

1^{Ni-B}

Ni	-0.04177100	-0.91207400	-0.45084200
C	-0.71764800	-2.27272100	0.91782200
B	0.07051600	-1.17146800	1.69221800
P	1.98054700	-0.15195300	-0.30874600
P	-1.55818000	0.64587700	-0.21254100
C	-2.14179100	-2.47741600	0.97823300
C	-2.80686800	-3.04419100	-0.09133500
H	-3.88491800	-3.18518100	-0.04024500
C	-2.12804500	-3.36296200	-1.29013500
C	-2.89862200	-3.85493900	-2.48216400
H	-3.39777000	-4.80705300	-2.25917500
H	-3.68419800	-3.14529800	-2.76528900
H	-2.24568000	-4.01032100	-3.34713600
C	-0.74209000	-3.30094300	-1.30802200
H	-0.20865100	-3.68650100	-2.17791000
C	0.02200400	-2.91497400	-0.16510100
C	1.35747000	-3.60885800	-0.00706500
H	1.95159700	-3.55013100	-0.92560800
H	1.95653500	-3.22003600	0.81205700
H	1.17474400	-4.67443500	0.19481000
C	-2.90738500	-2.11524800	2.22042800
H	-2.42666700	-2.53240500	3.11301300
H	-2.95481200	-1.03266600	2.36751600
H	-3.93422000	-2.49118600	2.16671900
C	1.59814500	-1.32896400	2.11681100
C	2.61309900	-0.86635300	1.25710600
C	2.27122700	1.63567000	-0.02074500
C	2.48409700	2.51176000	-1.09286000
H	2.51376600	2.12718100	-2.10928300
C	2.37322700	3.52075700	1.50314400
H	2.31874700	3.90912900	2.51722900
C	2.20701400	2.15408900	1.27968500
H	2.02648400	1.48923700	2.11930900
C	3.96342900	-0.99094300	1.59196600
H	4.73371200	-0.64584500	0.90833200
C	4.32808600	-1.58089500	2.80153300
H	5.37861400	-1.68843800	3.06024000
C	3.33715700	-2.04215600	3.67156100
H	3.61633600	-2.51527200	4.61037600
C	1.99006700	-1.91295000	3.33105400
H	1.23290200	-2.30684500	4.00691900
C	-0.65828300	0.08952800	2.34775200
C	-0.50451000	0.38546000	3.71287600

H	0.11368800	-0.26182100	4.32976500
C	-1.11762600	1.48926400	4.30255400
H	-0.98274900	1.68141700	5.36467100
C	-1.88889600	2.35807600	3.52735200
H	-2.35995500	3.22882900	3.97669300
C	-2.03419700	2.10973600	2.16474400
H	-2.60154900	2.80243100	1.54786300
C	-1.52121300	2.32135100	-0.97901200
C	-2.26849400	2.60397100	-2.13178200
H	-2.92796700	1.85140600	-2.55292500
C	-3.31136600	0.18610600	-0.51248600
C	-4.33753700	0.41102900	0.40932600
H	-4.11542900	0.86681500	1.36924300
C	-5.64951800	0.04002700	0.11270700
H	-6.43484200	0.20934000	0.84541900
C	-5.95475200	-0.53801700	-1.11968700
H	-6.97868500	-0.81787900	-1.35405200
C	-4.93641500	-0.76101300	-2.04826800
H	-5.16561400	-1.21373300	-3.00981800
C	-3.62227900	-0.42052400	-1.73674300
H	-2.82354900	-0.64157200	-2.44155900
C	-1.43307700	0.98837900	1.57946600
C	2.61542100	4.38315600	0.43272500
C	2.66765700	3.87364000	-0.86604800
H	2.75476500	5.44689400	0.60839600
H	2.83789800	4.54060200	-1.70740300
C	-0.69274100	3.32177000	-0.45466200
C	-2.19493600	3.85661300	-2.73944500
C	-1.38149900	4.85314300	-2.19805800
C	-0.63370200	4.57890000	-1.05315500
H	-0.09616700	3.12568900	0.42981400
H	0.00792500	5.34179000	-0.62159600
H	-1.33208900	5.83424700	-2.66379500
H	-2.78591400	4.05603400	-3.63020400
C	5.40918500	-0.33974100	-2.63266700
C	4.50619900	0.02939500	-1.63745900
C	3.22776600	-0.54410100	-1.59251200
C	2.86235500	-1.46881000	-2.57814600
C	3.76475100	-1.83934400	-3.57536000
C	5.04207100	-1.27860400	-3.60020800
H	6.39914200	0.10909500	-2.65694100
H	4.78964900	0.78106100	-0.90550700
H	1.85915600	-1.88933100	-2.56078900
H	3.46831900	-2.55859500	-4.33470300

