

1A-S0

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C	0.31193600	-2.09998800	0.13778400
C	0.75244400	-0.96598500	0.81729000
C	2.10463800	-0.51193700	0.69795300
C	3.00891600	-1.26757500	-0.07571000
C	1.28075500	-2.87735700	-0.63236800
H	2.00343200	1.31951500	1.86024700
C	2.64096100	0.66831700	1.27375400
C	4.33561900	-0.92712800	-0.26994700
C	4.86134600	0.24420600	0.32615000
C	3.95394900	1.04030200	1.09455700
H	4.93613300	-1.57850600	-0.88942100
H	4.29124900	1.95962800	1.55333600
C	-0.19305000	-0.19303700	1.70672600
H	-0.91439000	-0.84892700	2.19445700
H	0.34135300	0.34346300	2.48999400
O	-0.90192600	0.76385800	0.87489800
C	-1.79869400	1.54807100	1.51827200
O	-1.99808400	1.45830200	2.72438300
C	-2.48670100	2.49577300	0.61854000
C	-2.21463800	2.56469900	-0.76083800
C	-3.44681300	3.35823700	1.16547400
C	-2.88698700	3.47172300	-1.56272500
H	-1.47582100	1.90593500	-1.20186800
C	-4.12912200	4.27304100	0.37043600
H	-3.65901500	3.30759100	2.22793000
C	-3.84892700	4.33166300	-1.00332500
H	-2.68594400	3.53397600	-2.62701200
H	-4.86674600	4.92686400	0.81827500
O	-4.45492700	5.18463900	-1.87387400
C	-5.44881200	6.08453400	-1.36601200
H	-5.79341000	6.65818100	-2.22670900
H	-6.29088000	5.53773400	-0.92969500
H	-5.02272700	6.76371500	-0.62059400
O	1.07132000	-3.91735200	-1.24530900
O	2.58445000	-2.42049200	-0.69189800
N	6.18183100	0.58749800	0.19587200
C	7.08863900	-0.20869400	-0.64325600
C	6.98934100	0.06288900	-2.14708900
H	6.91246300	-1.26937000	-0.44098500
H	8.10437400	0.00162800	-0.29933800

H	7.67216500	-0.60384000	-2.68450400
H	5.97774900	-0.11486900	-2.52370200
H	7.26638900	1.09391000	-2.38403000
C	6.68926900	1.86997900	0.70641300
C	6.35044700	3.09005000	-0.15449800
H	7.77404300	1.76804600	0.78477500
H	6.32428700	2.01704800	1.72730400
H	6.74936500	3.99355000	0.31895900
H	6.79041700	3.00707200	-1.15217500
H	5.26966200	3.21714400	-0.26703000
C	-1.08635100	-2.50887500	0.16055400
H	-1.75823800	-1.78398100	0.61002000
C	-1.64712600	-3.64467700	-0.32573600
H	-1.02602400	-4.39863200	-0.79389900
C	-3.05376700	-3.97214000	-0.28471600
C	-3.63194900	-5.13134100	-0.76511700
S	-4.29688300	-2.92619300	0.40101400
C	-5.04321200	-5.18882800	-0.58942500
H	-3.04618200	-5.91624400	-1.23103600
C	-5.54705700	-4.07443400	0.02364400
H	-5.65885700	-6.02321400	-0.90566900
H	-6.57454000	-3.85138400	0.27872600

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C	0.29002300	-1.97951900	0.11169800
C	0.95957000	-0.97114500	0.80152500
C	2.37919300	-0.81373200	0.68970400
C	3.10569400	-1.73586200	-0.08924500
C	1.07713800	-2.94011900	-0.66068400
H	2.66498600	0.98666300	1.86963900
C	3.15166500	0.21874000	1.27966000
C	4.47587100	-1.68395800	-0.27718800
C	5.23662300	-0.66011100	0.33626000
C	4.51573000	0.30233800	1.11068300
H	4.92596500	-2.44330500	-0.90140900
H	5.03802000	1.12493900	1.57956400
C	0.19840000	-0.01692800	1.69036500
H	-0.66062100	-0.49697800	2.15963400
H	0.82726600	0.37721100	2.48790100
O	-0.26321800	1.08428100	0.86165000

C	-0.90921000	2.08061100	1.51079900
O	-1.09418400	2.06020800	2.72242200
C	-1.35106700	3.16393700	0.60872600
C	-1.12571500	3.13172400	-0.78046100
C	-2.02124900	4.26357400	1.16231500
C	-1.56125800	4.17114000	-1.58526500
H	-0.60995200	2.28996500	-1.22730900
C	-2.46258600	5.31411800	0.36463600
H	-2.19702400	4.29246900	2.23218400
C	-2.23284900	5.26921800	-1.01892800
H	-1.39387100	4.15671100	-2.65707200
H	-2.97723100	6.15173700	0.81812200
O	-2.62128600	6.23784800	-1.89295800
C	-3.30997400	7.38480100	-1.37751300
H	-3.52116600	8.01427100	-2.24225500
H	-4.25024200	7.09790700	-0.89566700
H	-2.68392800	7.93538300	-0.66798300
O	0.65499200	-3.91000800	-1.27920600
O	2.44769500	-2.76747600	-0.71685200
N	6.60216000	-0.60678600	0.21642600
C	7.31856900	-1.54398300	-0.65969000
C	7.25888200	-1.21206400	-2.15361400
H	6.93508600	-2.55384100	-0.48441300
H	8.35983400	-1.55315900	-0.32900500
H	7.78587400	-1.98637500	-2.72137600
H	6.22802800	-1.16992800	-2.51728700
H	7.73632800	-0.25151700	-2.36639000
C	7.37221700	0.51186300	0.77903600
C	7.34796600	1.79954400	-0.04902500
H	8.40259000	0.16325600	0.88308800
H	7.01681300	0.71164800	1.79406800
H	7.92255400	2.57690800	0.46603300
H	7.79347600	1.64646100	-1.03592500
H	6.32793500	2.16989600	-0.18821700
C	-1.16277800	-2.08337700	0.12483300
H	-1.66892100	-1.23200500	0.56993300
C	-1.94925600	-3.07759600	-0.36408100
H	-1.49764700	-3.94498300	-0.83111000
C	-3.38776800	-3.10987500	-0.32809000
C	-4.19765500	-4.11239000	-0.81754900
S	-4.38389800	-1.82503300	0.38369300
C	-5.59478500	-3.89644100	-0.64640400
H	-3.78652000	-4.99547200	-1.29508700
C	-5.85068000	-2.70572300	-0.01418200

