A-I**, **3A-II**, and **3A-III**.

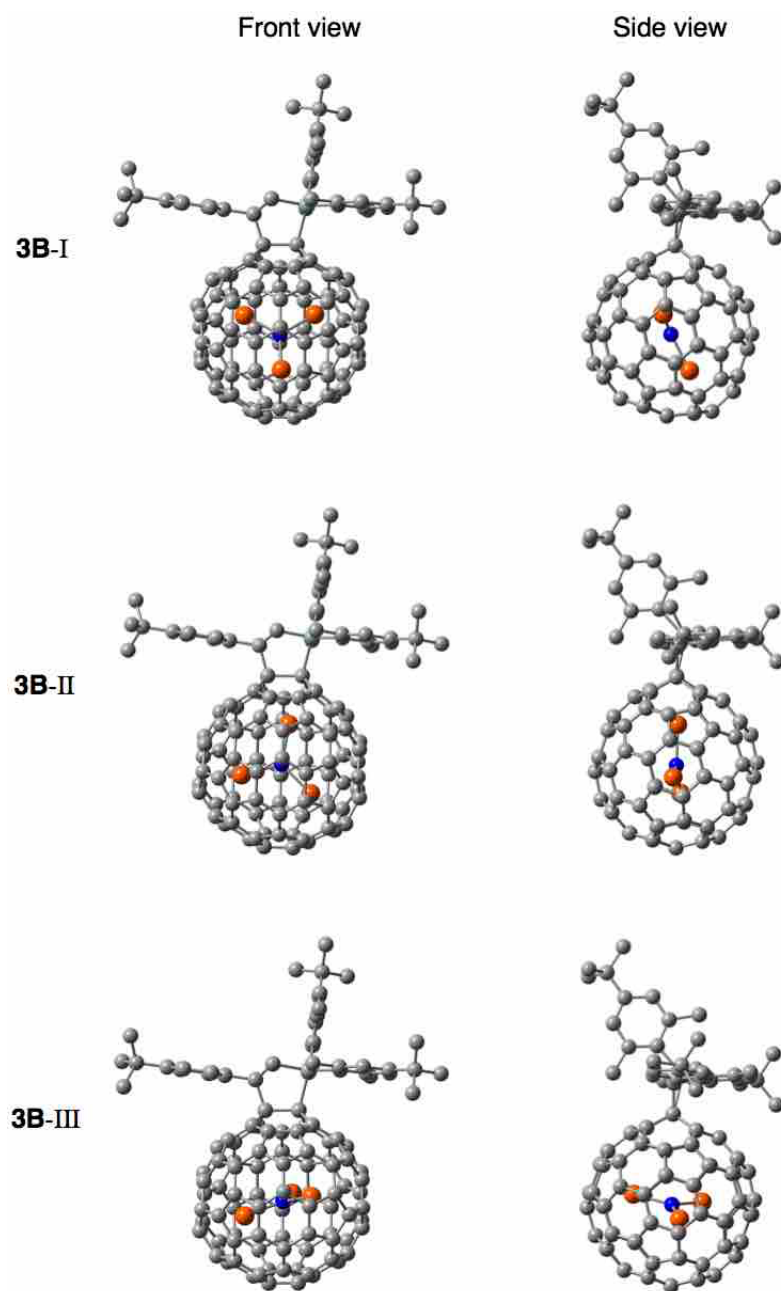


Figure S14. Optimized structures of **3B-I**, **3B-II**, and **3B-III**.

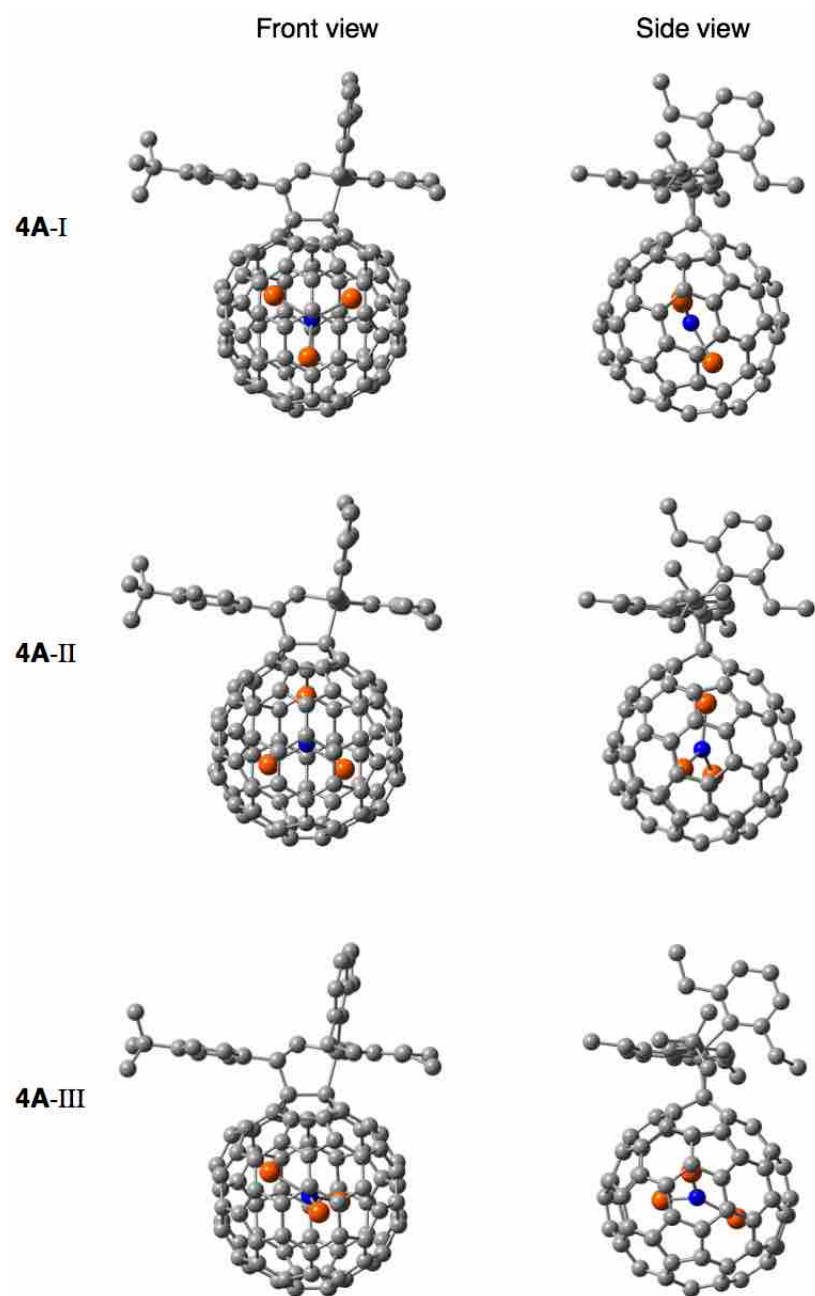


Figure S15. Optimized structures of **4A-I**, **4A-II**, and **4A-III**.

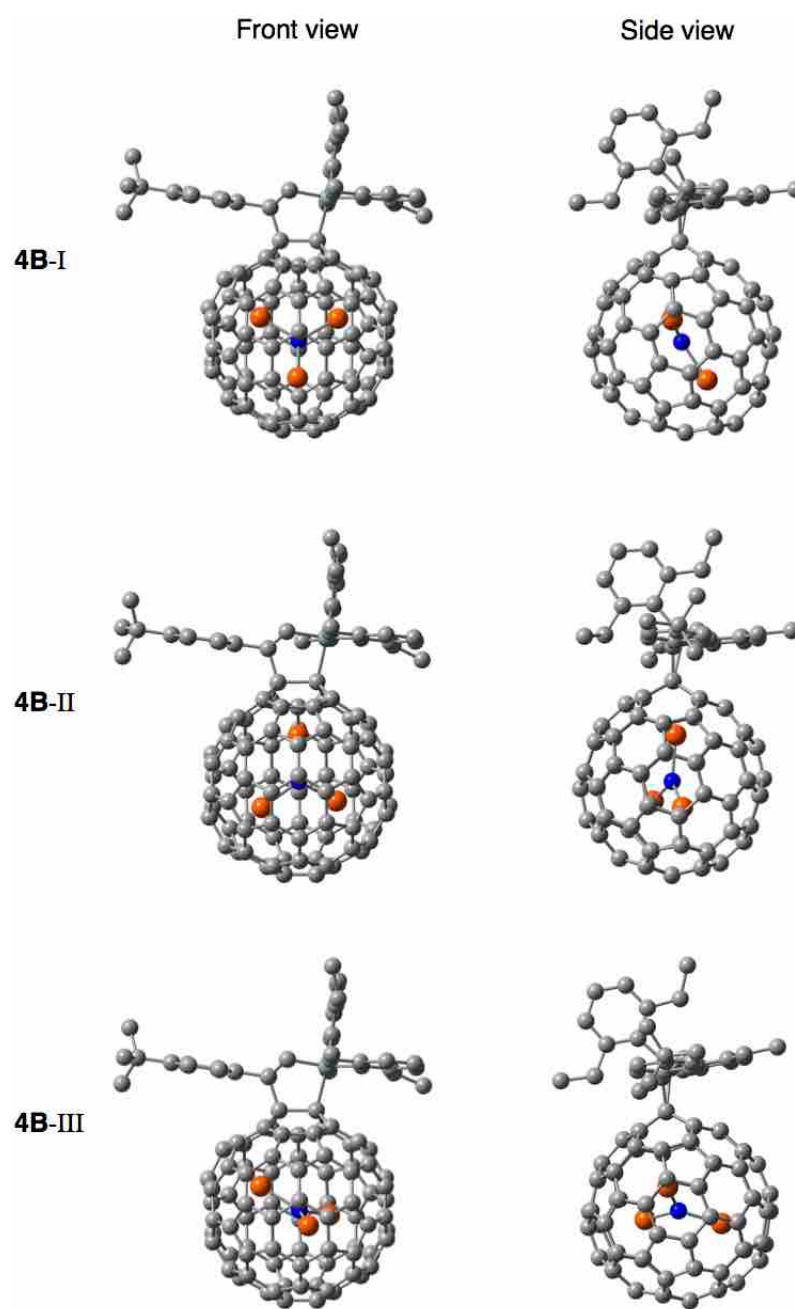


Figure S16. Optimized structures of **4B-I**, **4B-II**, and **4B-III**.

Table S1. Cartesian coordinates of optimized structures.**3A-I**

C	-2.44222900	2.73204800	2.98298300
C	-2.84686000	1.59785000	3.75725300
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C	-2.40383700	-0.75940100	4.18654200
C	-3.77729600	-1.07188900	3.83512500
C	-4.75667500	-0.06862000	3.49177900
C	-2.48056500	-0.97000200	-3.82105500
C	-1.99498000	0.37622300	-3.88885400
C	-0.64862000	0.69655100	-3.50959100
C	0.22395600	-0.32221100	-3.04173600
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C	3.31228400	5.29163400	-2.51856300
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C	4.32853600	1.19361800	-1.25384000
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H	3.89515100	1.11374700	-2.25325900
C	3.45451700	2.10686100	-0.36716800
H	3.88525900	2.11208700	0.64452800
Lu	-0.94908600	-1.82401600	-0.00029200
Lu	-3.90944300	-0.19971500	1.22925600
Lu	-1.47035700	1.57507000	-0.63704500

3A-II

C	-2.38151800	2.74544100	3.00686900
C	-2.79083300	1.61710200	3.78879100
C	-1.86441300	0.58304000	4.13303300
C	-0.50074700	0.75433000	3.74092400
C	-4.15771600	1.31366300	3.46258600
C	-2.36387700	-0.75537400	4.22410700
C	-3.72367500	-1.06365800	3.87889200
C	-4.61946900	-0.03886700	3.44829600
C	-2.53062700	-0.99588500	-3.81024600
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C	-0.25783400	-1.70664600	-3.09020200
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C	1.19543000	2.05813700	0.82776900
C	-0.08724200	1.88277900	2.96537300
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C	-0.83461100	3.46748800	1.28432500
C	1.00086100	1.47324200	2.10127500
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C	-5.38392100	-1.89399100	-1.80012100
C	-4.30961100	-2.30587600	-2.66473100
C	-3.36898100	-3.28626600	-2.23136700
C	-3.59782700	-3.90123800	-0.94084300
C	-4.73058200	-3.58755200	-0.09232900
C	-3.89978000	-1.17296300	-3.44540200
C	-2.02275700	-3.15703500	-2.67554000
C	-4.32823000	-3.79683400	1.31529100
C	-6.04842200	-1.58985300	0.51997200