H	5.74733700	-1.56301600	-4.37696300
2^{Ni-B}			
Ni	0.27643700	-0.10273000	-0.83544200
P	2.25982100	-0.53652600	-0.19725100
P	-1.33257700	1.18260000	-0.24471500
C	3.61116100	-0.95542300	-1.35756500
C	3.27557500	-1.58079200	-2.56453700
C	4.95932900	-0.71132500	-1.06481800
C	4.27057600	-1.96506300	-3.46271000
H	2.23017500	-1.76465500	-2.79836100
C	5.95434700	-1.09244600	-1.96407500
H	5.22982200	-0.21386700	-0.13696300
C	5.61192000	-1.72051300	-3.16359200
H	3.99863300	-2.44929100	-4.39722400
H	6.99787300	-0.89834400	-1.72882900
H	6.38868700	-2.01447100	-3.86485400
C	2.19333200	-1.91121500	0.98598300
C	3.28501600	-2.66738600	1.42151100
C	0.87160900	-2.21357900	1.35828800
C	3.06506500	-3.76150900	2.25749700
H	4.29319300	-2.41973900	1.09718600
C	0.67878000	-3.32856200	2.18819900
C	1.75899700	-4.09276500	2.63402200
H	3.90307600	-4.36343400	2.60042800
H	-0.33358600	-3.60462900	2.47892200
H	1.58506800	-4.95733200	3.27134900
C	2.89474500	0.93486100	0.67725800
C	2.73007200	1.06621600	2.05979700
C	3.37913200	2.02357300	-0.06359000
C	3.02662600	2.27399500	2.69104900
H	2.34958200	0.23057500	2.63702500
C	3.69338400	3.22242500	0.57174600
H	3.50385200	1.93539900	-1.14041600
C	3.50767500	3.35454400	1.95055900
H	2.87550300	2.36908400	3.76314700
H	4.07145900	4.05838300	-0.01157000
H	3.73676100	4.29581000	2.44358700
C	-1.09456300	1.16804000	1.55843000
C	-0.51732100	-0.03806700	2.00336100
C	-1.33796000	2.24039800	2.41644700
C	-0.16416800	-0.10996900	3.35742900
C	-0.99229200	2.13120400	3.76543800
H	-1.75872100	3.16749300	2.03297700

C	-0.39855500	0.95515000	4.22943800
H	0.30136700	-1.01805300	3.73714200
H	-1.16481500	2.96452600	4.44225500
H	-0.10854100	0.87303600	5.27508600
C	-1.05975000	2.92694600	-0.71310900
C	-1.93610200	3.64001300	-1.53608600
C	0.14126400	3.52437100	-0.30135400
C	-1.61644400	4.93808200	-1.94197100
H	-2.86839800	3.18333500	-1.85804300
C	0.45507500	4.81868000	-0.70304200
H	0.82939900	2.96982500	0.33172200
C	-0.42324400	5.52978600	-1.52699400
H	-2.30407100	5.48689200	-2.58091500
H	1.38730900	5.27114500	-0.37450200
H	-0.17701500	6.54035100	-1.84308800
C	-3.10193300	0.89472000	-0.57393000
C	-4.10908400	1.33378900	0.29206700
C	-3.44364200	0.18648900	-1.73004300
C	-5.44495600	1.06380900	0.00257400
H	-3.84685900	1.87135100	1.19958100
C	-4.78015100	-0.07270700	-2.02537600
H	-2.65584100	-0.18724000	-2.37896000
C	-5.78197100	0.36268300	-1.15790600
H	-6.22411800	1.39600200	0.68433000
H	-5.03663300	-0.63524200	-2.91915300
H	-6.82452400	0.14740700	-1.37878600
B	-0.32708000	-1.22933600	0.93706500
C	-1.65435600	-1.94218200	0.36434100
C	-1.60614300	-2.61224000	-0.88414900
C	-2.90654500	-1.94686300	1.03779100
C	-2.74639400	-3.18684900	-1.45012700
C	-4.03083800	-2.52617600	0.44065400
C	-3.98412400	-3.13630700	-0.81102500
H	-2.66695600	-3.67765000	-2.42010900
H	-4.97957500	-2.49612000	0.97575700
C	-0.32791000	-2.69301100	-1.67330000
H	-0.44331800	-3.32509200	-2.56101000
H	-0.02320300	-1.69161300	-2.04175100
H	0.50520100	-3.07735400	-1.07700300
C	-3.10663300	-1.38151800	2.42231000
H	-2.33912400	-1.72763300	3.12042100
H	-3.07062100	-0.28753300	2.43361700
H	-4.08321900	-1.68602200	2.81430600
C	-5.22393000	-3.70838800	-1.44075700