H	-6.36251700	-4.58477000	-0.97413100
O	-7.00951100	-2.11619400	0.34267200
C	-8.20599600	-2.85035600	0.02671900
H	-9.03281400	-2.23608100	0.38205300
H	-8.28965800	-3.00202300	-1.05385600
H	-8.20956800	-3.81678800	0.54014400

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C	0.26597800	-2.05322700	0.16618400
C	0.74380500	-0.92858100	0.83478200
C	2.10794200	-0.51400700	0.70611900
C	2.98553700	-1.30057000	-0.06729900
C	1.20566000	-2.85989500	-0.60913600
H	2.06584400	1.32606800	1.85837500
C	2.68123100	0.65321600	1.27252600
C	4.32101100	-1.00065200	-0.26930700
C	4.88357100	0.15852700	0.31692600
C	4.00358900	0.98546200	1.08474300
H	4.89846300	-1.67325800	-0.88808100
H	4.37016400	1.89697700	1.53643400
C	-0.17348300	-0.12465700	1.72678500
H	-0.89740000	-0.76127600	2.23565000
H	0.38219500	0.41511700	2.49264700
O	-0.87894100	0.83093800	0.89084800
C	-1.77310500	1.62129900	1.53023900
O	-1.97153200	1.53955300	2.73708200
C	-2.46008000	2.56445700	0.62494300
C	-2.18946300	2.62329000	-0.75521800
C	-3.41780100	3.43267000	1.16698500
C	-2.86090300	3.52605400	-1.56261500
H	-1.45243400	1.96006700	-1.19252700
C	-4.09925800	4.34322700	0.36634800
H	-3.62882000	3.38992600	2.23002500
C	-3.82051200	4.39176700	-1.00811700
H	-2.66092700	3.58051700	-2.62752500
H	-4.83505400	5.00164000	0.81045800
O	-4.42580600	5.23981900	-1.88387600
C	-5.41688800	6.14564500	-1.38110200
H	-5.76100900	6.71424400	-2.24532500
H	-6.25981200	5.60392600	-0.94012900

H	-4.98828000	6.82879600	-0.64078000
O	0.96334900	-3.89291300	-1.22141500
O	2.52350100	-2.44232000	-0.67624300
N	6.21266400	0.46323200	0.17837700
C	7.09328800	-0.36563600	-0.65691000
C	6.99900000	-0.10129500	-2.16236100
H	6.88554400	-1.41904500	-0.44696100
H	8.11575800	-0.18388800	-0.31645000
H	7.65948400	-0.79250700	-2.69675600
H	5.98138200	-0.25007900	-2.53532900
H	7.30732700	0.91899900	-2.40700900
C	6.75772700	1.73665100	0.67314100
C	6.44280700	2.95766600	-0.19539500
H	7.84008900	1.60701700	0.74256500
H	6.40632400	1.90200700	1.69606600
H	6.86977200	3.85438600	0.26635700
H	6.87096600	2.85455300	-1.19632500
H	5.36475700	3.11236100	-0.29910100
C	-1.14710200	-2.41956000	0.20637600
H	-1.78997800	-1.66016900	0.63744500
C	-1.74193000	-3.55185300	-0.23883400
H	-1.13370000	-4.33239000	-0.67914300
C	-3.17748600	-3.84553000	-0.17888700
C	-4.15037900	-2.94539400	0.30505900
C	-3.61683100	-5.10545400	-0.63317200
C	-5.49665900	-3.29760600	0.33540800
H	-3.85629100	-1.96183500	0.65788300
C	-4.96531100	-5.45740500	-0.60203700
H	-2.88332900	-5.81201900	-1.01263500
C	-5.91343800	-4.55463900	-0.11670600
H	-6.22715700	-2.58752700	0.71235000
H	-5.27511800	-6.43589200	-0.95749000
H	-6.96507900	-4.82377900	-0.09130100

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C	0.40468800	-1.78944300	0.21502800
C	1.23359200	-0.87335500	0.85764900
C	2.65727900	-0.92819100	0.70738400
C	3.21828600	-1.97038700	-0.05711100
C	1.01932200	-2.87436400	-0.54779100

H	3.23574800	0.84503700	1.81852000
C	3.58858600	-0.00292000	1.24316100
C	4.57573100	-2.12699400	-0.27665700
C	5.49498600	-1.20735800	0.28215000
C	4.94474200	-0.12479200	1.03801200
H	4.89268000	-2.96215500	-0.88556200
H	5.59462300	0.62579900	1.46636800
C	0.64187800	0.19580900	1.74566100
H	-0.24560100	-0.16304700	2.26746700
H	1.35208100	0.53080700	2.50082900
O	0.27887100	1.32384400	0.90459800
C	-0.29265100	2.37177000	1.54292200
O	-0.48558200	2.37364500	2.75353000
C	-0.64606200	3.47962500	0.63207100
C	-0.40551900	3.42743100	-0.75391000
C	-1.24504200	4.62501400	1.17448500
C	-0.75682900	4.49240500	-1.56640400
H	0.05647300	2.55064000	-1.19213800
C	-1.60265400	5.70098500	0.36886300
H	-1.43189900	4.66926500	2.24196200
C	-1.35831100	5.63608200	-1.01147300
H	-0.57669900	4.46338500	-2.63583900
H	-2.06419700	6.57320600	0.81414000
O	-1.66734900	6.62596300	-1.89314200
C	-2.28693100	7.81758000	-1.39169600
H	-2.44081900	8.45722500	-2.26104100
H	-3.25229100	7.59511400	-0.92579600
H	-1.63808200	8.32770600	-0.67248300
O	0.44441100	-3.78489800	-1.13237000
O	2.39971100	-2.91007700	-0.63663000
N	6.84947200	-1.36008400	0.12926600
C	7.39637400	-2.44362700	-0.69905800
C	7.37100100	-2.18521800	-2.20835200
H	6.85923900	-3.36830100	-0.46713300
H	8.42724900	-2.60130200	-0.37266200
H	7.76254200	-3.06155200	-2.73594100
H	6.35510900	-1.99973800	-2.56946200
H	7.99114400	-1.32460600	-2.47423600
C	7.79039300	-0.33325500	0.60104100
C	7.89611500	0.90903700	-0.28802000
H	8.76859900	-0.81441900	0.67315300
H	7.52022100	-0.04330600	1.62087600
H	8.59993800	1.61952700	0.15863600
H	8.26039200	0.65298000	-1.28686300