C	-5.61493400	-1.73441500	1.89464500
C	-4.73619400	-2.79915600	2.31990800
C	1.28641200	0.05972800	2.37942700
C	0.32507100	-0.36389300	3.38124300
C	-3.48890700	3.14698000	2.16869000
C	-4.58512700	2.24391500	2.45570900
C	0.17831200	-2.64863800	-2.09825700
C	-0.91852100	-3.54253500	-1.83349300
C	-4.71724600	-0.05009700	-3.06889600
C	-5.63185000	-0.49241500	-2.05162400
C	-0.20438400	-1.68426800	3.39749700
C	-1.54316500	-1.87540700	3.87071600
C	-1.12775800	-4.08190200	-0.53726200
C	-1.94174400	3.90101200	0.46216400
C	-3.31654200	3.77424600	0.88428300
C	-4.19551300	1.28035600	-3.07228400
C	1.11454500	-2.27164200	-1.08744100
C	-3.75709400	-2.38824500	3.29642500
C	-2.38937700	-2.87665300	3.28353900
C	-1.93166800	-3.73798300	2.24208000
C	-2.91319400	-4.20589000	1.27757100
C	-2.49133400	-4.28615900	-0.10669100
C	1.83161300	-0.83743000	1.40771500
C	1.75219200	-0.98108000	-1.15578900
C	1.23518100	-2.13880000	1.40369700
C	0.27808200	-2.57640400	2.40465000
C	-0.56266100	-3.58783300	1.83278200
C	-0.15669700	-3.76908000	0.46243900
C	0.94878400	-2.89475200	0.19266000
C	-5.58639200	-0.40225100	2.46923700
C	-6.02054000	0.53825900	1.46994600
C	-6.30248100	-0.19218500	0.26744300
C	-6.04762800	0.38005500	-1.01242300
C	-5.49521400	1.87196500	1.42730500
C	-0.17990900	3.23159600	-0.93070900
C	-1.53366400	3.72837000	-0.92073000
C	-2.49919500	3.38300200	-1.93289300
C	-2.85790200	1.45652600	-3.52708400
C	-2.01633200	2.46790000	-2.92890400
C	-3.91412800	3.33866300	-1.55984100
C	-4.33699500	3.54577200	-0.14796300
C	-5.35245800	2.52816100	0.13889100
C	-5.58037400	1.74891800	-1.05374700
C	-4.69379100	2.22229600	-2.08597800
N	-2.10422700	-0.19822600	0.16400100
C	2.44640200	-0.28385800	0.07928600
C	2.09303300	1.38098600	-0.23255100
Si	4.41430700	-0.45040100	-0.32566100
C	4.62159500	-2.14880200	-1.17263200
C	4.65771800	-2.33902500	-2.58191300
C	4.74926600	-3.30047500	-0.35395500
C	4.80769200	-3.62375400	-3.11050200
C	4.88686500	-4.57126000	-0.93195100
H	4.83096700	-3.72541600	-4.19229700
H	4.96960100	-5.42003900	-0.26188400
C	5.86837800	-0.19578400	0.91677400
C	7.16986100	-0.24913100	0.34204600
C	5.79093100	0.09518700	2.30378100
C	8.30640500	-0.01958300	1.13271600
C	6.95201500	0.31541500	3.05087100
H	9.27257200	-0.07036400	0.64230600
H	6.83633900	0.53740600	4.10856600
C	3.40936200	3.54182400	-0.83109800
C	3.48135200	4.56292600	0.12227600
C	3.27764800	3.92359600	-2.17435800
C	3.41367000	5.90931100	-0.24199800
H	3.59590400	4.30552000	1.17310100
C	3.20746800	5.26659700	-2.53509800
H	3.23019300	3.16849600	-2.95318000
C	3.27134500	6.29677500	-1.58057500

H	3.47720900	6.65691900	0.54089500
H	3.10286500	5.51201800	-3.58847300
C	3.18817000	7.76792200	-2.02480600
C	4.35340700	8.08184000	-2.99346600
H	4.32505100	7.44703100	-3.88533300
H	4.30185900	9.12591400	-3.32598400
H	5.32224000	7.92845200	-2.50431600
C	1.84166500	8.00911900	-2.74864100
H	1.73472000	7.37093600	-3.63193200
H	0.99624200	7.80224900	-2.08264500
H	1.76782300	9.05242500	-3.07938300
C	3.27669900	8.74427900	-0.83641500
H	2.45873600	8.59419200	-0.12248800
H	4.22530000	8.64472500	-0.29644000
H	3.21124600	9.77557900	-1.20115500
C	4.36938600	1.19280400	-1.28957800
H	5.36440300	1.63519700	-1.39215000
H	3.93053200	1.11846500	-2.28657200
C	3.49147000	2.08847000	-0.39108800
H	3.92586700	2.09601500	0.61881800
Lu	-0.05414600	-0.13095800	0.16189300
Lu	-3.05340600	1.59718300	-0.23826600
Lu	-3.23071500	-1.85103200	0.67668000
C	7.43916400	-0.56950500	-1.11746100
H	7.28546200	-1.63144300	-1.33663900
H	6.79971300	-0.00715000	-1.80457700
H	8.47469900	-0.32488300	-1.37321900
C	4.48086900	0.17363100	3.04990800
H	3.80328000	0.91861000	2.62306200
H	3.95040400	-0.78406900	3.04678900
H	4.64369300	0.44941200	4.09629900
C	4.53980200	-1.20480200	-3.58006200
H	3.55727300	-0.72233200	-3.53510500
H	5.29514500	-0.42755600	-3.42168000
H	4.66942400	-1.57956800	-4.59983400
C	4.91907400	-4.76897100	-2.31206600
C	8.23498000	0.26382000	2.49571800
C	4.77222200	-3.24229200	1.16188900
H	3.99577000	-2.59128800	1.57450100
H	4.60805300	-4.23843800	1.58456500
H	5.73437700	-2.87517700	1.53616500
C	5.06583200	-6.15543500	-2.96242800
C	9.47405700	0.51844000	3.37113700
C	10.78845800	0.40450000	2.57533700
H	11.63923400	0.58923900	3.24092300
H	10.91813900	-0.59417100	2.14281200
H	10.83979700	1.13884000	1.76339300
C	9.51520500	-0.51817900	4.51933200
H	8.62413700	-0.46179500	5.15324700
H	9.58088300	-1.53855800	4.12447800
H	10.39035400	-0.34350000	5.15696000
C	9.39409900	1.94319600	3.96979100
H	9.37661200	2.70049400	3.17760400
H	8.49594200	2.07832400	4.58138300
H	10.26527900	2.13777300	4.60728400
C	6.35187900	-6.18493100	-3.82278200
H	7.24023100	-6.00537800	-3.20621700
H	6.46480800	-7.16364200	-4.30495800
H	6.33231200	-5.42484200	-4.61073900
C	3.83873300	-6.43104200	-3.86446800
H	2.91143100	-6.41479400	-3.28068000
H	3.74271500	-5.68846000	-4.66349200
H	3.92754400	-7.41775800	-4.33533200
C	5.15769900	-7.28631500	-1.92012400
H	6.02905500	-7.16987300	-1.26552800
H	4.26093900	-7.33536100	-1.29212100
H	5.25607900	-8.25066900	-2.43128700

3A-III

C	-2.42895400	2.24569800	3.35965700
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C	-2.99828400	1.05594900	3.94834700
C	-2.19736900	-0.11295200	4.20563500
C	-0.80802200	-0.01312600	3.85400500
C	-4.38219900	0.94722700	3.50212300
C	-2.85228400	-1.41562300	4.11734800
C	-4.27316300	-1.54914200	3.69267000
C	-5.03723700	-0.33919500	3.32769200
C	-2.44057300	-0.28644300	-4.00723400
C	-1.81589100	0.99221200	-3.80881300
C	-0.47112300	1.09888600	-3.31302500
C	0.25802900	-0.06518900	-2.98674000
C	-0.33740400	-1.33872000	-3.27032600
C	-1.65621100	-1.49296300	-3.84470900
C	-0.34094200	2.31574800	-2.53536100
C	1.17009100	0.02073100	-1.88201000
C	1.33320700	1.24393200	-1.13376300
C	0.60098300	2.42966600	-1.43741900
C	0.45261800	2.77234500	1.00312000
C	1.20272600	1.56897200	1.27198200
C	-0.24305000	1.18322900	3.27505000
C	-1.04903500	2.30565200	2.98600300
C	-0.68652500	3.08759100	1.83836300
C	0.83923500	0.81382400	2.40115900
C	-5.80153700	-1.93049500	-1.14291900
C	-5.48711800	-1.19849300	-2.32565900
C	-4.40368400	-1.60472100	-3.19963100
C	-3.63539100	-2.81906800	-3.01137600
C	-3.96555100	-3.53046400	-1.79048100
C	-5.03574800	-3.11070800	-0.89968400
C	-3.83532100	-0.37829400	-3.73777000
C	-2.21300400	-2.78250300	-3.41088200
C	-4.70525100	-3.50345400	0.44365800
C	-6.30681400	-1.20954300	-0.01626400
C	-5.96936100	-1.60616700	1.32064100
C	-5.14411800	-2.73426100	1.57654300
C	0.95832600	-0.63680600	2.45084900
C	-0.06133900	-1.12894800	3.33783300
C	-3.42768500	2.87554600	2.54936600
C	-4.61877900	2.07171300	2.61305700
C	-0.05954600	-2.46807100	-2.44318600
C	-1.19250200	-3.37227400	-2.50402900
C	-4.57340900	0.74208600	-3.22476700
C	-5.58854800	0.23470000	-2.35057100
C	-0.70069700	-2.37126000	3.10798100
C	-2.09632200	-2.47582900	3.47599500
C	-1.55192700	-4.03624000	-1.26234200
C	-1.67102600	3.77446200	1.04561200
C	-3.07900300	3.60922400	1.36474500
C	-3.92838900	1.99614900	-2.95670900
C	0.84154100	-2.33744200	-1.31911000
C	-4.30499700	-2.68113000	2.75853500
C	-2.98446600	-3.25601300	2.66533600
C	-2.51607200	-3.98459400	1.50795200
C	-3.41960900	-4.13942200	0.41632500
C	-2.94752300	-4.15005700	-0.94958000
C	1.40533300	-1.37006900	1.34419400
C	1.52169400	-1.10805800	-1.11791700
C	0.80345800	-2.63705700	1.13672400
C	-0.23825700	-3.13222300	1.99966700
C	-1.12930800	-3.93540300	1.21582100
C	-0.64337800	-3.94245000	-0.14838900
C	0.55546500	-3.15521700	-0.18709900
C	-5.86809100	-0.41397500	2.15123300
C	-6.13231000	0.71686000	1.28121700
C	-6.39490700	0.22655300	-0.03888100
C	-6.00038000	0.97156000	-1.19370000
C	-5.48315000	1.97250500	1.47980700
C	0.21796300	3.33330000	-0.32917200
C	-1.14578200	3.93358300	-0.30230600
C	-2.10049700	3.71290900	-1.38615000

C	-2.54898800	2.11418600	-3.29497800
C	-1.64528200	2.94057200	-2.51861000
C	-3.50065800	3.58703900	-1.07601800
C	-3.99235600	3.57932600	0.28292100
C	-5.18409800	2.76662300	0.33349200
C	-5.42394100	2.26116800	-0.98665000
C	-4.39729600	2.77004200	-1.85872100
N	-2.32734400	-0.18296200	0.06637300
C	2.16469200	-0.69305100	0.21568400
C	2.07996100	0.96197000	0.17817200
C	4.37955700	0.64816900	-0.79041600
H	5.42657700	0.96362300	-0.78292500
H	4.00013400	0.77363500	-1.80661100
Si	4.13520100	-1.10090600	-0.07188100
C	3.55941500	1.51280200	0.19270600
H	3.92696600	1.31347100	1.21001400
C	4.23656000	-2.68649300	-1.13723200
C	4.20250700	-3.94726000	-0.48690500
C	4.34736100	-2.68626200	-2.55566400
C	4.25886400	-5.13405100	-1.23375800
C	4.40802800	-3.89419000	-3.25551500
C	4.36110500	-5.14346500	-2.62431500
H	4.21931900	-6.07101500	-0.68861500
H	4.49158700	-3.84739500	-4.33824000
C	5.52180700	-1.19322700	1.27460500
C	5.37663800	-1.08550300	2.68196000
C	6.84922700	-1.32262400	0.77502800
C	6.49641400	-1.10293200	3.51892800
C	7.94331000	-1.33204100	1.65464400
C	7.80375500	-1.22468200	3.03736100
H	6.32717100	-1.01630000	4.58909900
H	8.93200500	-1.42857900	1.21896300
C	3.69775100	3.01188800	-0.02112300
C	3.78167400	3.87181900	1.08387400
C	3.76623500	3.59532000	-1.29105000
C	3.90946200	5.24884900	0.92416000
H	3.74983000	3.45485700	2.08822100
C	3.89152800	4.97753800	-1.44995800
H	3.72540200	2.97166700	-2.17915000
C	3.96286000	5.84140000	-0.34899600
H	3.97364500	5.86944200	1.81381600
H	3.93701800	5.37377400	-2.45844200
C	4.10558900	7.36763300	-0.48635700
C	5.43389500	7.81985000	0.16605600
H	6.29225800	7.34736800	-0.32527300
H	5.55002300	8.90762900	0.08257300
H	5.47334000	7.56066300	1.22933700
C	2.92177100	8.06281500	0.22783900
H	1.96574300	7.76362800	-0.21671200
H	2.88606600	7.81574100	1.29405800
H	3.01166100	9.15269300	0.14140000
C	4.11198400	7.82519900	-1.95741300
H	4.95370200	7.39866800	-2.51509200
H	3.18486500	7.55039100	-2.47328200
H	4.20559100	8.91615900	-2.00413300
C	4.40999700	-1.41917200	-3.38492000
H	3.48911600	-0.83198500	-3.30288000
H	5.23948400	-0.76833200	-3.08786300
C	4.12933100	-4.10475500	1.02039500
H	5.09067700	-3.88207500	1.49621600
H	3.37894700	-3.45348600	1.47767000
C	4.03180500	-0.95824700	3.35468100
H	4.14454300	-0.87706000	4.44029800
H	3.48339800	-0.07276300	3.02068600
C	7.19231300	-1.48183200	-0.69563700
H	6.93474100	-2.47912000	-1.06726800
H	6.67701200	-0.76065300	-1.33684200
H	8.26603900	-1.33733400	-0.85023100
H	3.39214000	-1.82393700	3.15855900
H	3.85755300	-5.13220800	1.28220000