H	-5.93941700	-2.91291300	-1.68777200
H	-4.99123300	-4.24829400	-2.36498100
H	-5.73679100	-4.40210300	-0.76324300
C	0.79272800	1.12040200	-3.11622900
H	0.14971500	0.23454000	-3.16985700
H	0.23084000	1.98608300	-3.47006400
H	1.68807800	0.95371700	-3.71714400
H	1.10309300	1.32376700	-2.07713100

TS_{2/3}^{Ni-B}

Ni	0.37426200	0.22034700	-0.85042000
P	2.43692200	-0.31530600	-0.33026600
P	-1.27458400	1.65012800	-0.71336100
C	3.82113000	-0.54534300	-1.50274100
C	3.72514300	-1.53649600	-2.49157300
C	4.92401200	0.31859700	-1.51425300
C	4.71388700	-1.66425600	-3.46450300
H	2.88358800	-2.22387300	-2.48645600
C	5.91205700	0.19067200	-2.49085500
H	5.01453000	1.08912800	-0.75336600
C	5.81111500	-0.79975100	-3.46884700
H	4.62904500	-2.44254400	-4.21896000
H	6.76579500	0.86397300	-2.48239900
H	6.58282100	-0.90023700	-4.22765900
C	2.12506800	-2.02139900	0.29460900
C	3.17157700	-2.94089800	0.43161400
C	0.78552000	-2.39249000	0.58762800
C	2.92423800	-4.23839700	0.87874100
H	4.18560400	-2.64938000	0.16710000
C	0.57258500	-3.70857300	1.02868100
C	1.61678400	-4.62092700	1.18070800
H	3.74476700	-4.94453600	0.98132400
H	-0.44569100	-4.01891400	1.25423200
H	1.40984900	-5.63149200	1.52622600
C	3.20371700	0.60718100	1.05066300
C	3.99508400	0.00781700	2.03658000
C	2.94658100	1.98077900	1.11679200
C	4.51735700	0.77419900	3.07675800
H	4.18445500	-1.06123000	2.00482800
C	3.47851700	2.75005200	2.15016500
H	2.29726000	2.43260000	0.37062300
C	4.26178500	2.14674900	3.13430700
H	5.12186500	0.30013200	3.84630900

H	3.26327400	3.81448300	2.19804200
H	4.66669900	2.74145700	3.94943100
C	-0.74877200	1.29375800	1.01380400
C	-0.19360300	-0.00257900	1.28797600
C	-0.58177100	2.34438000	1.93433900
C	0.57974200	-0.11475700	2.47014200
C	0.09251900	2.14451600	3.13211500
H	-0.99777000	3.32174800	1.70906000
C	0.69539400	0.91122000	3.39293300
H	1.05545500	-1.06747000	2.68365100
H	0.17031000	2.95712500	3.85042900
H	1.26450600	0.76035600	4.30624300
C	-1.49999700	3.46508700	-0.72401900
C	-2.73670300	4.08974800	-0.52454300
C	-0.36160000	4.25114300	-0.94841000
C	-2.82860500	5.48223600	-0.53595900
H	-3.62637300	3.48779200	-0.35966800
C	-0.45105100	5.64141900	-0.94498000
H	0.59424000	3.76035300	-1.12494700
C	-1.68720600	6.25974700	-0.74006100
H	-3.79292700	5.96035300	-0.38210700
H	0.43902200	6.24253100	-1.11358000
H	-1.76141600	7.34420700	-0.74768600
C	-2.94807300	0.99064900	-0.97603300
C	-3.83480300	0.73909600	0.07487000
C	-3.34026500	0.70872800	-2.29188100
C	-5.09825900	0.21217300	-0.18559800
H	-3.52819100	0.94165100	1.09662800
C	-4.60653500	0.18852800	-2.55178200
H	-2.65130700	0.89867600	-3.11184500
C	-5.48584100	-0.06296300	-1.49667600
H	-5.77294300	0.00045500	0.63890800
H	-4.90301000	-0.03093200	-3.57443000
H	-6.46848200	-0.48282600	-1.69620700
B	-0.44973000	-1.36669300	0.47845100
C	-1.93277500	-1.99743800	0.51938800
C	-2.43581400	-2.81241200	-0.52476500
C	-2.77827700	-1.83848000	1.65374700
C	-3.74315400	-3.30978500	-0.49411200
C	-4.07067100	-2.37243200	1.66066400
C	-4.59607900	-3.07589700	0.57916800
H	-4.09604300	-3.90699100	-1.33499000
H	-4.69223000	-2.22439700	2.54344500
C	-1.61013800	-3.21358400	-1.72023300