H	6.93092300	1.41274200	-0.39534900
C	-1.04984300	-1.66878500	0.26638900
H	-1.40264600	-0.72478700	0.66721000
C	-1.98841000	-2.55774400	-0.14073800
H	-1.67134900	-3.50852200	-0.55173800
C	-3.43779200	-2.36646400	-0.07979100
C	-4.06905500	-1.18972000	0.38410300
C	-4.27204700	-3.41473400	-0.50786800
C	-5.44943200	-1.07924200	0.41821300
H	-3.47457300	-0.34660100	0.72176500
C	-5.66336500	-3.31992300	-0.47974100
H	-3.81774300	-4.33218800	-0.87261800
C	-6.26129100	-2.14378300	-0.01231900
H	-5.92637700	-0.17199400	0.77575900
H	-6.26226000	-4.15593700	-0.81931000
O	-7.61052800	-1.93256900	0.06415700
C	-8.49612200	-2.98557100	-0.36267300
C	-9.91611200	-2.49490000	-0.16797600
H	-8.30470300	-3.88681800	0.23220700
H	-8.30091800	-3.22206200	-1.41571100
H	-10.61826500	-3.27185700	-0.48459900
H	-10.10930800	-2.26398300	0.88392000
H	-10.10481900	-1.59673900	-0.76365200

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C	-1.24044600	1.50110200	0.65998100
C	-1.44233300	0.07990800	0.94669000
C	-2.79017800	-0.45125700	0.72121600
C	-3.85376000	0.43135000	0.51896000
C	-2.44400700	2.38939700	0.75536300
H	-2.33943700	-2.56221800	0.77333500
C	-3.12016200	-1.81796600	0.65606900
C	-5.15833600	0.03878600	0.27291100
C	-5.48346800	-1.33809400	0.22116700
C	-4.40914200	-2.25487900	0.41029100
H	-5.90010400	0.81344700	0.13697900
H	-4.58338200	-3.32060900	0.35296700
C	-0.41535200	-0.66093300	1.44702900
H	0.55901800	-0.23727700	1.66125400
H	-0.55532800	-1.70572400	1.70191900

O	2.30268200	-0.32804100	-0.47383000
C	3.10629100	-0.57539600	0.47862100
O	2.95309800	-0.20641200	1.68193500
C	4.35064000	-1.37804800	0.14623900
C	4.62433600	-1.77965100	-1.17169700
C	5.25870000	-1.74122000	1.14671100
C	5.76293600	-2.51329700	-1.47753300
H	3.93016700	-1.50717000	-1.95945800
C	6.40785100	-2.48052700	0.86177700
H	5.05849700	-1.43774300	2.16881000
C	6.66257400	-2.86866200	-0.45981900
H	5.97634000	-2.82242600	-2.49619000
H	7.08788400	-2.74549400	1.66233800
O	7.75685800	-3.59264200	-0.85734900
C	8.70495700	-3.98021300	0.14112200
H	9.48044500	-4.53799600	-0.38540200
H	9.15247900	-3.10623100	0.62690500
H	8.24538800	-4.62391000	0.89907400
O	-2.41336500	3.58826900	0.96210100
O	-3.66190700	1.81385800	0.60318300
N	-6.77802800	-1.76567800	0.03006600
C	-7.84330500	-0.80992300	-0.29861700
C	-7.84403600	-0.30131800	-1.74362400
H	-7.78708100	0.03615700	0.39419100
H	-8.79181400	-1.30983300	-0.08741200
H	-8.64954900	0.42927500	-1.87494600
H	-6.90024100	0.18884400	-2.00023400
H	-8.00801400	-1.11788200	-2.45234800
C	-7.08780300	-3.19478400	-0.10637100
C	-6.78560300	-3.80316400	-1.47920400
H	-8.15165600	-3.30945100	0.11706400
H	-6.55452200	-3.74763300	0.67291500
H	-7.01145900	-4.87496300	-1.46387300
H	-7.39337600	-3.34061800	-2.26197900
H	-5.73210300	-3.68420000	-1.74954900
C	-0.00384700	1.99754300	0.29031300
H	0.79596700	1.26774200	0.16025300
C	0.27701100	3.34912200	-0.00060900
H	-0.53017900	4.07210100	0.04883800
C	1.51565900	3.87148000	-0.35652600
C	1.74551400	5.23552500	-0.64489800
S	3.03405700	2.96101300	-0.48648400
C	3.07334100	5.52377500	-0.95043700
H	0.94134200	5.96208300	-0.61986500

C	3.87682300	4.39052300	-0.89940000
H	3.45242500	6.50658400	-1.19959900
H	4.94152100	4.34336400	-1.09536500

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C	-2.59815900	-0.67156000	0.82443000
C	-1.12961300	-0.57043700	0.80867600
C	-0.41264500	-1.82771600	0.56128000
C	-1.08639900	-3.04396000	0.69239700
C	-3.18855200	-1.97758300	1.25091500
H	1.51628800	-1.02014500	0.00133900
C	0.93418900	-1.92243900	0.16322700
C	-0.50909600	-4.28349300	0.47299100
C	0.85186900	-4.37150700	0.09323000
C	1.54861600	-3.14053200	-0.06946100
H	-1.12756000	-5.15931400	0.61228500
H	2.58113700	-3.13257300	-0.39167700
C	-0.51925800	0.61666700	1.04752100
H	-1.09156700	1.50885200	1.27524900
H	0.56119900	0.71666200	1.06617600
O	3.47520200	0.41651600	-0.63266100
C	3.66335300	1.34471600	0.21151300
O	2.88315600	1.63787800	1.16759200
C	4.92552300	2.17533600	0.06345100
C	5.84582100	1.91367500	-0.96486300
C	5.20601200	3.22512400	0.94480800
C	7.00137000	2.67066000	-1.10646700
H	5.64209500	1.10418800	-1.65750000
C	6.36169700	3.99859700	0.82090300
H	4.50416000	3.44090900	1.74347600
C	7.26578600	3.71975400	-0.21182300
H	7.71267100	2.46884400	-1.90153100
H	6.54641600	4.80363500	1.52190100
O	8.42971100	4.41135500	-0.43059400
C	8.74282200	5.49413000	0.44983200
H	9.69359100	5.89748600	0.09893500
H	7.97796900	6.27730000	0.40685200
H	8.85420900	5.14885500	1.48345800
O	-4.30557400	-2.12124000	1.71433800
O	-2.42090100	-3.08715400	1.11634200