H	4.54961300	-1.66136800	-4.44293800
C	4.42051800	-6.43608900	-3.45655300
C	5.74839900	-6.47569600	-4.25028600
H	5.80022400	-7.38563500	-4.86075200
H	6.61029100	-6.47154600	-3.57308400
H	5.84726000	-5.61699300	-4.92255800
C	3.23119200	-6.46424700	-4.44654800
H	3.25246800	-5.61317400	-5.13521000
H	2.27534300	-6.43732700	-3.91094600
H	3.25833400	-7.38095200	-5.04846900
C	4.34616400	-7.70197100	-2.58176500
H	3.41005500	-7.75138800	-2.01405100
H	5.18002700	-7.75734100	-1.87269200
H	4.39441100	-8.59292700	-3.21804400
C	8.99458500	-1.23269800	4.01154000
C	10.34658200	-1.37057800	3.28577300
H	11.16031900	-1.37020300	4.01997700
H	10.52552100	-0.53937200	2.59423900
H	10.41294400	-2.30705600	2.72028800
C	8.84921400	-2.42243200	4.99020200
H	8.84759900	-3.37628700	4.45022800
H	7.92072500	-2.36385300	5.56763200
H	9.68488300	-2.43502300	5.70065900
C	9.01083200	0.09081800	4.81317700
H	8.09021500	0.22990000	5.38947100
H	9.12036400	0.95254000	4.14477300
H	9.85086700	0.09826700	5.51862600
Lu	-1.32913200	1.58751900	-0.26748900
Lu	-3.15898300	-0.60948700	1.88224800
Lu	-2.36863100	-1.55332700	-1.45063900

3B-I

C	2.64446300	1.39186600	-3.50710000
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C	2.17051400	-1.04302600	-3.69971700
C	0.78802000	-0.74962300	-3.51686500
C	4.43247300	-0.08395900	-3.19163600
C	2.66410000	-2.29071200	-3.20619600
C	4.01247300	-2.41421200	-2.67972100
C	4.96995600	-1.33045400	-2.69676700
C	2.20031700	0.71760300	4.20206000
C	1.72261500	1.96943800	3.69708500
C	0.40786700	2.08060200	3.13458400
C	-0.43946300	0.94288600	3.05545700
C	-0.02452500	-0.27304000	3.66295800
C	1.29122300	-0.38862100	4.22320300
C	0.42408100	3.08899600	2.09622500
C	-1.27702200	0.83817100	1.90031000
C	-1.32449900	1.86391000	0.90615700
C	-0.46010800	3.00770300	0.95515700
C	-0.20532700	2.71754900	-1.47186200
C	-1.09281800	1.57987500	-1.49945500
C	0.34562600	0.59439300	-3.27561000
C	1.26762300	1.66648500	-3.22580100
C	0.96988900	2.72415600	-2.30608100
C	-0.79514800	0.55640000	-2.39677500
C	5.43788500	-1.88393600	2.01849200
C	5.18613400	-0.85575800	2.96755800
C	4.04186500	-0.91456600	3.83728800
C	3.12105100	-2.00383400	3.76974000
C	3.42130000	-3.07568700	2.88138100
C	4.57060900	-3.01755700	2.02113600
C	3.58576100	0.43106700	4.05417200
C	1.73701700	-1.73316000	4.01762600
C	4.25330300	-3.69319600	0.79271900
C	6.04898400	-1.50983800	0.75743600
C	5.83366200	-2.23100400	-0.48155400
C	4.81296200	-3.27441100	-0.46128200
C	-1.05420700	-0.85459000	-2.07933800
C	-0.06336200	-1.63611900	-2.77526900

C	3.68251900	2.11274600	-2.82716000
C	4.78167600	1.20180700	-2.62073600
C	-0.43454600	-1.56073200	3.14437900
C	0.67632700	-2.47587100	3.35916400
C	4.45242400	1.32642300	3.33737400
C	5.43853600	0.53102400	2.65755100
C	0.44339000	-2.83269100	-2.21936600
C	1.80884500	-3.17847500	-2.47993700
C	0.96820600	-3.54632000	2.43061800
C	1.99134100	3.50530600	-1.66374800
C	3.37989300	3.13080200	-1.86852300
C	3.95071800	2.53062300	2.75636000
C	-1.32711200	-1.66274700	2.00638700
C	3.95040200	-3.37727100	-1.59765800
C	2.59053700	-3.85545300	-1.48677100
C	2.03453600	-4.22250100	-0.22172000
C	2.89544600	-4.17593000	0.90221000
C	2.37052900	-3.79297800	2.19461200
C	-1.60862000	-1.24635000	-0.85989300
C	-1.74577100	-0.42499300	1.41351400
C	-1.16545300	-2.50188000	-0.30385700
C	-0.12405300	-3.24379400	-0.96979700
C	0.62272200	-3.97731700	0.01292500
C	0.02736900	-3.73683400	1.32244900
C	-1.13072100	-2.82733500	1.12111800
C	5.95739100	-1.26847300	-1.60419900
C	6.21735800	0.04718900	-0.98554500
C	6.28830500	-0.12339300	0.44835700
C	5.94683000	0.92303100	1.38971600
C	5.63013700	1.28693900	-1.47735100
C	0.04701300	3.56381600	-0.30964300
C	1.45059500	4.04215600	-0.41790700
C	2.35139100	4.02014100	0.74074900
C	2.57976300	2.87121100	2.98803200
C	1.78753000	3.58524400	2.00187000
C	3.72976000	3.64824500	0.53014400
C	4.25557100	3.26117100	-0.76208400
C	5.35946900	2.35263100	-0.55875900
C	5.52026600	2.17749000	0.85838800
C	4.52703400	2.96965400	1.52948500
N	2.16497800	-0.16439700	0.23354400
C	-2.35600300	-0.25010900	0.02295200
C	-2.05745200	1.35175700	-0.33607300
Si	-4.31398900	-0.49816200	-0.42712500
C	-3.46072000	2.03450700	-0.58090300
H	-3.94461800	2.05143200	0.40631900
C	-4.26933300	1.08536600	-1.49043200
H	-3.76451000	0.96527800	-2.45205500
H	-5.26329500	1.50001200	-1.68194400
C	-3.41126700	3.48164600	-1.04505400
C	-3.51148300	4.51910300	-0.10697600
C	-3.28340200	3.84444200	-2.39031900
C	-3.46701100	5.85533300	-0.49602100
H	-3.62806300	4.27638600	0.94703200
C	-3.24021000	5.18526800	-2.77906500
H	-3.21694300	3.07714600	-3.15631700
C	-3.32678500	6.22586200	-1.84406800
H	-3.54759400	6.62080000	0.27099200
H	-3.13898500	5.40821200	-3.83554100
C	-3.27935000	7.71361300	-2.23526600
C	-4.59076000	8.40626200	-1.79371800
H	-4.56886900	9.46986600	-2.06163500
H	-5.45923000	7.95031200	-2.28289200
H	-4.74310800	8.33879200	-0.71136800
C	-3.11836000	7.91524200	-3.75409900
H	-2.18933700	7.47026500	-4.12825800
H	-3.95550700	7.48334500	-4.31454300
H	-3.08678100	8.98660200	-3.98266500
C	-2.08025200	8.39118600	-1.52943600
H	-2.15496400	8.31824000	-0.43937700

H	-1.13444700	7.92664700	-1.83082100
H	-2.03578800	9.45573200	-1.79032700
C	-4.50720300	-2.23573000	-1.20022400
C	-4.66968100	-3.34554900	-0.33171700
C	-4.51366600	-2.49434900	-2.59911000
C	-4.81887500	-4.64025800	-0.85006700
C	-4.67417900	-3.80076600	-3.06909300
C	-4.82738700	-4.90349800	-2.21973900
H	-4.93129000	-5.45421500	-0.14193500
H	-4.67505000	-3.95378300	-4.14511900
C	-5.80009800	-0.19070400	0.76685300
C	-5.75377100	0.16745000	2.14059700
C	-7.09038100	-0.28662300	0.17194000
C	-6.93263100	0.40742200	2.85340400
C	-8.24506500	-0.03110700	0.92784000
C	-8.20365500	0.31591500	2.27712000
H	-6.84171200	0.67907400	3.90176800
H	-9.20079900	-0.11584900	0.42194100
C	-4.72066900	-3.21472900	1.17885600
H	-3.97418600	-2.51882800	1.57192100
H	-5.70113000	-2.86246800	1.51919600
H	-4.53028000	-4.18286600	1.65269900
C	-4.35354700	-1.41199200	-3.64762000
H	-5.10025900	-0.61766700	-3.54461000
H	-3.36466200	-0.94249000	-3.59942200
H	-4.46320400	-1.83399500	-4.65125700
C	-7.32980500	-0.68631000	-1.27335300
H	-8.36080300	-0.45953800	-1.56216700
H	-6.67721800	-0.16163500	-1.97715300
H	-7.16990000	-1.75833100	-1.43007300
C	-4.46323400	0.31235600	2.91316700
H	-3.87020400	-0.60709700	2.90606500
H	-3.82956200	1.10909100	2.51016600
H	-4.66444700	0.56129800	3.95960300
C	-4.99365700	-6.31633600	-2.80592100
C	-3.75579300	-6.66393000	-3.66744600
H	-3.62437300	-5.95993800	-4.49563100
H	-2.84085300	-6.64532800	-3.06438300
H	-3.86043000	-7.66804600	-4.09649200
C	-6.26190400	-6.35687600	-3.69203300
H	-6.39232800	-7.35636300	-4.12466700
H	-7.15743600	-6.12070000	-3.10577300
H	-6.20435200	-5.64043800	-4.51811200
C	-5.13537500	-7.39278900	-1.71287400
H	-4.25284600	-7.43390400	-1.06442800
H	-6.01576400	-7.22173300	-1.08290100
H	-5.24925300	-8.37813300	-2.17879900
C	-9.46176700	0.59278200	3.11808900
C	-10.75934700	0.43709600	2.30211700
H	-10.87310300	-0.57861100	1.90630800
H	-11.62446300	0.64018100	2.94351300
H	-10.80035200	1.13866700	1.46104600
C	-9.40649400	2.03925900	3.66515800
H	-8.52315400	2.20521600	4.29060300
H	-9.37822800	2.76723700	2.84626900
H	-10.29281500	2.24892800	4.27648800
C	-9.51601600	-0.40084700	4.30318300
H	-9.56545900	-1.43570000	3.94542900
H	-8.63719900	-0.31256600	4.95046100
H	-10.40436100	-0.21067800	4.91780000
Lu	1.50602800	1.77998000	0.19301200
Lu	0.84220500	-1.55652400	0.96473200
Lu	3.93907300	-0.75297800	-0.58942500

3B-II

C	2.53014700	1.32443400	-3.58914900
C	2.97212500	-0.01937300	-3.81456100
C	2.06006800	-1.11840500	-3.74203500
C	0.67899900	-0.82456400	-3.51864000
C	4.32125500	-0.13665600	-3.33234900