H	-1.77554400	-2.53895200	-2.56726500
H	-0.54086100	-3.23004100	-1.50015500
H	-1.89438300	-4.21824400	-2.05305400
C	-2.35514700	-1.15309400	2.93146600
H	-1.40454700	-1.54390900	3.30594700
H	-2.22643700	-0.07226200	2.81682600
H	-3.11032100	-1.31563000	3.70810000
C	-6.02176000	-3.55229800	0.57094700
H	-6.68296900	-2.78923700	0.13694300
H	-6.13992600	-4.46221600	-0.02798700
H	-6.38397800	-3.75860200	1.58434200
C	0.17946000	-0.74059700	-2.57187500
H	-0.79558800	-0.70281300	-3.05833500
H	0.83866500	0.01406100	-3.01314300
H	0.62296800	-1.72816800	-2.70588800
H	-0.34777300	-1.04654400	-1.21522100

3Ni-B

Ni	0.54532400	0.54627400	-0.91151000
P	2.39319600	-0.42503800	-0.35856300
P	-1.31409100	1.54169400	-0.39010100
C	3.53602900	-0.87781800	-1.69894800
C	3.41227700	-2.12540400	-2.32546700
C	4.43873600	0.06311200	-2.21281900
C	4.19473800	-2.43318900	-3.43673800
H	2.70738900	-2.85678500	-1.93920800
C	5.22027200	-0.24880700	-3.32431300
H	4.53371900	1.03751700	-1.74209400
C	5.10217000	-1.49732000	-3.93720200
H	4.09588800	-3.40607800	-3.91127200
H	5.92211800	0.48544100	-3.71134600
H	5.71362600	-1.73973800	-4.80244000
C	2.09108300	-1.96382900	0.57962800
C	3.16022500	-2.81672500	0.88666200
C	0.77792600	-2.23601400	1.00966200
C	2.93947000	-3.97546900	1.62528500
H	4.16282200	-2.58798000	0.53321300
C	0.58870900	-3.41975400	1.74273900
C	1.64369400	-4.27657100	2.05285200
H	3.76710900	-4.64185000	1.85521300
H	-0.41861500	-3.67596100	2.06432800
H	1.45670700	-5.18489600	2.62163600
C	3.36500400	0.61696200	0.78590900
C	4.72478300	0.39010600	1.03245300