N	1.47352600	-5.58924200	-0.07916300
C	0.70138500	-6.83695500	-0.04404200
C	-0.12993300	-7.12981700	-1.29725900
H	0.05307800	-6.82861100	0.83854500
H	1.41744400	-7.64705500	0.11558200
H	-0.69445400	-8.05775600	-1.15500300
H	-0.84585100	-6.32871200	-1.50351600
H	0.50739000	-7.25245700	-2.17746400
C	2.85984300	-5.66631100	-0.55615900
C	3.04813900	-5.46512300	-2.06304200
H	3.23722900	-6.65167800	-0.27033000
H	3.46423300	-4.93961100	-0.00466600
H	4.11529100	-5.50007800	-2.30801800
H	2.54399900	-6.24897700	-2.63543600
H	2.65847400	-4.49717400	-2.39214500
C	-3.39747700	0.37520900	0.43824700
H	-2.87756500	1.26247500	0.08685700
C	-4.81829400	0.39124400	0.39379500
H	-5.36230200	-0.50917600	0.65771700
C	-5.58716200	1.46895800	0.02573600
C	-7.00978700	1.46490100	-0.04419900
S	-4.95795700	3.07594700	-0.42075500
C	-7.57317400	2.65822800	-0.43229300
H	-7.57487800	0.57103800	0.19526600
C	-6.58769500	3.64117900	-0.67573900
H	-8.63277500	2.84322300	-0.54318000
O	-6.72487000	4.88004700	-1.05496100
C	-8.06867700	5.40288000	-1.28151400
H	-7.91597200	6.43648900	-1.58282400
H	-8.54883800	4.83229900	-2.07781300
H	-8.63927100	5.34844000	-0.35331400

1a-IM1

0 1			
C	1.25075300	1.44033300	-0.71248900
C	1.43864000	0.00364500	-0.88683700
C	2.78981600	-0.52150500	-0.67912900
C	3.86191800	0.36735800	-0.56115900
C	2.45531000	2.30851900	-0.92404100
H	2.33190900	-2.63074000	-0.59551500
C	3.11675500	-1.88374000	-0.54130100

C	5.16975500	-0.01471200	-0.31964500
C	5.49030100	-1.38748000	-0.18641100
C	4.40938600	-2.30984100	-0.29877200
H	5.91803200	0.76282000	-0.25303500
H	4.58196700	-3.37076500	-0.18050500
C	0.38334600	-0.76350700	-1.28715400
H	-0.59554500	-0.34686200	-1.49769500
H	0.50600100	-1.82526300	-1.47170600
O	-2.48198100	-0.27275500	0.55790000
C	-3.20612600	-0.61415700	-0.43147200
O	-2.95826800	-0.34595100	-1.64394400
C	-4.46435800	-1.40412900	-0.12836800
C	-4.82082800	-1.71895800	1.19334600
C	-5.30259100	-1.84284600	-1.15911900
C	-5.97147200	-2.44373600	1.47361000
H	-4.18085900	-1.38654700	2.00364000
C	-6.46343000	-2.57302700	-0.89957500
H	-5.03853700	-1.60711900	-2.18453700
C	-6.80053600	-2.87570200	0.42595200
H	-6.24831800	-2.68756700	2.49468900
H	-7.08927300	-2.89721000	-1.72226000
O	-7.91276600	-3.58449700	0.79930700
C	-8.78931100	-4.05064900	-0.23059400
H	-9.59321400	-4.58159400	0.28077900
H	-9.21096400	-3.21721700	-0.80292100
H	-8.27509100	-4.73798200	-0.91113100
O	2.42321000	3.47944000	-1.25041600
O	3.67197700	1.74101700	-0.73710800
N	6.78555100	-1.80751900	0.00860700
C	7.85628100	-0.83845300	0.27692900
C	7.86127500	-0.24561300	1.68928900
H	7.80283200	-0.03453700	-0.46466500
H	8.80165800	-1.35492200	0.09430100
H	8.67203100	0.48566900	1.77696100
H	6.92129200	0.26576900	1.91676900
H	8.01979800	-1.02012300	2.44488200
C	7.09689800	-3.22922700	0.20714100
C	6.82884200	-3.76824300	1.61544800
H	8.15456200	-3.35748100	-0.03733500
H	6.54319400	-3.81755600	-0.53056800
H	7.05487900	-4.83960100	1.64765100
H	7.45571900	-3.26796000	2.35895200
H	5.78229400	-3.63517100	1.90557700
C	0.02649700	1.97059100	-0.32689500

H	-0.76027300	1.25214100	-0.11114200
C	-0.23745400	3.33368400	-0.12726100
H	0.56760000	4.03804000	-0.30306300
C	-1.47240500	3.89245800	0.29259100
C	-2.63349100	3.11968400	0.58525400
C	-1.53717600	5.30992500	0.41546400
C	-3.79917200	3.75341000	0.97763600
H	-2.60730300	2.03656400	0.51447200
C	-2.71100000	5.93021200	0.80635000
H	-0.65077600	5.89570900	0.19299700
C	-3.84243500	5.15228400	1.08674700
H	-4.68366100	3.16752900	1.20372100
H	-2.75642800	7.01002800	0.89646600
H	-4.76368500	5.63710600	1.39483700