C	2.56011300	-2.36599800	-3.24806100
C	3.90096300	-2.48054500	-2.74571700
C	4.77812300	-1.35349200	-2.73943500
C	2.34311900	0.74480400	4.16178300
C	1.84877900	1.98953800	3.66507100
C	0.51815900	2.08879700	3.12943700
C	-0.35600600	0.96498100	3.10042700
C	0.10373200	-0.23725800	3.70000600
C	1.43612700	-0.35169600	4.23100200
C	0.53193100	3.03827200	2.05588000
C	-1.30980900	0.85854400	2.00400400
C	-1.32960700	1.84416900	0.96755800
C	-0.34642600	2.89265200	0.94946400
C	-0.21340100	2.62403400	-1.48794600
C	-1.14480700	1.53554100	-1.48046800
C	0.23398400	0.51711900	-3.29806600
C	1.16372700	1.59743800	-3.28484600
C	0.90738800	2.66487800	-2.38723000
C	-0.89569700	0.48406300	-2.39264700
C	5.52982100	-1.91026500	1.89970300
C	5.28862200	-0.85566300	2.83684200
C	4.17123000	-0.89107500	3.74322900
C	3.24756800	-1.97673000	3.71051200
C	3.53277300	-3.06275100	2.79870600
C	4.70262900	-3.10703700	1.94695000
C	3.72715400	0.45611500	3.96440800
C	1.88244600	-1.69879900	4.00180800
C	4.37477300	-3.89612200	0.74229600
C	6.06224600	-1.52749500	0.62858200
C	5.69433200	-2.23751600	-0.58031500
C	4.83855800	-3.40171600	-0.56689200
C	-1.18093300	-0.92398300	-2.07999100
C	-0.17014700	-1.70886200	-2.77051500
C	3.59755300	2.05454300	-2.94481500
C	4.70403500	1.13463100	-2.78510100
C	-0.28801000	-1.51226700	3.16949900
C	0.81831700	-2.41691000	3.34703500
C	4.56727100	1.33682900	3.19585300
C	5.52932300	0.52765600	2.49666500
C	0.35902900	-2.90489600	-2.21038900
C	1.71985800	-3.25115500	-2.49871700
C	1.08721900	-3.44087900	2.40185700
C	1.97308900	3.42012900	-1.77109300
C	3.36336200	3.14507400	-2.03661300
C	4.05134500	2.54140200	2.62500900
C	-1.17399500	-1.60208200	2.05152400
C	3.90546300	-3.44744800	-1.66805200
C	2.53504600	-3.90683900	-1.51302400
C	2.02510100	-4.26928700	-0.22983600
C	2.95782300	-4.28157500	0.88439600
C	2.46859900	-3.78165900	2.15403800
C	-1.75454600	-1.34258500	-0.83987900
C	-1.81801300	-0.41098600	1.55091600
C	-1.16991900	-2.51460100	-0.27257500
C	-0.17072000	-3.31312400	-0.95841900
C	0.63845300	-3.98256300	0.01838400
C	0.16604300	-3.58631100	1.32090000
C	-0.94625300	-2.69656300	1.15319900
C	5.69514700	-1.26199200	-1.65492300
C	6.08299100	0.01477400	-1.11685800
C	6.30746100	-0.14729300	0.29123500
C	5.99362600	0.89861400	1.20814200
C	5.56067500	1.23585000	-1.65441800
C	0.14630200	3.36074400	-0.30800800
C	1.50100100	3.83641800	-0.46284600
C	2.41744900	3.96836100	0.64338300
C	2.69207300	2.86453000	2.90331000
C	1.88358600	3.52705500	1.90344500
C	3.85174400	3.79598800	0.38792000
C	4.33146400	3.38562200	-0.96054000

C	5.35267300	2.35873200	-0.75665300
C	5.52867200	2.15435500	0.66006000
C	4.60371000	3.00751700	1.36447800
N	2.11046100	-0.18067400	0.19580500
C	-2.44449400	-0.29583500	0.12358500
C	-2.09648800	1.35334100	-0.27527800
Si	-4.41314500	-0.47942000	-0.31117200
C	-3.49941000	2.03627600	-0.49928800
H	-3.95676200	2.06782000	0.49980200
C	-4.34127300	1.09475600	-1.38290200
H	-3.85989000	0.95347400	-2.35358600
H	-5.32993200	1.52902600	-1.55758000
C	-3.42396700	3.47826500	-0.97586700
C	-3.44047100	4.52308300	-0.04079000
C	-3.34537100	3.82714500	-2.32831900
C	-3.36665100	5.85418300	-0.44219800
H	-3.51291100	4.29048700	1.01928000
C	-3.27266500	5.16313700	-2.72873900
H	-3.34190600	3.05347900	-3.09079400
C	-3.27748600	6.21125300	-1.79829400
H	-3.38263800	6.62699100	0.32143600
H	-3.21243700	5.37589100	-3.79035300
C	-3.19432200	7.69396300	-2.20265900
C	-4.46117400	8.43481200	-1.71223500
H	-4.41225500	9.49607100	-1.98586700
H	-5.36423800	8.00863300	-2.16428600
H	-4.57228800	8.37618600	-0.62437700
C	-3.08996800	7.87993000	-3.72839500
H	-2.19441500	7.39870800	-4.13766100
H	-3.96525700	7.47576200	-4.24986800
H	-3.02900000	8.94784900	-3.96670900
C	-1.94334700	8.33267300	-1.55273100
H	-1.97652200	8.27411300	-0.45974700
H	-1.02854200	7.82965200	-1.88614700
H	-1.86954800	9.39195800	-1.82771600
C	-4.62909700	-2.21776900	-1.06822900
C	-4.73588100	-3.32264100	-0.18495700
C	-4.69758300	-2.48413200	-2.46353800
C	-4.90148100	-4.62124900	-0.68679700
C	-4.87256100	-3.79493200	-2.91622500
C	-4.97753800	-4.89257000	-2.05326500
H	-4.97027400	-5.43208900	0.03040800
H	-4.92204600	-3.95618700	-3.98980900
C	-5.87245000	-0.14512400	0.90644400
C	-5.80687800	0.21005600	2.28052300
C	-7.17005100	-0.21795300	0.32295700
C	-6.97546800	0.47216000	3.00266000
C	-8.31256600	0.06037100	1.08867000
C	-8.25279700	0.40761600	2.43710100
H	-6.86980700	0.74007000	4.05060300
H	-9.27397400	-0.00731500	0.59116100
C	-4.69309400	-3.17659700	1.32417800
H	-3.88586100	-2.51910900	1.66274600
H	-5.63035700	-2.76762200	1.71797000
H	-4.52791600	-4.14886300	1.79860000
C	-4.58023100	-1.40956800	-3.52591000
H	-5.31137200	-0.60526800	-3.39353100
H	-3.58458200	-0.95127700	-3.53148800
H	-4.74382300	-1.83689200	-4.51981300
C	-7.43119300	-0.61495100	-1.11897800
H	-8.46429600	-0.38121200	-1.39389000
H	-6.78580700	-0.09285100	-1.83118200
H	-7.28008600	-1.68764900	-1.27920000
C	-4.50855600	0.33075500	3.04312500
H	-3.91099500	-0.58365000	2.99348700
H	-3.88198900	1.14403500	2.66241000
H	-4.69942700	0.54042300	4.10003900
C	-5.16541700	-6.30971800	-2.62193800
C	-3.97531900	-6.65461600	-3.54920300
H	-3.89480900	-5.95676200	-4.38911100

H	-3.02819100	-6.62538300	-2.99863500
H	-4.09695000	-7.66266200	-3.96416500
C	-6.48153900	-6.36396200	-3.43440700
H	-6.62729100	-7.36605500	-3.85590000
H	-7.34430600	-6.13406300	-2.79855000
H	-6.47838600	-5.64974000	-4.26459800
C	-5.23787300	-7.38058700	-1.51677000
H	-4.32068600	-7.41102100	-0.91768800
H	-6.08380000	-7.21286200	-0.84038500
H	-5.36906600	-8.36959300	-1.97009300
C	-9.49813100	0.71081800	3.28774700
C	-10.80493900	0.58357200	2.48159100
H	-10.94409900	-0.42941600	2.08694100
H	-11.66039500	0.80571300	3.12952700
H	-10.83692900	1.28599600	1.64083900
C	-9.40703700	2.15566200	3.83435900
H	-8.51456200	2.30264900	4.45148000
H	-9.37108700	2.88313000	3.01530700
H	-10.28296100	2.38384900	4.45392400
C	-9.56437500	-0.28201900	4.47284000
H	-9.63809600	-1.31542600	4.11512000
H	-8.67937600	-0.21249900	5.11391600
H	-10.44406400	-0.07348800	5.09385700
Lu	0.06078000	-0.14613900	0.07980100
Lu	3.23647800	-1.89604700	0.42048800
Lu	3.02244400	1.65819900	-0.06462500

3B-III

C	3.03732100	2.82092500	2.96797700
C	2.17701000	1.96295300	3.76086700
C	2.63588400	0.72897900	4.35339300
C	4.00059900	0.39548200	4.03584700
C	0.83772100	2.08563700	3.19587800
C	1.67002800	-0.37432400	4.48758700
C	0.30765400	-0.22858500	3.89252800
C	-0.08350800	0.99225500	3.19987800
C	2.40836400	-1.13177300	-3.72007100
C	3.34550000	-0.04123600	-3.75908500
C	4.68053300	-0.17572400	-3.24871100
C	5.10432600	-1.40206600	-2.65455900
C	4.17716400	-2.51283800	-2.67065800
C	2.85971300	-2.43168300	-3.25123100
C	5.09781000	1.10409600	-2.72460300
C	6.02180400	-1.32843800	-1.57991800
C	6.43190100	-0.05188400	-1.03712800
C	5.97613500	1.19503500	-1.58885500
C	5.90710400	2.07306300	0.72271600
C	6.33158200	0.81020200	1.28762200
C	4.87095600	1.26242000	3.26062800
C	4.38436800	2.46629100	2.68106400
C	4.93350000	2.87358500	1.40908600
C	5.83260600	0.44811200	2.57831700
C	-1.29034100	-1.23459200	-0.79583900
C	-0.76973500	-0.87235100	-2.03905700
C	0.18600900	-1.70512800	-2.75282600
C	0.60958700	-2.99656500	-2.29131500
C	0.09828800	-3.32875600	-0.98075400
C	-0.83509900	-2.47043700	-0.26681800
C	1.04193100	-0.81000500	-3.50792400
C	1.99105900	-3.42161500	-2.61203000
C	-0.65190900	-2.66139700	1.14307900
C	-1.40846700	-0.36061900	1.52400600
C	-0.86329000	-1.54657300	2.03812000
C	5.56933900	-0.92769200	2.91198300
C	4.44577100	-0.96343500	3.79988000
C	2.24175600	3.48312400	1.97186300
C	0.89080700	3.01991300	2.10356500
C	4.14798400	-3.49383900	-1.62435100
C	2.81552700	-4.07544100	-1.56166300
C	0.61298100	0.54027100	-3.28861000

C	-0.49687000	0.52053000	-2.37286500
C	3.50685200	-2.04020000	3.77972100
C	2.13013600	-1.71693700	4.11388300
C	2.28299300	-4.34016100	-0.22378200
C	4.18410400	3.62136300	0.42564800
C	2.77914800	3.84656900	0.69075900
C	1.55656800	1.60702300	-3.26010200
C	5.03161500	-3.35117500	-0.48504900
C	-0.00972600	-1.46546100	3.21214000
C	1.08769300	-2.38072800	3.37305200
C	1.34716300	-3.43834700	2.42198100
C	0.43970600	-3.56284200	1.32235500
C	0.90260400	-4.00396600	0.01917400
C	5.78161300	-1.96976000	1.95537800
C	5.98384900	-2.28843600	-0.50508600
C	4.89532700	-3.08801300	1.98661500
C	3.76453800	-3.11679100	2.87875800
C	2.69370600	-3.81313300	2.20979900
C	3.16293100	-4.22789200	0.90398600
C	4.52800900	-3.76845200	0.77731600
C	-0.93759500	0.89391300	2.02433000
C	-0.95784800	1.88293700	0.99966900
C	-0.73720300	1.55537700	-1.46362800
C	0.01668300	2.89998400	0.97923500
C	5.81337000	2.34010800	-0.70150200
C	4.74139600	3.35305000	-0.91091200
C	3.78125100	3.17214300	-2.01973600
C	2.92655000	1.31519400	-3.54477000
C	4.01158600	2.05713000	-2.92585900
C	2.38558200	3.40188200	-1.72764600
C	1.88098900	3.79623100	-0.41760600
C	0.52429200	3.37038700	-0.28599700
C	0.17545500	2.64408300	-1.47481500
C	1.30649400	2.67165200	-2.35981400
N	2.56655000	-0.21996100	0.25043400
Si	-3.95573000	-0.44886500	-0.32351800
C	-1.97930500	-0.21483800	0.11536000
C	-1.66736000	1.36230600	-0.25842900
C	6.63590700	-0.23618800	0.37696900
C	6.36406900	-1.61332800	0.70291100
C	-3.89743800	1.12295900	-1.39950900
H	-4.88775500	1.54960000	-1.58410400
H	-3.40454800	0.98550100	-2.36481500
C	-3.06586400	2.06565500	-0.50514200
H	-3.54265300	2.10002500	0.48505500
C	-4.16721300	-2.19272100	-1.08067000
C	-4.29814900	-3.29526700	-0.19796100
C	-4.20983600	-2.46409200	-2.47619800
C	-4.45409800	-4.59558700	-0.69921900
C	-4.37475900	-3.77639600	-2.92921000
C	-4.49748900	-4.87180900	-2.06582700
H	-4.54144800	-5.40365100	0.01920900
H	-4.40299600	-3.94016200	-4.00332600
C	-2.99689100	3.50788000	-0.98291400
C	-3.03626700	4.55419600	-0.05559000
C	-2.90886700	3.85584800	-2.33891900
C	-2.97537100	5.89093000	-0.45715500
H	-3.11530500	4.32404400	1.00451200
C	-2.85082600	5.18810500	-2.73794100
H	-2.88535000	3.07963400	-3.09807600
C	-2.87842700	6.24318400	-1.80930000
H	-3.00955100	6.65932600	0.30758400
H	-2.78233600	5.40513600	-3.80064600
C	-5.44455800	-0.12603300	0.86794800
C	-5.40302200	0.23536500	2.24101300
C	-6.73344300	-0.21197800	0.26746400
C	-6.58340300	0.48874000	2.94703500
C	-7.88941200	0.05790100	1.01633600
C	-7.85206600	0.40964600	2.36431900
H	-6.49488800	0.76218900	3.99520200