C	2.69402800	1.61997000	1.49635400
C	5.40373900	1.15976700	1.97549000
H	5.25787000	-0.38128100	0.48347900
C	3.37267400	2.38341500	2.44431400
H	1.63669500	1.79097600	1.31529200
C	4.72840800	2.15638700	2.68414700
H	6.46022000	0.98041800	2.15802200
H	2.83808000	3.15298900	2.99471300
H	5.25950200	2.75407900	3.42060600
C	-1.04576600	1.27350000	1.40042200
C	-0.47179700	0.02867200	1.76868900
C	-1.14549100	2.33106500	2.31352900
C	0.07603000	-0.05154000	3.05628400
C	-0.63491400	2.19166500	3.60356800
H	-1.59410200	3.27293200	2.01038800
C	0.00402300	1.00393800	3.96317400
H	0.57087200	-0.97373000	3.35392000
H	-0.71170600	3.01454100	4.30999000
H	0.44739200	0.90210000	4.95125500
C	-1.53730200	3.33799400	-0.58019400
C	-2.75247900	3.90102000	-0.98449500
C	-0.44356400	4.17611500	-0.31582000
C	-2.87356500	5.28515300	-1.11915600
H	-3.60421100	3.25934500	-1.19092200
C	-0.56980600	5.55662500	-0.44167700
H	0.50303000	3.74289700	-0.00475900
C	-1.78545200	6.11424400	-0.84692600
H	-3.82164600	5.71397400	-1.43354600
H	0.28218000	6.19758000	-0.23013600
H	-1.88170700	7.19184000	-0.95166000
C	-2.89068700	0.81807100	-0.91532800
C	-3.89263800	0.47990100	-0.00252600
C	-3.08078300	0.58136500	-2.28234100
C	-5.08112400	-0.08817300	-0.45578400
H	-3.73104500	0.64202300	1.05913500
C	-4.27483700	0.02426600	-2.73343700
H	-2.29020600	0.82797300	-2.98801400
C	-5.27450800	-0.31194600	-1.81896600
H	-5.84791300	-0.37346000	0.25855300
H	-4.41906300	-0.16212400	-3.79456600
H	-6.19951400	-0.76328400	-2.16844100
B	-0.46179700	-1.23345900	0.75800400
C	-1.87336200	-2.00012300	0.53359700
C	-2.15354000	-2.55546300	-0.74099900

C	-2.84744000	-2.18133200	1.54218000
C	-3.37070200	-3.19235800	-0.99380000
C	-4.05037600	-2.84102300	1.26017800
C	-4.34642300	-3.33405500	-0.00804900
H	-3.56248500	-3.58793400	-1.99111000
H	-4.78266700	-2.96211500	2.05867000
C	-1.16081900	-2.48683400	-1.87403100
H	-1.06914800	-1.46655000	-2.27097200
H	-0.15835900	-2.79454100	-1.55615400
H	-1.47189900	-3.13586800	-2.69989600
C	-2.66178500	-1.68878300	2.95613900
H	-1.70450500	-2.00474700	3.38155000
H	-2.68145300	-0.59456900	3.01709000
H	-3.45884700	-2.07382700	3.60188400
C	-5.67562500	-3.96792500	-0.31418400
H	-6.34918300	-3.24752800	-0.79919500
H	-5.57009200	-4.81948300	-0.99640300
H	-6.17267700	-4.31971300	0.59659300
C	1.44545300	1.93470000	-1.88104700
H	0.74325000	2.68267600	-2.26016100
H	2.21225100	2.44090900	-1.28262500
H	1.93583700	1.43405000	-2.72670400
H	-0.30031300	-0.79377400	-0.44575100

1^{BPh}

Ni	-0.08504900	-0.17951600	0.73899400
P	1.73918600	-0.05396600	-0.48023400
C	3.02686900	0.81840600	0.63576400
C	1.58859700	0.91471800	-2.12182700
C	2.35930900	-1.81867300	-0.88030900
C	2.71948500	2.32332700	0.66567100
H	1.66895500	2.51475300	0.90564700
H	3.32985900	2.78464800	1.45317900
H	2.96185000	2.83043500	-0.27017400
C	2.79483000	0.32612700	2.07730500
H	1.75490400	0.48847800	2.38867200
H	3.01819900	-0.73053700	2.21921200
H	3.44542300	0.89790100	2.75340100
C	4.49813600	0.62093700	0.25805300
H	4.71574900	0.94536600	-0.76236200
H	5.12278700	1.21908600	0.93577700
H	4.81823200	-0.41872500	0.36113600
C	0.66416300	2.11932300	-1.88191100
H	1.05725300	2.83765000	-1.16414700