1b-IM1

0 1			
C	1.71392400	-0.88024300	0.95200300
C	2.19292800	0.50704900	0.90548300
C	3.61845800	0.68151800	0.60005400
C	4.48126100	-0.41348600	0.67775200
C	2.71108600	-1.92392600	1.35154300
H	3.59398400	2.77286700	0.07272800
C	4.21138200	1.88734000	0.18289000
C	5.83310400	-0.36444500	0.38147400
C	6.42347800	0.85568400	-0.02707700
C	5.55672300	1.98162800	-0.12654700
H	6.40342500	-1.27745600	0.48136600
H	5.93670400	2.93833500	-0.45822700
C	1.34494900	1.53453000	1.16648800
H	0.30468100	1.38213400	1.43170400
H	1.69672700	2.56049600	1.15990700
O	-1.94330700	1.31499300	-0.50945100
C	-2.49228000	1.95570200	0.44302300
O	-2.03544100	2.04561600	1.62072300
C	-3.79866600	2.66359000	0.13926800
C	-4.36870700	2.61068200	-1.14351100
C	-4.47028600	3.39000200	1.12856400
C	-5.56392300	3.25843400	-1.42599700
H	-3.85982800	2.05211100	-1.92179900
C	-5.67292000	4.04820500	0.86619000

H	-4.04117700	3.43930700	2.12384400
C	-6.22379100	3.98235900	-0.42008000
H	-6.00502500	3.21842800	-2.41723500
H	-6.16600800	4.60081200	1.65676600
O	-7.39609200	4.58747700	-0.79265000
C	-8.10502900	5.34377300	0.19306200
H	-8.99112700	5.73218800	-0.31061700
H	-8.41246300	4.71360900	1.03471800
H	-7.50209600	6.17976000	0.56395500
O	2.43857000	-2.99065600	1.87015900
O	4.02217700	-1.65790000	1.12401600
N	7.77383500	0.95238900	-0.28307400
C	8.62518700	-0.24345300	-0.27803600
C	8.52071800	-1.12997600	-1.52313800
H	8.40239300	-0.83164500	0.61802400
H	9.65543900	0.10267800	-0.16265600
H	9.16018900	-2.01097600	-1.40130700
H	7.49636700	-1.47754100	-1.68709300
H	8.84749700	-0.59593100	-2.41982000
C	8.35100500	2.18787100	-0.82803200
C	8.11010400	2.42114800	-2.32278200
H	9.42590200	2.14481500	-0.63481000
H	7.97514000	3.03963400	-0.25258800
H	8.54767500	3.38041900	-2.62002500
H	8.57249600	1.63610900	-2.92769700
H	7.04235400	2.45021800	-2.55958600
C	0.42008300	-1.21137600	0.60889700
H	-0.21140400	-0.39398600	0.27336100
C	-0.11608100	-2.52149000	0.58942100
H	0.54173900	-3.33732700	0.86651900
C	-1.42277700	-2.87382300	0.23142100
C	-2.43869500	-1.93590100	-0.15556800
C	-1.76557600	-4.26415900	0.25987100
C	-3.69299700	-2.37224700	-0.48328900
H	-2.22183700	-0.87193200	-0.19889900
C	-3.02278700	-4.70811500	-0.06744200
H	-1.00296000	-4.97950100	0.55128600
C	-4.00691100	-3.75935900	-0.44369800
H	-4.47295900	-1.67975300	-0.77959000
H	-3.25457800	-5.76446300	-0.03596100
O	-5.25286100	-4.07036100	-0.77914700
C	-5.69631700	-5.46072800	-0.77680400
C	-7.15045000	-5.46458000	-1.18994600
H	-5.55825600	-5.86389700	0.23052000

H	-5.07234100	-6.02160900	-1.47871600
H	-7.51507400	-6.49581500	-1.19847100
H	-7.75939500	-4.88898200	-0.48726700
H	-7.27455500	-5.04643600	-2.19275900

1A-IM2

1 1			
C	1.28086200	1.33767300	-0.38441000
C	0.75385400	0.00204000	-0.37320800
C	-0.58822800	-0.20770500	-0.14878200
C	-1.42348600	0.93830300	0.09033400
C	0.42901400	2.50141200	-0.13240900
H	-0.63509900	-2.37214000	-0.31046300
C	-1.23468000	-1.48660100	-0.12929600
C	-2.76418400	0.83617300	0.32769000
C	-3.39589900	-0.44999400	0.34961300
C	-2.56884900	-1.61138100	0.10303300
H	-3.32148700	1.74664500	0.49224400
H	-3.00993800	-2.59751300	0.09714800
C	1.86900700	-0.96590700	-0.63302300
H	1.63909300	-1.62972600	-1.47159300
H	2.02997300	-1.60026900	0.24438000
O	0.77448800	3.66190000	-0.10506500
O	-0.90602000	2.21989700	0.09343100
N	-4.70941300	-0.57343400	0.60235000
C	-5.57343300	0.61124500	0.80590300
C	-6.01097800	1.29584600	-0.48946300
H	-5.05409400	1.31429600	1.46057800
H	-6.44817200	0.26376100	1.35651500
H	-6.62576400	2.16593700	-0.23894500
H	-5.15477300	1.64177900	-1.07528000
H	-6.60741300	0.62424300	-1.11198500
C	-5.38836300	-1.88942400	0.57991300
C	-5.77555900	-2.36630100	-0.81996200
H	-6.27996500	-1.78672500	1.20003000
H	-4.74892200	-2.62217600	1.07481200
H	-6.25715300	-3.34582800	-0.73956100
H	-6.47939900	-1.67816100	-1.29483600
H	-4.89992900	-2.46861200	-1.46741100
C	2.60698300	1.33410200	-0.68199900
H	3.23672100	2.21309900	-0.76001200

C	3.11591500	-0.06105000	-0.91100400
H	3.38837900	-0.13686100	-1.97279100
C	4.33801100	-0.35849600	-0.07542200
C	4.52142400	-0.13876000	1.26668500
S	5.76585900	-1.07937000	-0.77968800
C	5.80476800	-0.55258100	1.73697500
H	3.76013200	0.30353400	1.90035600
C	6.58854500	-1.08111500	0.74895600
H	6.12889900	-0.45902300	2.76721300
H	7.59497100	-1.47154800	0.82047700