H	-8.84310700	-0.01954600	0.50549100
C	-2.80398000	7.70150300	-2.29561300
C	-3.99633300	7.99563800	-3.23700200
H	-3.95007800	9.02994400	-3.59989600
H	-3.99853000	7.33638200	-4.11147000
H	-4.95057200	7.86099600	-2.71475200
C	-2.85240700	8.70985800	-1.13220100
H	-3.78461800	8.62919400	-0.56142900
H	-2.01396300	8.57384400	-0.43959300
H	-2.79345900	9.73092400	-1.52596200
C	-1.47905500	7.91793000	-3.06567400
H	-0.61502000	7.72571400	-2.41942400
H	-1.39978700	7.25545200	-3.93392900
H	-1.41143400	8.95162700	-3.42705000
C	-4.07976500	-1.39215900	-3.53997000
H	-4.81795200	-0.59234500	-3.42110900
H	-3.08797100	-0.92648600	-3.52857100
H	-4.22431400	-1.82348500	-4.53529800
C	-4.29641400	-3.14732700	1.31168700
H	-5.25170300	-2.75643300	1.67990400
H	-4.12496700	-4.11642600	1.79072000
H	-3.51135000	-2.47444300	1.67012500
C	-4.66776600	-6.29147400	-2.63407500
C	-5.95912300	-6.35185800	-3.48477100
H	-6.09145000	-7.35621000	-3.90550600
H	-6.84040800	-6.11964800	-2.87577900
H	-5.93212800	-5.64162400	-4.31786000
C	-4.77073800	-7.35833000	-1.52735700
H	-3.87065900	-7.38604100	-0.90273000
H	-5.63503100	-7.18781300	-0.87538200
H	-4.88920000	-8.34920500	-1.98031600
C	-3.45038700	-6.63776800	-3.52480000
H	-3.34766000	-5.94242900	-4.36433700
H	-2.51989100	-6.60349300	-2.94657800
H	-3.55672400	-7.64781900	-3.93934800
C	-6.97193800	-0.61328200	-1.17721900
H	-6.32034800	-0.08681100	-1.88021200
H	-6.80970900	-1.68486200	-1.33369600
H	-8.00322300	-0.38837400	-1.46639200
C	-4.11581800	0.37529400	3.01903400
H	-3.50458700	-0.53061700	2.97614900
H	-3.49809800	1.19846600	2.64457000
H	-4.32188100	0.58211400	4.07387200
C	-9.11201400	0.70391300	3.19653400
C	-10.40635600	0.56054000	2.37316700
H	-11.27301600	0.77613800	3.00842800
H	-10.43376000	1.25948700	1.52937500
H	-10.52955600	-0.45514600	1.98014200
C	-9.18532200	-0.28473700	4.38463900
H	-9.24428800	-1.32015700	4.02995000
H	-8.30962800	-0.20438900	5.03718400
H	-10.07530200	-0.08240100	4.99308500
C	-9.04320600	2.15167100	3.73863300
H	-8.16135800	2.30967700	4.36822300
H	-9.00166900	2.87603300	2.91712000
H	-9.93049400	2.37411000	4.34410900
Lu	2.19351200	-1.88614100	-0.87808900
Lu	1.93162500	-0.12169800	2.18736100
Lu	3.63998600	1.35450600	-0.50233800

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C	-1.96579600	2.38089200	3.25056900
C	-2.62760500	1.22531000	3.77482400
C	-1.90629500	0.01219000	4.00563100
C	-0.50048100	0.01556600	3.77555100
C	-3.99203300	1.21021700	3.27959100
C	-2.61555000	-1.21106300	3.80569600
C	-3.97359000	-1.21407400	3.29479200
C	-4.73543800	-0.01160500	3.05996100
C	-1.86416800	-0.08579000	-4.08689500

C	-1.16511500	1.14648800	-3.87322600
C	0.16597300	1.15784600	-3.33806400
C	0.80793200	-0.06200200	-2.99444300
C	0.17129200	-1.29143800	-3.31064000
C	-1.15854000	-1.30754600	-3.84738100
C	0.35924200	2.36929500	-2.56523300
C	1.65071700	-0.04323700	-1.83748900
C	1.89422500	1.16064600	-1.09899000
C	1.26003900	2.40548400	-1.42868400
C	1.02485400	2.71741000	1.00808700
C	1.70056500	1.47604800	1.30234000
C	0.15937800	1.17285800	3.23839100
C	-0.56872100	2.34600200	2.93297000
C	-0.11875500	3.10023900	1.80218000
C	1.24965600	0.74153600	2.40267600
C	-5.42608900	-1.52545900	-1.40095500
C	-5.03625600	-0.80067600	-2.55911500
C	-3.94657400	-1.25114700	-3.38183900
C	-3.22176800	-2.43773000	-3.05553700
C	-3.67135200	-3.21120600	-1.94727800
C	-4.76840800	-2.76486800	-1.13451700
C	-3.27352400	-0.08791800	-3.89256400
C	-1.81997800	-2.47390500	-3.34368200
C	-4.53363400	-3.19145900	0.21681500
C	-5.91649700	-0.76787800	-0.26868500
C	-5.75979400	-1.20758900	1.09801400
C	-4.95685900	-2.39976300	1.33192500
C	1.24845400	-0.72554900	2.41586200
C	0.16324000	-1.14829400	3.26388300
C	-2.88605200	3.09253300	2.41343600
C	-4.13969200	2.36828800	2.41992900
C	0.36173800	-2.46912100	-2.49597400
C	-0.88432200	-3.21846600	-2.51805200
C	-3.95297600	1.08104500	-3.40548200
C	-5.04344600	0.64223000	-2.57551500
C	-0.55299500	-2.33835300	2.99713200
C	-1.94664800	-2.37842600	3.31941400
C	-1.32044600	-4.00196500	-1.38040200
C	-1.01704300	3.86574000	0.98516300
C	-2.44185900	3.80170800	1.25486300
C	-3.23784300	2.28089400	-3.11058900
C	1.24444400	-2.45657600	-1.35495900
C	-4.10832500	-2.40158400	2.47603100
C	-2.86118700	-3.12476200	2.50184500
C	-2.40996100	-3.85307800	1.35516800
C	-3.28129900	-3.90829100	0.23763800
C	-2.73490800	-3.92632000	-1.10429500
C	1.70813200	-1.47700600	1.33531600
C	1.90423600	-1.21654800	-1.06779000
C	1.02710800	-2.72452700	1.07339400
C	-0.09990600	-3.11599900	1.88155600
C	-0.98297900	-3.92642500	1.08718200
C	-0.39412300	-4.09353600	-0.24097800
C	0.88962000	-3.34537000	-0.24062800
C	-5.73075500	-0.02468300	1.97536200
C	-5.83742400	1.15766300	1.08075400
C	-5.95095200	0.67274300	-0.28426700
C	-5.44737500	1.39482100	-1.43847400
C	-5.01238300	2.34806300	1.28300400
C	0.88523400	3.30942600	-0.32318900
C	-0.42932400	4.00382800	-0.34060600
C	-1.35522700	3.87127700	-1.46572100
C	-1.83613100	2.31799600	-3.39890500
C	-0.90519500	3.08734100	-2.59335700
C	-2.77288200	3.81976100	-1.19742800
C	-3.31647500	3.83233400	0.14131800
C	-4.56273300	3.09737200	0.14237000
C	-4.79090100	2.63972900	-1.20199200
C	-3.69781700	3.07981500	-2.02436600
N	-1.87351200	-0.03154000	-0.03721500

C	2.57733900	-0.84672500	0.26375700
C	2.57562700	0.82305300	0.23574900
Si	4.52852800	-1.35545500	0.02116400
C	4.55987700	-2.94076900	-1.07287900
C	4.71595100	-2.92151700	-2.49055100
C	4.44007800	-4.20232900	-0.42042100
C	4.75423100	-4.12761600	-3.20049000
C	4.48631900	-5.38441100	-1.17165300
C	4.64361600	-5.35195600	-2.55068200
H	4.86967700	-4.11501900	-4.27806500
H	4.39252500	-6.34266500	-0.67319800
C	5.88327500	-1.52522100	1.40726400
C	7.22225500	-1.71588200	0.94207300
C	5.67364000	-1.41066400	2.80898100
C	8.27754900	-1.77167100	1.86328700
C	6.75774100	-1.47264000	3.69320700
C	8.05437600	-1.65036000	3.22808800
H	9.29183700	-1.91271600	1.50793400
H	6.58706200	-1.38136200	4.75980600
C	4.84276600	-1.61651200	-3.27082700
H	3.94753100	-1.01006300	-3.08964100
H	5.67924800	-1.03603900	-2.86338200
C	4.28044100	-4.31477700	1.09273300
H	5.25466300	-4.15120400	1.57049400
H	3.64197300	-3.49821900	1.44514300
C	4.27813000	-1.22763700	3.37971800
H	3.84629900	-0.30334900	2.97894200
H	3.63794900	-2.03199600	3.00252600
C	7.56207600	-1.90085000	-0.53593400
H	7.24577900	-2.90298200	-0.85042100
H	6.96384800	-1.21045300	-1.13858900
C	4.31220300	2.78155200	0.12166300
C	4.40148300	3.61852100	1.23934200
C	4.46366800	3.37775700	-1.13909700
C	4.61315100	4.99284100	1.11015500
H	4.30603800	3.19113700	2.23527800
C	4.67410200	4.74841400	-1.26632600
H	4.42191300	2.77000900	-2.03810800
C	4.75116000	5.59517100	-0.14709900
H	4.67341100	5.59021000	2.01322800
H	4.78473500	5.16213200	-2.26503800
C	4.98575200	7.10434600	-0.33521400
C	6.32753900	7.32993000	-1.07258400
H	6.33581000	6.85386500	-2.05870500
H	6.50676000	8.40228300	-1.21843100
H	7.16523300	6.92030200	-0.49649300
C	3.83234000	7.70212200	-1.17610400
H	3.76575700	7.23716100	-2.16532400
H	2.86801400	7.56014200	-0.67503200
H	3.98509800	8.77844700	-1.32326000
C	5.04234500	7.85905200	1.00666500
H	4.10604500	7.76192700	1.56791000
H	5.86133100	7.50264100	1.64200700
H	5.20808200	8.92661300	0.82274700
C	4.88356900	0.39374900	-0.65959900
H	5.94499900	0.65232200	-0.61095800
H	4.54758800	0.55888300	-1.68512900
C	4.08125400	1.28950200	0.30760200
H	4.40262800	1.05850800	1.33286700
Lu	-0.92047900	-1.81899600	-0.36765400
Lu	-3.69791600	0.12913700	0.86615200
Lu	-0.78907700	1.67153500	-0.43225100
H	8.88672400	-1.69488900	3.92590500
H	4.67538300	-6.27735000	-3.12019400
C	4.13545100	-1.18874400	4.90461800
H	4.50215700	-2.10904900	5.37309000
H	4.67603200	-0.34457300	5.34716000
H	3.07840300	-1.07975200	5.16944000
C	9.03006800	-1.70577600	-0.93980800
H	9.68353800	-2.47708500	-0.51869600

H	9.12095400	-1.76748700	-2.02978600
H	9.41334400	-0.72831000	-0.62525500
C	5.03927700	-1.72519200	-4.78742600
H	5.12555500	-0.72207700	-5.21908600
H	5.95137800	-2.27515400	-5.04497500
H	4.19404900	-2.22150900	-5.27669800
C	3.68192700	-5.62379100	1.62449200
H	4.34846100	-6.47882200	1.46870600
H	3.51257200	-5.54048400	2.70355200
H	2.72184600	-5.85004100	1.14754300

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C	-0.03630300	1.28920400	-3.27497900
C	1.30784300	1.31549800	-3.77694300
C	2.01333400	0.09750700	-4.01608300
C	1.30867300	-1.12926900	-3.85824700
C	1.97249200	2.47993400	-3.22895200
C	3.41766100	0.10684600	-3.75845700
C	4.06847100	1.26993600	-3.19560700
C	3.38927600	2.51814000	-2.95275600
C	1.79860800	-0.12856500	4.09811400
C	0.39445600	-0.12849300	3.82744200
C	-0.26009300	-1.27775800	3.27548100
C	0.48048900	-2.45447500	2.97302100
C	1.87353300	-2.49959700	3.31503600
C	2.52022000	-1.34556700	3.85893400
C	-1.36353000	-0.83224300	2.44224100
C	0.07655400	-3.18927600	1.83253600
C	-1.01385900	-2.73873600	0.99785200
C	-1.79294700	-1.57904000	1.30344200
C	-1.89972500	-1.17935300	-1.17281900
C	-1.09297300	-2.34209900	-1.44250000
C	-0.73667000	-3.19549700	-0.35187300
C	-0.03802600	-1.14073800	-3.34571000
C	-0.70936200	0.05976500	-3.00774600
C	-1.66033400	0.02452100	-1.90464200
C	-0.21951500	-2.33206900	-2.56475300
C	4.90308900	2.30502200	1.55537300
C	4.04372400	2.30390800	2.68758000
C	3.86850300	1.12056000	3.48569100
C	4.54880200	-0.08793000	3.15717100
C	5.47824400	-0.05995500	2.08041000
C	5.66407500	1.12611300	1.29251100
C	2.50558100	1.09865900	3.94830200
C	3.87921100	-1.33282200	3.39942000
C	5.96231900	0.73096200	-0.05735300
C	4.52091100	3.12041900	0.42289800
C	4.86428800	2.78300300	-0.93842000
C	5.51444800	1.50411800	-1.17609800
C	1.02687700	-3.05117900	-2.56397600
C	1.97164600	-2.30003300	-3.35245300
C	-0.22764800	2.42433900	-2.42411700
C	1.01215600	3.16137000	-2.38160200
C	2.83442700	-3.23067300	2.51750900
C	4.10221400	-2.50582100	2.57851000
C	1.84648900	2.27532700	3.46087300
C	2.79299600	3.02260800	2.67378400
C	3.34724300	-2.26290400	-3.00341000
C	4.07983700	-1.06451200	-3.26552400
C	5.02499900	-2.48834100	1.46093800
C	-1.93401000	1.19217300	-1.11382400
C	-1.11203600	2.35582600	-1.30386800
C	0.46337500	2.24300800	3.10883200
C	2.43226300	-3.95423400	1.33539300
C	5.13726400	0.78676700	-2.34630500
C	5.14901600	-0.65144900	-2.39933100
C	5.51710100	-1.41854500	-1.25109200
C	5.95390700	-0.70896900	-0.10229100
C	5.65888400	-1.21516700	1.22305200
C	1.43479800	-3.80066400	-1.42746800