1B-IM2

1 1			
C	0.48984600	1.54713700	-0.38075700
C	0.04152700	0.18491700	-0.44607600
C	-1.27809800	-0.12001200	-0.19670400
C	-2.17096100	0.95530300	0.14048600
C	-0.41880200	2.63761900	-0.02414300
H	-1.20257800	-2.26696500	-0.50496000
C	-1.84654500	-1.43430600	-0.24320300
C	-3.49489200	0.75641900	0.40986600
C	-4.04653600	-0.56594500	0.37387800
C	-3.16161200	-1.65587200	0.02420300
H	-4.09815200	1.61911300	0.65184400
H	-3.54204300	-2.66489700	-0.03902900
C	1.20061400	-0.69506600	-0.80537400
H	0.97268800	-1.33684800	-1.66125000
H	1.44650100	-1.35251700	0.03473400
O	-0.14058200	3.81230900	0.07603600
O	-1.72880800	2.26269400	0.21486800
N	-5.33897000	-0.78588800	0.66790300
C	-6.27182400	0.33115200	0.94073900
C	-6.76750500	1.04957600	-0.31479200
H	-5.78792200	1.03277000	1.62382100
H	-7.11616800	-0.09709000	1.48160600
H	-7.43849700	1.86098000	-0.01618000
H	-5.94289500	1.48397900	-0.88671900
H	-7.32139200	0.37055300	-0.96788800
C	-5.92998700	-2.14294100	0.63288300
C	-6.38030800	-2.59096200	-0.75737500
H	-6.78203700	-2.12431100	1.31406500

H	-5.21309600	-2.84889600	1.05498100
H	-6.78996900	-3.60352600	-0.68818700
H	-7.15881700	-1.93466400	-1.15467300
H	-5.54588000	-2.60768500	-1.46448800
C	1.79938400	1.64442200	-0.73410600
H	2.37308900	2.56316600	-0.77742000
C	2.37357300	0.30315000	-1.09120400
H	2.56980000	0.32304800	-2.17295500
C	3.66815200	0.02753300	-0.36949700
C	3.97052900	0.23619100	0.94785000
S	5.04555400	-0.66841300	-1.21747800
C	5.29634100	-0.15287500	1.32045200
H	3.25990900	0.65814900	1.65101900
C	5.99631500	-0.65980800	0.25773300
H	5.69811300	-0.05798100	2.32067900
O	7.25538600	-1.14133500	0.15952400
C	8.01704100	-1.13417800	1.37930600
H	7.53148800	-1.75362000	2.14003900
H	8.99021100	-1.55277600	1.12401000
H	8.13610200	-0.11224500	1.75287100

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C	1.32183900	1.33812600	-0.40076700
C	0.78989300	0.00572100	-0.44250500
C	-0.54913400	-0.21058700	-0.20212200
C	-1.37515500	0.92593700	0.10173800
C	0.47995900	2.49173500	-0.08188700
H	-0.60670800	-2.36486100	-0.45998800
C	-1.19965700	-1.48679900	-0.22740100
C	-2.71234000	0.81741200	0.35775300
C	-3.34771800	-0.46659600	0.33759200
C	-2.52997600	-1.61817900	0.02475600
H	-3.26337400	1.72107300	0.57319700
H	-2.97409200	-2.60207000	-0.01783400
C	1.89910600	-0.94989900	-0.76386900
H	1.64826800	-1.59125600	-1.61385500
H	2.07892500	-1.61148300	0.09052100
O	0.82971600	3.64910100	-0.00763000
O	-0.85275900	2.20458800	0.15319800
N	-4.65667700	-0.59634700	0.61266000

C	-5.51282500	0.58239400	0.87494500
C	-5.96382600	1.32171400	-0.38535200
H	-4.98242200	1.25635200	1.55122500
H	-6.38239000	0.21605800	1.42142600
H	-6.57500000	2.18070100	-0.09132900
H	-5.11424700	1.69220900	-0.96564400
H	-6.56781300	0.67742500	-1.02906100
C	-5.33945100	-1.90899900	0.56074400
C	-5.77901000	-2.32717400	-0.84250200
H	-6.20749400	-1.83124900	1.21723000
H	-4.68457100	-2.66232200	1.00138400
H	-6.25591000	-3.31069400	-0.78645700
H	-6.50119000	-1.62154500	-1.26086400
H	-4.92801000	-2.39862900	-1.52607200
C	2.64322800	1.34092300	-0.72347000
H	3.27304900	2.22265000	-0.76894200
C	3.13738900	-0.03894600	-1.04519700
H	3.36224000	-0.05327500	-2.12098000
C	4.41666600	-0.40907800	-0.30697700
C	4.47837900	-0.34413500	1.09300400
C	5.55047200	-0.81756000	-1.01866300
C	5.65143200	-0.68690000	1.76573200
H	3.60533400	-0.02676900	1.65729500
C	6.72458900	-1.16249300	-0.34552600
H	5.51198200	-0.86731100	-2.10344000
C	6.77807500	-1.09729200	1.04794500
H	5.68635800	-0.63152100	2.84974400
H	7.59563200	-1.48060600	-0.91072500
H	7.69090400	-1.36391500	1.57218100

1b-IM2

1 1

C	-0.05194700	1.64275500	0.41332500
C	0.36972100	0.28523300	0.60888600
C	1.66351800	-0.08510600	0.31327200
C	2.55424000	0.91682800	-0.20451800
C	0.85451400	2.65829700	-0.12288200
H	1.56220100	-2.17911500	0.87202400
C	2.20578500	-1.40058400	0.47692200
C	3.85331600	0.65036900	-0.53201300
C	4.37965600	-0.67259300	-0.37136200

C	3.49652100	-1.68882800	0.15795700
H	4.45803700	1.46216200	-0.90888800
H	3.85827500	-2.69487000	0.31315500
C	-0.78638900	-0.51162700	1.13403500
H	-0.52493500	-1.04806200	2.05108400
H	-1.08183300	-1.26757300	0.39847100
O	0.59710000	3.82217300	-0.33981400
O	2.13666800	2.21953200	-0.40212300
N	5.64727800	-0.96155600	-0.71255300
C	6.57728900	0.08486500	-1.19303100
C	7.19727400	0.92842500	-0.07838500
H	6.05037700	0.71819100	-1.90990500
H	7.36061100	-0.42992300	-1.75047900
H	7.85337400	1.68070800	-0.52723000
H	6.43486300	1.44868600	0.50810800
H	7.79577300	0.31404700	0.59896100
C	6.21940600	-2.31328600	-0.51905600
C	6.70918600	-2.58482600	0.90345100
H	7.04906800	-2.39967700	-1.22196900
H	5.47877100	-3.05492800	-0.82324600
H	7.09479400	-3.60775600	0.95694100
H	7.51499400	-1.90177700	1.18371600
H	5.90171200	-2.48613400	1.63458000
C	-1.34036200	1.81084300	0.81720200
H	-1.88970800	2.74512800	0.77892100
C	-1.92415100	0.53731600	1.35501000
H	-2.07676700	0.68744100	2.43320200
C	-3.27549600	0.19347900	0.74648300
C	-3.43002000	0.06876500	-0.64482600
C	-4.39580500	-0.00474200	1.55632000
C	-4.66155700	-0.25055000	-1.20095800
H	-2.57683400	0.22105600	-1.30052400
C	-5.64293000	-0.32816800	1.01384000
H	-4.30071400	0.09019200	2.63465100
C	-5.77827700	-0.45230900	-0.37383700
H	-4.78115600	-0.34762600	-2.27535800
H	-6.48763300	-0.47909800	1.67454600
O	-6.94563700	-0.76535300	-1.01620600
C	-8.12917100	-0.98239300	-0.22434800
C	-9.26001300	-1.31425800	-1.17623900
H	-8.35228800	-0.07761900	0.35409700
H	-7.95197900	-1.80424100	0.47989600
H	-10.17908500	-1.48520800	-0.60792800
H	-9.43582500	-0.49208400	-1.87641800

H	-9.03592200	-2.21927100	-1.74888300
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C	1.09054700	1.21096900	0.13103800
C	0.58267300	-0.05570500	0.05957700
C	-0.82200200	-0.28177400	0.14008500
C	-1.65087000	0.85402700	0.28597500
C	0.25998700	2.36097500	0.28590000
H	-0.87400900	-2.43170500	-0.03823900
C	-1.47208300	-1.53320900	0.07773900
C	-3.03093700	0.77308200	0.36807000
C	-3.67426400	-0.48847100	0.31911800
C	-2.84346500	-1.64225900	0.15791600
H	-3.58508500	1.69632100	0.46431900
H	-3.28582600	-2.62726500	0.09982300
C	1.69694000	-1.06195500	-0.06800200
H	1.48903500	-1.84578700	-0.80159400
H	1.84877300	-1.55841600	0.89772000
O	0.62613200	3.53366300	0.35802500
O	-1.11063500	2.12644700	0.34732700
N	-5.03617900	-0.60409000	0.45113400
C	-5.88704700	0.58818800	0.56432200
C	-6.20120400	1.29324500	-0.75840500
H	-5.41819500	1.28901800	1.26141200
H	-6.81872500	0.26877700	1.03791400
H	-6.79966200	2.18945800	-0.56252200
H	-5.28937100	1.60280800	-1.27761700
H	-6.77279800	0.64445000	-1.42802700
C	-5.71163300	-1.89400900	0.24642400
C	-5.84873400	-2.33107200	-1.21474300
H	-6.70384600	-1.80273100	0.69441000
H	-5.19031000	-2.66574500	0.82107900
H	-6.34245400	-3.30776400	-1.26000100
H	-6.45024600	-1.61977200	-1.78759400
H	-4.87362600	-2.42366500	-1.70198100
C	2.92380500	-0.19048000	-0.46657500
H	2.90786700	-0.08987400	-1.55807900
C	4.25991800	-0.73278400	-0.03998700
C	4.60798500	-1.41234200	1.09999200
S	5.67826100	-0.46473200	-1.03478500

C	6.00153700	-1.72238100	1.18120300
H	3.89248100	-1.68935600	1.86614000
C	6.71111700	-1.27623000	0.10204600
H	6.45147100	-2.25924000	2.00899000
H	7.76933000	-1.37497000	-0.09984400
C	2.59627100	1.23770000	0.06414200
H	3.02645400	1.38422600	1.06631600
O	3.12389200	2.21980800	-0.82943100
H	2.77347200	3.07314400	-0.52638000

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0 1

C	-0.36324500	1.33256400	-0.06656800
C	0.09052100	0.04858700	0.04557700
C	1.47995200	-0.24587200	-0.07013400
C	2.35276800	0.84261200	-0.29643900
C	0.51114200	2.43489200	-0.30559500
H	1.44127500	-2.38587100	0.20239200
C	2.07468600	-1.52238400	0.02478100
C	3.72384600	0.69391500	-0.42348800
C	4.31106100	-0.59300500	-0.34157000
C	3.43582400	-1.69874900	-0.09935000
H	4.31450800	1.58527300	-0.58221800
H	3.83526200	-2.69975400	-0.01207700
C	-1.06157000	-0.90232700	0.24361900
H	-0.86466000	-1.66750000	0.99930500
H	-1.26021300	-1.42366100	-0.70102500
O	0.19709400	3.61785700	-0.42916400
O	1.86792300	2.13420300	-0.39826200
N	5.66045500	-0.77753500	-0.51749900
C	6.56137500	0.36811400	-0.70276000
C	6.94608500	1.10863500	0.58147400
H	6.10565700	1.06297500	-1.41456400
H	7.46279800	-0.01393100	-1.18835700
H	7.58143700	1.96581200	0.33392500
H	6.06489500	1.48325500	1.11068300
H	7.50361500	0.45931100	1.26233200
C	6.28254200	-2.09057100	-0.29246800
C	6.46629000	-2.47960400	1.17712200
H	7.25619400	-2.06510000	-0.78732600
H	5.69870300	-2.85607700	-0.81274500

H	6.90988900	-3.47919900	1.23873600
H	7.13086000	-1.78088200	1.69292700
H	5.51197200	-2.50096900	1.71162500
C	-2.23768200	0.03707800	0.63070400
H	-2.18913900	0.18684900	1.71822600
C	-3.59909500	-0.47815000	0.26057300
C	-3.96757500	-1.68075600	-0.27212400
S	-5.03160700	0.51820600	0.55695200
C	-5.38000000	-1.84803500	-0.46604200
H	-3.25252000	-2.45649800	-0.52166100
C	-6.08113700	-0.74629500	-0.06330200
H	-5.83196000	-2.73886900	-0.88225100
O	-7.40854300	-0.47122300	-0.07193100
C	-8.24724300	-1.50868800	-0.60404500
H	-8.15299700	-2.42451000	-0.01133100
H	-9.26737200	-1.13004400	-0.54133600
H	-7.98993500	-1.71630000	-1.64789800
C	-1.86436400	1.42411700	0.03413900
H	-2.31157100	1.55225100	-0.96297200
O	-2.33210400	2.45959400	0.90173600
H	-2.01421200	3.29497600	0.52322600