C	1.02623100	-3.90127600	1.01872300
C	0.51809200	-3.88114300	-0.33687400
C	2.84391800	-3.84695000	-1.10983900
C	3.76438900	-3.05791900	-1.87669800
C	4.86486800	-2.69124700	-1.02585800
C	4.67693100	-3.29916300	0.28807100
C	3.38359100	-4.02631400	0.23228600
C	3.85568900	3.35787700	-1.83845100
C	2.85627500	4.03171900	-0.96861400
C	3.29252200	3.87186700	0.41131800
C	2.37813900	3.76450000	1.53307200
C	1.42485500	3.90197400	-1.22466200
C	-1.81176300	1.44720200	1.39798400
C	-0.27219900	1.04146300	3.34334200
C	-1.37810600	0.63793500	2.49176400
C	-1.03355300	2.62082400	1.15245200
C	-0.74010200	3.13178600	-0.16860300
C	0.51101100	3.84361600	-0.11446100
C	0.98062000	3.80556700	1.24850000
C	0.04164900	3.04993000	2.02004300
N	1.80280200	-0.02849900	0.03534000
C	-4.92193500	0.40363300	-0.74005900
H	-4.57195100	0.64115900	-1.74617000
H	-5.98853900	0.64122100	-0.69116300
C	-2.62782500	-0.90676300	0.18145200
C	-2.64401700	0.83305300	0.22767100
C	-4.38355800	2.75279700	0.17970400
C	-4.78717800	4.89448500	1.27644000
C	-4.63044400	4.80284000	-1.10677500
C	-4.81599700	5.57556300	0.05295200
H	-4.93137600	5.43244700	2.20665400
H	-4.65011300	5.28101500	-2.08235900
C	-4.51816800	-2.87981200	-1.38372600
C	-4.38100900	-4.18009900	-0.81965100
C	-4.64926500	-2.76211700	-2.79987700
C	-4.39624700	-5.30819500	-1.65141900
C	-4.65525000	-3.91644700	-3.59128900
H	-4.29255200	-6.29740500	-1.21909400
H	-4.75144700	-3.83145500	-4.66747600
C	-5.03974900	7.09421500	-0.05802600
C	-6.31120700	7.36887900	-0.89628300
H	-7.19545300	6.92497300	-0.42462300
H	-6.48073500	8.44877800	-0.98849600
H	-6.22979300	6.95728700	-1.90783900
C	-5.21879100	7.76162300	1.31891700
H	-6.08979900	7.36629100	1.85404500
H	-4.33613600	7.62803500	1.95467700
H	-5.37235500	8.83893800	1.18951400
C	-3.81836400	7.74277200	-0.75291700
H	-2.90182000	7.56743200	-0.17820300
H	-3.66245100	7.34275300	-1.76031400
H	-3.96218500	8.82655300	-0.84274000
C	-4.57662200	3.51513400	1.33638300
H	-4.56469900	3.02493800	2.30757400
C	-4.42242100	3.42718400	-1.04963000
H	-4.28984000	2.87814600	-1.97694000
C	-4.53536700	-5.18182000	-3.02632800
H	-4.54375000	-6.06522500	-3.65972500
C	-4.15504500	1.25276100	0.29223300
H	-4.49284200	0.96618100	1.29787100
Si	-4.56779000	-1.38565900	-0.17387200
C	-5.95892200	-1.69247500	1.14683800
C	-7.27322000	-1.88998300	0.61939400
C	-5.80066200	-1.68068600	2.56007900
C	-8.35514000	-2.06345800	1.49389100
C	-6.91016400	-1.85661700	3.39585900
C	-8.18183500	-2.04872300	2.87098500
H	-9.35077100	-2.21116000	1.09129900
H	-6.78009900	-1.84206500	4.47189000
H	-9.03393100	-2.18333600	3.53240400

C	-7.55879600	-1.95236000	-0.87959900
H	-6.93570000	-1.21975600	-1.40097900
H	-7.23637200	-2.92790100	-1.26413000
C	-9.01013200	-1.71050500	-1.31781800
H	-9.40072500	-0.76371000	-0.92764800
H	-9.06083700	-1.67065500	-2.41141000
H	-9.68205300	-2.51250800	-0.99480100
C	-4.43414200	-1.49002600	3.19558600
H	-3.77471800	-2.29979200	2.86118900
H	-3.98591700	-0.57093500	2.80444500
C	-4.36571000	-1.42953800	4.72497000
H	-4.71760300	-2.35779200	5.18860500
H	-3.32733000	-1.27794500	5.03801100
H	-4.95945900	-0.60188100	5.12900200
C	-4.23721000	-4.39988200	0.68312400
H	-3.71575800	-3.54482400	1.12384800
H	-5.23306100	-4.40464900	1.14610600
C	-3.48242600	-5.66513200	1.11534300
H	-2.50085300	-5.72855600	0.63348900
H	-3.32810700	-5.65149900	2.19982000
H	-4.03631400	-6.58034100	0.88180200
C	-4.78173900	-1.40855000	-3.49147800
H	-5.64768700	-0.87677600	-3.07850200
H	-3.90895100	-0.79690500	-3.23558800
C	-4.92046200	-1.41481000	-5.01827500
H	-5.00967200	-0.38544200	-5.38212400
H	-4.04831300	-1.86213200	-5.50739200
H	-5.81211600	-1.95971900	-5.34794200
Lu	-0.23810200	-0.01542200	0.25598400
Lu	2.63862300	1.68117000	-0.77333500
Lu	2.96849000	-1.68850200	0.45366700

4A-III

C	-1.81861400	2.50410000	3.26629600
C	-2.51609500	1.38019600	3.84698000
C	-1.84063600	0.13997300	4.13032600
C	-0.44128200	0.10088100	3.80891300
C	-3.89230400	1.40467400	3.36739500
C	-2.61820800	-1.09296600	4.03364200
C	-4.03397800	-1.08861500	3.57270000
C	-4.66567500	0.18766600	3.18180800
C	-1.90352600	-0.06639900	-4.08789900
C	-1.16160900	1.14688200	-3.87878400
C	0.17531900	1.12492200	-3.35097800
C	0.77766200	-0.10302800	-3.00003700
C	0.06697300	-1.31346000	-3.29233700
C	-1.24540000	-1.34307600	-3.90086200
C	0.40526300	2.32820200	-2.57526300
C	1.66466300	-0.09960800	-1.87175800
C	1.93055500	1.10693200	-1.12766400
C	1.32774700	2.35757500	-1.45561900
C	1.15709500	2.73101000	0.97949500
C	1.77947200	1.46149200	1.27206800
C	0.25323600	1.23153400	3.23850300
C	-0.43056100	2.42637100	2.92677800
C	0.03426600	3.16160600	1.78499300
C	1.31470700	0.75217000	2.39376600
C	-5.47828400	-1.35198300	-1.29666800
C	-5.06574500	-0.66268800	-2.47553000
C	-4.00775900	-1.18066600	-3.32226700
C	-3.36794100	-2.46469800	-3.11109800
C	-3.79284300	-3.12885800	-1.89275900
C	-4.83621200	-2.59834000	-1.02902400
C	-3.30717000	-0.01956700	-3.85029400
C	-1.93770600	-2.56776300	-3.47208600
C	-4.57703700	-3.01066800	0.32363600
C	-5.93805700	-0.57718100	-0.18625000
C	-5.67174200	-0.99518600	1.16008000
C	-4.96637300	-2.19593100	1.44164300
C	1.29041200	-0.70346500	2.45528600

C	0.20595600	-1.08678100	3.31980200
C	-2.73114400	3.22357600	2.42977400
C	-3.99682100	2.54073700	2.46827600
C	0.21116500	-2.45584600	-2.45023900
C	-1.00386200	-3.24246100	-2.53316200
C	-3.94320800	1.17161100	-3.36012800
C	-5.02506400	0.77324800	-2.50962500
C	-0.54775600	-2.26127800	3.07882800
C	-1.95500600	-2.22656000	3.41478600
C	-1.45495900	-3.86172000	-1.29965700
C	-0.85959700	3.93480200	0.96500200
C	-2.28429600	3.91133100	1.25064700
C	-3.18484400	2.35818200	-3.08185900
C	1.09497400	-2.40982600	-1.30683000
C	-4.15411800	-2.21760300	2.64309700
C	-2.89537800	-2.92109500	2.58552900
C	-2.47375800	-3.70102900	1.44369300
C	-3.36221900	-3.77265500	0.33074500
C	-2.86119000	-3.83789800	-1.02248700
C	1.68858700	-1.48510100	1.36210400
C	1.89045400	-1.25277100	-1.09511400
C	0.96969300	-2.68802300	1.14653500
C	-0.13616100	-3.07171900	1.98642900
C	-1.08240900	-3.79107000	1.18566300
C	-0.56683200	-3.85574900	-0.16596800
C	0.70363100	-3.18964900	-0.17992400
C	-5.47289800	0.18666500	1.98694300
C	-5.60548100	1.33234400	1.10651200
C	-5.88311000	0.86074800	-0.21766800
C	-5.39023300	1.55536000	-1.36622200
C	-4.83998700	2.51914400	1.31515900
C	1.00989800	3.30245100	-0.36128100
C	-0.28925000	4.03270200	-0.37018600
C	-1.23542700	3.89850900	-1.47564500
C	-1.79316900	2.33912900	-3.38799200
C	-0.83134900	3.07782700	-2.59353200
C	-2.64793800	3.91203600	-1.19891700
C	-3.17062300	3.96270700	0.14714000
C	-4.43757400	3.27219800	0.17270400
C	-4.69444800	2.78325100	-1.15061000
C	-3.60151900	3.18170700	-1.99949500
N	-1.86113900	0.04687600	-0.00406500
C	2.54068700	-0.89206100	0.25137900
C	2.61870300	0.76425100	0.20150700
C	4.89704300	0.21605600	-0.71741100
H	5.96964400	0.42922000	-0.69066500
H	4.55258700	0.36462900	-1.74270500
Si	4.47980500	-1.49242200	0.02237400
C	4.14441200	1.16822200	0.23993700
H	4.47179600	0.94972300	1.26619500
C	4.40432400	-3.12194000	-0.99665600
C	4.21853800	-4.34016000	-0.28255800
C	4.53367500	-3.17700800	-2.41586800
C	4.16531100	-5.55597700	-0.97846700
C	4.47430000	-4.41356500	-3.06875500
C	4.29170300	-5.59668300	-2.36009000
H	4.01979400	-6.48191900	-0.43324000
H	4.57009300	-4.45857900	-4.14753400
C	5.87102200	-1.66769900	1.38178800
C	5.73978600	-1.40270000	2.76724600
C	7.18001300	-1.99906700	0.89148400
C	6.85615400	-1.46433700	3.61760200
C	8.26112700	-2.06171000	1.77706300
C	8.10978000	-1.79752900	3.13558200
H	6.72465200	-1.23600500	4.67284600
H	9.24653700	-2.31190800	1.40142300
C	4.43058500	2.64470500	0.01210200
C	4.57439300	3.50575000	1.11012200
C	4.57421400	3.20492000	-1.26204200
C	4.82895200	4.86362800	0.93950600

H	4.48666700	3.10450500	2.11752500
C	4.82710700	4.56832000	-1.43188100
H	4.49183600	2.57778300	-2.14485200
C	4.95644700	5.43460300	-0.33818700
H	4.93307400	5.48636200	1.82384800
H	4.92579700	4.94811200	-2.44292300
C	5.23607100	6.94061300	-0.48720000
C	6.58577700	7.28170600	0.18864900
H	7.40949400	6.73311000	-0.28248900
H	6.79724200	8.35457700	0.10123200
H	6.58235500	7.02821100	1.25406500
C	4.10359800	7.74443800	0.19556400
H	3.13428800	7.52577300	-0.26684000
H	4.02409300	7.51201200	1.26270300
H	4.29080900	8.82126400	0.10230900
C	5.31176400	7.37922800	-1.96209400
H	6.12374300	6.87440400	-2.49807600
H	4.37442500	7.18102800	-2.49446600
H	5.50137700	8.45721400	-2.01735800
C	4.73958900	-1.91968400	-3.25481200
H	3.89019600	-1.24694200	-3.09053800
H	5.61820000	-1.37959400	-2.88140400
C	4.10833000	-4.37498100	1.23892300
H	5.11573100	-4.31328900	1.67097800
H	3.58942900	-3.47595500	1.58497000
C	4.43603500	-1.03052700	3.44296500
H	4.57163600	-0.08053700	3.97922600
H	3.66372500	-0.84720200	2.70161100
C	7.45232100	-2.29874900	-0.58117500
H	6.99056500	-3.25710600	-0.84392200
H	6.94122400	-1.55309400	-1.20045300
C	8.92062000	-2.33223600	-1.02529700
H	9.44396300	-1.40060700	-0.78180100
H	9.47259300	-3.16067300	-0.56845200
H	8.97065700	-2.47108500	-2.11082000
C	3.38276300	-5.58436200	1.84382500
H	3.93923300	-6.51711300	1.70327000
H	3.26368800	-5.44183500	2.92363300
H	2.38564100	-5.71303000	1.40898000
C	4.91005900	-2.10870400	-4.76688300
H	5.77825300	-2.73213300	-5.00852600
H	4.02666400	-2.56608000	-5.22610800
H	5.06052000	-1.13411700	-5.24403600
H	8.96724100	-1.84184600	3.80225100
H	4.24686500	-6.54681600	-2.88650000
C	3.92385800	-2.08523900	4.43982100
H	4.64703500	-2.26056400	5.24362900
H	2.98378200	-1.75663800	4.89593100
H	3.74100300	-3.04443700	3.94411800
Lu	-0.69649700	1.71480700	-0.32675700
Lu	-2.03721800	-1.29886100	-1.53341700
Lu	-2.77943800	-0.27796100	1.79065700

4B-I

C	1.72567500	2.21596100	-3.33134000
C	2.35681600	1.03501700	-3.83650300
C	1.63010100	-0.19066500	-3.95408400
C	0.24315200	-0.18045600	-3.62603200
C	3.75271300	1.04976400	-3.43521000
C	2.36149900	-1.39888300	-3.73808000
C	3.75494900	-1.37067600	-3.32842700
C	4.52488800	-0.15380500	-3.21403900
C	2.14864300	0.14532200	4.12107500
C	1.42832600	1.36251700	3.89162700
C	0.06368400	1.33965000	3.44941100
C	-0.59228100	0.10105000	3.21473100
C	0.07114400	-1.10861700	3.55344600
C	1.43607900	-1.08997700	3.99565400
C	-0.18967200	2.50665300	2.62848900
C	-1.51192300	0.05438100	2.11941800

C	-1.81985000	1.21678400	1.34141100
C	-1.16299400	2.47517700	1.55498800
C	-1.09318900	2.65197100	-0.90072700
C	-1.78010300	1.39643600	-1.08221700
C	-0.38295100	1.00221100	-3.10522500
C	0.35589900	2.19286300	-2.91385500
C	-0.01656700	3.00277400	-1.79364200
C	-1.40938200	0.61258000	-2.17436700
C	5.52767400	-1.42553500	1.27329500
C	5.21117100	-0.64003100	2.41453500
C	4.18419300	-1.04960300	3.33333800
C	3.44785900	-2.25480600	3.12231300
C	3.82675700	-3.08515400	2.02873400
C	4.86226100	-2.67910600	1.11971600
C	3.54080900	0.13705900	3.82866500
C	2.06964700	-2.27828600	3.50908900
C	4.53868200	-3.17790600	-0.18856800
C	5.93526400	-0.73124700	0.06956300
C	5.70201700	-1.24685600	-1.26126500
C	4.88394600	-2.44744500	-1.37200900
C	-1.40747300	-0.85484500	-2.11339200
C	-0.37770000	-1.31777700	-3.01004100
C	2.69592800	2.97608300	-2.59912900
C	3.94587500	2.25290900	-2.64884700
C	-0.16974100	-2.33178400	2.82066400
C	1.08440900	-3.06660800	2.79002700
C	4.17746300	1.28096100	3.23537900
C	5.20826400	0.80171600	2.35429900
C	0.36536100	-2.48661800	-2.72676300
C	1.73530900	-2.53807000	-3.14037300
C	1.44927300	-3.89976800	1.66348600
C	0.92679500	3.82059000	-1.08444700
C	2.32965000	3.74499600	-1.45010300
C	3.43570600	2.46143000	2.92758200
C	-1.13566700	-2.38709800	1.74537300
C	3.95258200	-2.50789700	-2.45138700
C	2.70940000	-3.23317300	-2.34800600
C	2.34555200	-3.90307100	-1.13708200
C	3.29313300	-3.90121200	-0.08348600
C	2.84161500	-3.84654800	1.29103100
C	-1.77257800	-1.54448400	-0.95744500
C	-1.81595500	-1.16358500	1.43321300
C	-1.07735300	-2.77874500	-0.67968900
C	-0.00326400	-3.20254900	-1.54157200
C	0.94148600	-3.96020900	-0.76783800
C	0.44741400	-4.05868400	0.60228700
C	-0.84844400	-3.33211600	0.65206600
C	5.58899900	-0.10730800	-2.19535500
C	5.72119700	1.11381100	-1.36483500
C	5.94245500	0.70747100	0.00859700
C	5.52475400	1.49299200	1.15336400
C	4.88529200	2.29143100	-1.57138100
C	-0.87095200	3.31788300	0.38076900
C	0.43035700	4.02978500	0.27047400
C	1.43138800	3.96448800	1.33788700
C	2.05654400	2.50985500	3.31035100
C	1.06658000	3.23494900	2.53332600
C	2.82579200	3.89331400	0.97187500
C	3.27691600	3.83561300	-0.40136000
C	4.52522800	3.10923000	-0.44824400
C	4.85072000	2.72483200	0.89801400
C	3.81293300	3.20160400	1.77021900
N	1.89636600	-0.01744500	0.11632100
C	-2.58020400	-0.86253600	0.14600400
C	-2.58035200	0.80481800	0.07647400
Si	-4.51554900	-1.37487100	-0.21557900
C	-4.09105200	1.26284500	0.05493100
H	-4.47608400	1.02651400	1.05668700
C	-4.81937600	0.35844200	-0.96046200
H	-4.39639500	0.50014700	-1.95731900

H	-5.88015500	0.62105400	-1.00476400
C	-4.32252300	2.75346100	-0.13850000
C	-4.50429700	3.58293700	0.97748100
C	-4.38403500	3.35508300	-1.40042400
C	-4.71770900	4.95168600	0.83653600
H	-4.48019500	3.14959900	1.97498900
C	-4.59879800	4.72804400	-1.53999600
H	-4.26607100	2.75277600	-2.29667300
C	-4.76735500	5.56344100	-0.42731500
H	-4.85261600	5.54980400	1.73359700
H	-4.63612300	5.14066300	-2.54222800
C	-5.00633300	7.07937700	-0.54278400
C	-6.37724700	7.43270600	0.08207900
H	-6.56086900	8.51221700	0.01571100
H	-7.19071300	6.91669700	-0.44085500
H	-6.42766700	7.15053000	1.13902200
C	-5.00596400	7.56305500	-2.00545000
H	-4.04944800	7.36175600	-2.50127500
H	-5.80238000	7.09138500	-2.59257900
H	-5.17206200	8.64585600	-2.03585600
C	-3.88789800	7.83481900	0.21432800
H	-3.86146600	7.56740700	1.27588000
H	-2.90398900	7.60763100	-0.21170000
H	-4.04662100	8.91811900	0.14711800
C	-4.48175400	-2.97632600	-1.28422400
C	-4.37915000	-4.22456000	-0.60347300
C	-4.57328900	-2.98383600	-2.70754700
C	-4.37331800	-5.42033700	-1.33288000
C	-4.56320500	-4.20391500	-3.39509300
C	-4.46585900	-5.41438400	-2.71848900
H	-4.29154400	-6.36796400	-0.81254500
H	-4.62907900	-4.21251100	-4.47682100
C	-5.94433200	-1.52399100	1.09771200
C	-5.81698300	-1.38699100	2.50834100
C	-7.25337000	-1.73522200	0.56077200
C	-6.94939800	-1.45402800	3.32950000
C	-8.35881200	-1.79449400	1.42100300
C	-8.21506600	-1.65590700	2.79452600
H	-6.84217600	-1.34727800	4.40285400
H	-9.34950600	-1.95284100	1.01042300
C	-4.29751100	-4.30425000	0.91805700
H	-3.67202700	-3.48394400	1.28632800
H	-5.29412600	-4.12308900	1.33973700
C	-4.67915100	-1.69610500	-3.51895800
H	-5.53287700	-1.11124100	-3.15576500
H	-3.79303500	-1.08253000	-3.31852100
C	-7.50817600	-1.93987000	-0.93129000
H	-6.86846100	-1.26460500	-1.50696200
H	-7.18456700	-2.94972200	-1.21212800
C	-4.46273500	-1.16636900	3.16215400
H	-3.77709800	-1.95021200	2.82422800
H	-4.03726100	-0.22808100	2.78731800
H	-4.45868100	-6.35014300	-3.27172900
H	-9.08463100	-1.70483800	3.44501000
C	-3.74041500	-5.60452700	1.51181300
H	-3.63926900	-5.49958600	2.59755200
H	-4.40097700	-6.45934800	1.33118900
H	-2.75258900	-5.84301900	1.10291100
C	-4.81845300	-1.83833800	-5.03919300
H	-5.71447100	-2.40354600	-5.31956900
H	-4.89836100	-0.84512000	-5.49435600
H	-3.95018800	-2.33476300	-5.48616100
C	-8.94775600	-1.73470200	-1.42298200
H	-8.97451600	-1.80219500	-2.51607700
H	-9.63240700	-2.49750500	-1.03758700
H	-9.33956400	-0.75202200	-1.13662300
C	-4.41268800	-1.12441100	4.69328800
H	-5.00194500	-0.29628600	5.10254800
H	-4.77985300	-2.05525400	5.13985300
H	-3.37698200	-0.98505800	5.02122400

Lu	0.90672800	-1.75711600	0.58261100
Lu	0.85302000	1.72074300	0.46951000
Lu	3.61642700	-0.00010900	-0.98393000

4B-II

C	-0.24619500	-1.20271900	-3.50346700
C	-1.62576600	-1.19882600	-3.90022700
C	-2.33490000	0.03272100	-4.03520500
C	-1.60747600	1.24660000	-3.88115000
C	-2.25789400	-2.38066700	-3.35191600
C	-3.71614100	0.02272900	-3.67175100
C	-4.33287400	-1.15884000	-3.10809200
C	-3.64992000	-2.42152100	-2.96981400
C	-1.49407800	-0.08208300	4.04384300
C	-0.11366100	-0.08083300	3.66670300
C	0.51025300	1.08661400	3.11285700
C	-0.24338800	2.27928300	2.91308900
C	-1.60507400	2.31892100	3.36453700
C	-2.21978100	1.14864700	3.91038500
C	1.54741300	0.67269600	2.18467000
C	0.07662600	3.05663600	1.77562100
C	1.09498200	2.63252100	0.84112200
C	1.88799900	1.46234600	1.04468700
C	1.81481900	1.17215800	-1.46222000
C	0.98979600	2.34422100	-1.61345200
C	0.71961300	3.14611400	-0.46077100
C	-0.22503600	1.22828500	-3.47534200
C	0.45750600	0.00997400	-3.23717200
C	1.48999100	-0.00413900	-2.21029300
C	0.02822500	2.38597700	-2.66285400
C	-4.80849600	-2.38541200	1.64854800
C	-3.86528400	-2.43749100	2.71050000
C	-3.61874300	-1.29054000	3.54265400
C	-4.30892500	-0.06469800	3.31605300
C	-5.31750700	-0.04036800	2.31240200
C	-5.57514800	-1.19127900	1.49336800
C	-2.22320000	-1.29680500	3.89881700
C	-3.61032500	1.16417600	3.55790800
C	-5.97225300	-0.73859700	0.18780000
C	-4.52312600	-3.15571400	0.45709100
C	-4.96719700	-2.75955600	-0.85894300
C	-5.62017100	-1.46697400	-0.99282000
C	-1.20788400	3.11017500	-2.53396200
C	-2.21823200	2.39915100	-3.27682500
C	-0.00182400	-2.37280400	-2.71791800
C	-1.24221200	-3.10371200	-2.60995800
C	-2.61639400	3.08506400	2.67010000
C	-3.88255000	2.36938400	2.80004800
C	-1.61506600	-2.45574200	3.31279700
C	-2.62616300	-3.16291800	2.57018800
C	-3.56390800	2.35837000	-2.82646200
C	-4.32679400	1.17720600	-3.08139400
C	-4.89083600	2.40903600	1.75986700
C	1.80523500	-1.20347100	-1.48541700
C	0.96387000	-2.35623100	-1.66587300
C	-0.26213000	-2.41853800	2.85914300
C	-2.30080400	3.85590200	1.49274500
C	-5.32647500	-0.70392500	-2.15822800
C	-5.32854800	0.73581500	-2.15120000
C	-5.60042200	1.45701900	-0.94780200
C	-5.95160800	0.70181000	0.20128700
C	-5.55249300	1.15039800	1.51967200
C	-1.52083400	3.81485300	-1.33892600
C	-0.92416100	3.81122500	1.06900900
C	-0.52368800	3.84064100	-0.32100400
C	-2.90179300	3.85916900	-0.91337500
C	-3.88686200	3.11005500	-1.63939200
C	-4.92487400	2.71849300	-0.72247200
C	-4.62966900	3.26900800	0.59856900
C	-3.33494300	3.98571300	0.47258700