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0 1			
C	1.11481500	1.27928100	0.01101300
C	0.63232400	0.00253500	-0.05542400
C	-0.76401800	-0.25498600	0.06985300
C	-1.61214700	0.86043900	0.25459800
C	0.26442500	2.40891600	0.20385900
H	-0.77436800	-2.40355700	-0.12693400
C	-1.38815000	-1.51987500	0.01740800
C	-2.98677100	0.74820400	0.38149000
C	-3.60366600	-0.52662700	0.34053800
C	-2.75356500	-1.66019500	0.14166800
H	-3.55727300	1.65810500	0.50516500
H	-3.17599100	-2.65422000	0.08871500
C	1.76343200	-0.97699400	-0.23065800
H	1.55036800	-1.74780600	-0.97723100
H	1.94974000	-1.49579800	0.71791600
O	0.60570500	3.58940500	0.27360400
O	-1.09817900	2.14377000	0.30957700

N	-4.95816600	-0.67349900	0.51430900
C	-5.83144700	0.49868800	0.66124700
C	-6.19714800	1.20767200	-0.64612700
H	-5.35952000	1.20415200	1.35160400
H	-6.74244700	0.15449800	1.15721300
H	-6.80949100	2.08879300	-0.42615700
H	-5.30670200	1.54165500	-1.18690000
H	-6.77231200	0.55201900	-1.30592300
C	-5.61094800	-1.97619800	0.31789800
C	-5.78557900	-2.40229200	-1.14256100
H	-6.58989600	-1.91197200	0.79862000
H	-5.05373000	-2.74129200	0.86719500
H	-6.25658200	-3.39040400	-1.18194000
H	-6.42273300	-1.70051400	-1.68794500
H	-4.82504700	-2.46608500	-1.66231100
C	2.97130500	-0.07736700	-0.63548900
H	2.95399800	0.02178200	-1.72640400
C	4.33262300	-0.59806400	-0.22414200
C	4.64046700	-0.84992200	1.12277200
C	5.32316900	-0.83147100	-1.18705600
C	5.90070700	-1.31987200	1.49298300
H	3.88876900	-0.67691300	1.88854300
C	6.58655500	-1.30270000	-0.82044100
H	5.10164100	-0.64175200	-2.23410800
C	6.87976100	-1.54838700	0.52164300
H	6.11902200	-1.50793100	2.54036800
H	7.33931500	-1.47637400	-1.58409600
H	7.86065000	-1.91469200	0.81002700
C	2.61733700	1.33891200	-0.09861700
H	3.06711200	1.50773500	0.89151200
O	3.09658500	2.33428000	-1.00801200
H	2.72886400	3.17725700	-0.69716900

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C	0.12552800	1.57022700	-0.01764100
C	0.46426300	0.25010400	0.08511800
C	1.82072200	-0.16629700	-0.04921700
C	2.78552200	0.84028800	-0.27966300
C	1.09362500	2.59008000	-0.26114400
H	1.59241800	-2.29512800	0.21599800

C	2.29921700	-1.49130400	0.03512500
C	4.13668800	0.56970000	-0.42004100
C	4.60669000	-0.76512300	-0.34845600
C	3.63779400	-1.78889300	-0.10285000
H	4.80419200	1.40451300	-0.58174300
H	3.94592800	-2.82215600	-0.02154200
C	-0.76610500	-0.59051900	0.30622300
H	-0.62727800	-1.36231300	1.06914900
H	-1.02938200	-1.10735800	-0.62526700
O	0.88680300	3.79831400	-0.37258800
O	2.41703800	2.17056000	-0.37106400
N	5.93309400	-1.06789800	-0.53692400
C	6.93288900	-0.00454500	-0.70652700
C	7.37025300	0.69026600	0.58635400
H	6.54640700	0.73330800	-1.41640300
H	7.80134400	-0.46122700	-1.18759700
H	8.08516100	1.48597800	0.35085800
H	6.52215700	1.14287900	1.10858500
H	7.85707100	-0.01175900	1.26907900
C	6.43535300	-2.43599200	-0.34399000
C	6.61511000	-2.86365800	1.11530200
H	7.39566700	-2.49305100	-0.86180700
H	5.77165100	-3.13563400	-0.86081700
H	6.96365600	-3.90139100	1.15274400
H	7.35453700	-2.23905000	1.62427400
H	5.67527600	-2.80309300	1.67207900
C	-1.85639900	0.45066100	0.70569600
H	-1.79527400	0.58506400	1.79154200
C	-3.27702000	0.06654300	0.35223200
C	-3.66610400	-0.17093100	-0.97839200
C	-4.25182800	-0.06482500	1.34481400
C	-4.97121200	-0.52466300	-1.29706900
H	-2.93736200	-0.07877200	-1.77942600
C	-5.57157000	-0.42109300	1.04574600
H	-3.98207300	0.11326400	2.38261200
C	-5.93483700	-0.65414500	-0.28436600
H	-5.26538200	-0.70693100	-2.32607500
H	-6.29359900	-0.51161100	1.84806800
O	-7.19296300	-1.01153600	-0.69905400
C	-8.22062800	-1.17069500	0.29545300
C	-9.49338800	-1.57274400	-0.42186000
H	-8.35593300	-0.22676800	0.83770900
H	-7.91636800	-1.93862600	1.01735000
H	-10.29937200	-1.70321000	0.30640000

H	-9.79790600	-0.80384500	-1.13831400
H	-9.35812500	-2.51658600	-0.95864400
C	-1.36015500	1.79762200	0.10837300
H	-1.80481100	1.97521300	-0.88266200
O	-1.71528200	2.87403500	0.98174300
H	-1.27548600	3.66221000	0.62471100