C	-4.03661000	-3.30281800	-1.85716900
C	-2.97963900	-4.01805100	-1.09568900
C	-3.30646500	-3.91306900	0.31970200
C	-2.30799500	-3.85896700	1.37113600
C	-1.57169100	-3.88821300	-1.45613100
C	1.86685900	-1.55698000	1.00138000
C	0.50086500	-1.23411900	3.08608000
C	1.53960800	-0.79987000	2.16484800
C	1.07042600	-2.72081900	0.77503600
C	0.67490900	-3.17967300	-0.53943400
C	-0.57385800	-3.88527100	-0.41785700
C	-0.93710700	-3.89725400	0.97797900
C	0.06455700	-3.17887200	1.70488100
N	-1.81398600	-0.01422300	-0.00043700
C	2.62851600	0.83573300	-0.18406200
C	2.62205500	-0.90408100	-0.20122300
Si	4.58481000	-1.37722800	0.12234400
C	4.55325600	-2.92672500	1.25888400
C	4.71983900	-2.88503100	2.67423000
C	4.37223400	-4.19228500	0.62946900
C	4.72037000	-4.07997400	3.40441500
C	4.38059700	-5.36156400	1.40031100
C	4.55742100	-5.30997000	2.77697200
H	4.84504900	-4.05333600	4.48072400
H	4.24168300	-6.32408000	0.92072900
H	4.56083500	-6.22572800	3.36267600
C	4.88462200	-1.57001000	3.42971600
H	5.71587700	-1.00503300	2.99256200
H	3.99019100	-0.95759000	3.26346700
C	4.18144900	-4.31772700	-0.87930100
H	3.58537300	-3.47197900	-1.24025900
H	5.15612600	-4.21737400	-1.37365900
C	3.50445500	-5.60025100	-1.38093300
H	2.53733400	-5.76266300	-0.89280400
H	3.32887400	-5.52589300	-2.45963500
H	4.12406000	-6.48811300	-1.21578400
C	5.98302000	-1.62382700	-1.20967000
C	7.30861200	-1.79119900	-0.68157300
C	5.83127700	-1.63672700	-2.61917400
C	8.39216500	-1.94053800	-1.55344200
C	6.94733700	-1.80645800	-3.45497600
C	8.22164900	-1.95204600	-2.93466600
H	9.39073900	-2.06096300	-1.14964800
H	6.79748700	-1.82978900	-4.53171300
H	9.07745300	-2.08148700	-3.59222500
C	7.59452900	-1.86240600	0.81655600
H	6.99799900	-1.10973700	1.33960200
H	7.23849400	-2.82718400	1.19807800
C	9.05277000	-1.67477700	1.25689900
H	9.69680000	-2.49534100	0.92364700
H	9.47559700	-0.73664800	0.87961400
H	9.10374900	-1.65005700	2.35089600
C	4.50427100	-1.49970000	-3.33913100
H	4.36028100	-2.38052100	-3.98096000
H	3.68019600	-1.51357200	-2.62920600
C	5.11946000	-1.65898300	4.94208800
H	5.23955000	-0.65131900	5.35454600
H	4.27645300	-2.12731200	5.46162600
H	6.02540800	-2.22603900	5.18424200
C	4.38342700	2.74809600	-0.14978400
C	4.49814700	3.51436100	-1.31402100
C	4.51076700	3.41668900	1.07659700
C	4.71900400	4.89258800	-1.26253000
H	4.41519900	3.02913700	-2.28407900
C	4.73121700	4.79057600	1.12547200
H	4.44126000	2.86298900	2.00853200
C	4.83916100	5.56759700	-0.04128900
H	4.79990100	5.43430000	-2.19827500
H	4.82314800	5.26359700	2.09938200
C	5.08298500	7.08377400	0.05992500

C	6.41309200	7.34335700	0.80711300
H	6.59726700	8.42125500	0.89358600
H	6.40043700	6.92544500	1.81929100
H	7.25797200	6.89597100	0.27099100
C	3.91967200	7.73954600	0.84199700
H	2.96316200	7.57302600	0.33366000
H	3.83283200	7.33776000	1.85693600
H	4.07809500	8.82191100	0.92427600
C	5.16963300	7.75608300	-1.32355300
H	5.99645200	7.35566800	-1.92136800
H	4.24265100	7.63337000	-1.89520800
H	5.34184600	8.83138800	-1.20108800
C	4.39292700	-0.23720300	-4.21261300
H	3.41543600	-0.19397600	-4.70541100
H	4.51008300	0.67332600	-3.61429600
H	5.16254000	-0.21802000	-4.99167700
C	4.14073800	1.24987800	-0.25021700
H	4.46599700	0.95401300	-1.25733900
C	4.90486800	0.38958600	0.77374500
H	4.52468000	0.57534700	1.78090200
H	5.96567900	0.65458300	0.75990100
Lu	0.23719900	-0.03007500	0.05520700
Lu	-2.72759300	-1.67630000	-0.82489300
Lu	-2.94286900	1.63494900	0.54328100

4B-III

C	-1.55763700	2.25381700	3.40099500
C	-2.22271300	1.09292900	3.94559700
C	-1.54241200	-0.16937100	4.08630000
C	-0.16980500	-0.19390700	3.65967400
C	-3.63022200	1.16276100	3.57173300
C	-2.33950200	-1.38632500	3.95336900
C	-3.78491000	-1.33708200	3.59760000
C	-4.42881100	-0.03159600	3.35172900
C	-2.21342400	0.25277600	-4.09689600
C	-1.44272200	1.44098800	-3.85498400
C	-0.07058900	1.37109200	-3.43253100
C	0.54217400	0.11616800	-3.21947900
C	-0.20452700	-1.06377600	-3.54761100
C	-1.55930800	-1.03757900	-4.05307500
C	0.23104000	2.51269600	-2.59054500
C	1.51259900	0.02735600	-2.16692100
C	1.84790600	1.17511900	-1.35772400
C	1.23350300	2.44958700	-1.54279700
C	1.23616200	2.62897900	0.91902400
C	1.86080300	1.33736000	1.06807100
C	0.49140200	0.97393200	3.12460900
C	-0.20024900	2.19277200	2.95342800
C	0.18513700	3.00732100	1.83703100
C	1.48185200	0.55401200	2.17032700
C	-5.58644000	-1.22049100	-1.15696700
C	-5.25352800	-0.44581300	-2.30708100
C	-4.26590500	-0.90351700	-3.26519300
C	-3.62816600	-2.20340900	-3.19921100
C	-3.97287700	-2.95996600	-2.00941700
C	-4.94245100	-2.48910400	-1.03300900
C	-3.59522200	0.29065600	-3.75687300
C	-2.23038900	-2.28827700	-3.67273300
C	-4.58855200	-3.00432600	0.26197500
C	-5.95386500	-0.53004000	0.03986300
C	-5.59395300	-1.05084100	1.32697400
C	-4.88467000	-2.27401500	1.46401000
C	1.45480900	-0.90344600	2.12731500
C	0.42777700	-1.34500300	3.03699800
C	-2.52054200	3.04069500	2.69076800
C	-3.78716400	2.36427600	2.77094800
C	-0.00998500	-2.27028200	-2.81267300
C	-1.23639800	-3.04411800	-2.86550200
C	-4.17991600	1.44437900	-3.13333000
C	-5.19979100	0.98840300	-2.23627100

C	-0.35752600	-2.49108800	2.76225800
C	-1.73637200	-2.47291400	3.20237100
C	-1.60465500	-3.75325000	-1.65122600
C	-0.75475700	3.84938500	1.14757500
C	-2.15415300	3.81398500	1.53692200
C	-3.38838200	2.60122200	-2.82339500
C	0.95776800	-2.31391200	-1.73720300
C	-3.98545300	-2.39018700	2.59599200
C	-2.74348100	-3.09576800	2.39396800
C	-2.41702300	-3.78950500	1.16808500
C	-3.38513500	-3.77182500	0.12159000
C	-2.98728400	-3.74040600	-1.26831300
C	1.74411600	-1.59333700	0.94320500
C	1.78454800	-1.18458400	-1.49830400
C	1.00102900	-2.77233000	0.69204800
C	-0.04015800	-3.21555700	1.58093100
C	-1.04987100	-3.86894400	0.80185300
C	-0.63771300	-3.83133300	-0.58615100
C	0.63479700	-3.17124100	-0.64246100
C	-5.32159600	0.06327800	2.22369100
C	-5.50514700	1.27335700	1.44452100
C	-5.88539900	0.90563000	0.11296800
C	-5.47008300	1.68247200	-1.01317000
C	-4.71384600	2.43644900	1.68547900
C	1.00398700	3.30630600	-0.35724600
C	-0.28242800	4.04631000	-0.21495900
C	-1.30768400	4.00448700	-1.25522600
C	-2.02249000	2.59673700	-3.23183000
C	-0.99565300	3.26912400	-2.45923600
C	-2.69558100	4.00294000	-0.87330500
C	-3.11699200	3.95266600	0.50820900
C	-4.38661000	3.27074200	0.57556900
C	-4.74659500	2.88669800	-0.75809000
C	-3.71458400	3.34210100	-1.65359500
N	-1.88105800	0.05920000	-0.03899600
C	2.53093300	-0.92906700	-0.18958800
C	2.61717300	0.72567500	-0.11110300
Si	4.46120600	-1.53207000	0.16348300
C	4.14487200	1.11630300	-0.12150200
H	4.50121700	0.85167300	-1.12744500
C	4.84819100	0.19088800	0.89139400
H	4.44400000	0.35622400	1.89260200
H	5.92005700	0.40649300	0.92140100
C	4.44336800	2.59731000	0.04790100
C	4.64354700	3.40254400	-1.08266100
C	4.54419700	3.21480100	1.29956100
C	4.91008600	4.76407600	-0.96553800
H	4.59001700	2.95529900	-2.07286900
C	4.81113400	4.58096000	1.41535300
H	4.41490500	2.63052300	2.20618600
H	5.05633100	5.34346300	-1.87307600
H	4.87559500	5.00738500	2.41048300
C	4.38196700	-3.12147300	1.24702500
C	4.19949500	-4.36422700	0.57462700
C	4.52499700	-3.13020300	2.66561200
C	4.17823000	-5.55888000	1.30487300
C	4.49591400	-4.34897600	3.35523100
H	4.03705800	-6.50269000	0.79015400
H	4.60190700	-4.35924900	4.43381300
C	5.87976600	-1.76128100	-1.15667200
C	5.75363900	-1.64500200	-2.56949900
C	7.18168200	-2.02242100	-0.62247900
C	6.87693000	-1.78281000	-3.39450700
C	8.27818700	-2.15065800	-1.48677100
H	6.76842000	-1.69207800	-4.46920100
H	9.26239400	-2.34661700	-1.07704400
C	4.03600000	-4.43448900	-0.94026200
H	3.41881100	-3.59130900	-1.27031300
H	5.01431500	-4.28580900	-1.41450500
C	4.70209400	-1.84625400	3.47060900

H	5.56309800	-1.29126200	3.08006700
H	3.83179700	-1.20305800	3.29674100
C	7.44053000	-2.20535600	0.87150100
H	6.84424300	-1.48244100	1.43502500
H	7.06678900	-3.18916300	1.17988200
C	4.41003900	-1.36869100	-3.22193400
H	3.68357800	-2.10108500	-2.85615900
H	4.03811000	-0.39869000	-2.87179100
C	8.13443600	-2.03421600	-2.86211000
H	8.99720200	-2.13805400	-3.51525400
C	4.99617000	5.39275500	0.28787900
C	4.32848700	-5.55560900	2.68553200
H	4.30917100	-6.49007100	3.24075800
C	5.28860100	6.90107800	0.37574800
C	5.32062800	7.40814000	1.83019700
H	4.36313700	7.24815300	2.33913700
H	6.10645200	6.91851200	2.41689200
H	5.52422100	8.48489700	1.84119800
C	4.18826600	7.68212000	-0.38198700
H	4.14203400	7.39964700	-1.43895100
H	3.20179700	7.49400400	0.05695800
H	4.38352200	8.76046000	-0.33313200
C	6.66369600	7.19723900	-0.26945100
H	6.69358300	6.89344700	-1.32122300
H	6.88320300	8.27113900	-0.22594700
H	7.46548700	6.66484100	0.25508100
C	4.88450300	-1.99165300	4.98611000
H	5.76904900	-2.58675300	5.23998300
H	5.01260200	-1.00114500	5.43630700
H	4.01436500	-2.45774000	5.46137600
C	3.40154900	-5.71140000	-1.50639700
H	3.24635300	-5.59891200	-2.58502000
H	4.03936500	-6.59016700	-1.36263900
H	2.42897700	-5.91582600	-1.04559500
C	8.89361100	-2.06531400	1.34655500
H	8.92617800	-2.10825500	2.44077800
H	9.53365800	-2.87231100	0.97467700
H	9.33434100	-1.11177700	1.03399200
C	4.35165800	-1.36874800	-4.75321700
H	4.98043400	-0.58544300	-5.19102100
H	4.66579800	-2.33033500	-5.17462500
H	3.32237200	-1.18354800	-5.07946600
Lu	-0.72307200	1.73740100	-0.33232500
Lu	-2.16148000	-1.19917400	-1.62522400
Lu	-2.64842800	-0.39937800	1.79782400