H	0.52249300	2.64656900	-2.83498800
H	-0.31728200	1.80098200	-1.52100700
C	2.91550100	1.39580500	-2.71942800
H	2.71380800	1.86548200	-3.69191300
H	3.40721200	2.14656200	-2.09670800
H	3.62032400	0.57837500	-2.88849000
C	0.87133400	0.04341000	-3.16307600
H	-0.04851300	-0.39251400	-2.76463900
H	0.59499800	0.68199300	-4.01239100
H	1.50060400	-0.75847900	-3.55448100
C	3.50726700	-1.91513300	-1.89092200
H	3.80844900	-2.96772600	-1.98300000
H	3.21707600	-1.57693300	-2.88825600
H	4.38800100	-1.34761100	-1.58077700
C	2.79999900	-2.49151600	0.42750000
H	2.96537100	-3.55872700	0.22985800
H	3.73602500	-2.08771300	0.81927700
H	2.02879000	-2.40931200	1.19893300
C	1.15810300	-2.63733700	-1.38861300
H	0.81089500	-2.33302500	-2.37506400
H	1.45658300	-3.69218200	-1.45571700
H	0.31247000	-2.56431800	-0.69880300
B	-2.21636700	0.06944300	0.63219400
C	-2.78070800	-0.89121100	-0.47954700
C	-2.59382300	-0.62150100	-1.84905900
C	-3.43458800	-2.09505100	-0.15311800
C	-3.01189500	-1.50877300	-2.83945000
C	-3.87224100	-2.98365900	-1.13479300
C	-3.65468200	-2.69691800	-2.48465200
C	-1.62254200	-0.51974700	1.94052200
C	-1.49111200	0.17825800	3.18472300
C	-0.87293600	-1.74389000	1.81377800
C	-0.73032800	-0.31250100	4.22469800
C	-0.10511100	-2.24012100	2.90134500
C	-0.02387300	-1.53167400	4.08086300
C	-2.22515100	1.62591900	0.40223100
C	-1.27838500	2.47228100	1.02122800
C	-3.09766100	2.23376800	-0.52593300
C	-1.18565300	3.82970500	0.71574500
C	-3.02276300	3.59083100	-0.82843400
C	-2.05663500	4.39454400	-0.21504400
H	-2.09764800	0.30037600	-2.14087400
H	-2.83842300	-1.27474400	-3.88775600
H	-3.98642000	-3.39151900	-3.25292000

H	-4.37999200	-3.90249600	-0.84922100
H	-3.60204000	-2.33467800	0.89515000
H	-1.08404500	-2.42140100	0.98906600
H	0.40657400	-3.19456000	2.79995300
H	0.56896400	-1.91242800	4.90935000
H	-0.67623300	0.23264800	5.16430400
H	-2.03668600	1.11018700	3.31552000
H	-3.85111200	1.62296500	-1.01711200
H	-3.71518500	4.02597700	-1.54574700
H	-1.98921000	5.45223300	-0.45873800
H	-0.43076300	4.44461200	1.20093800
H	-0.58391600	2.05315800	1.74676300

2^{BPh}

Ni	-0.21103800	-0.82618300	0.23370100
B	1.91725500	-1.01251400	0.60489100
C	2.86947500	-0.74357900	-0.62913400
C	2.38214700	-0.30351100	-1.87033800
C	4.25969900	-0.92222000	-0.51642400
C	3.22986600	-0.06067600	-2.95197000
C	5.11819100	-0.68166100	-1.59033100
C	4.60537800	-0.25036700	-2.81602800
C	1.90490000	0.03064200	1.77849900
C	0.88723100	0.05655900	2.76002600
C	2.82190800	1.10537700	1.79630300
C	0.79183700	1.08516300	3.69786900
C	2.73811500	2.13118600	2.73138700
C	1.71639500	2.12812900	3.68658600
C	1.03266800	-2.28587700	0.66194000
C	0.36536500	-2.64027400	-0.56336500
C	0.60298900	-2.97466500	1.84301900
C	-0.62309100	-3.66084800	-0.58296400
C	-0.36582100	-3.95552600	1.80510000
C	-0.99400200	-4.29688300	0.58217000
C	3.50940800	3.19432100	-1.01246000
H	3.41213800	3.78916800	-1.92405100
H	2.54392100	3.13662500	-0.50716300
H	4.23919000	3.66306800	-0.34766000
H	3.83726400	2.18554500	-1.26982500
P	-1.80361400	0.55227100	-0.41089300
C	-3.19056100	0.39364600	0.89986700
C	-3.26282300	-1.08966500	1.31090100
C	-2.77093000	1.15079700	2.16819600
C	-4.58192900	0.87865800	0.48016400

H	-3.60968300	-1.74644800	0.51406000
H	-2.28279400	-1.45826200	1.63973100
H	-3.96276800	-1.18888800	2.15192100
H	-2.80557800	2.23568500	2.05027900
H	-3.47009600	0.88897300	2.97334100
H	-1.76657900	0.86632900	2.49366400
H	-5.26313300	0.78359500	1.33699100
H	-4.58364100	1.92759500	0.17399800
H	-5.00553200	0.28548100	-0.33334900
C	-1.27599500	2.38618200	-0.53218200
C	-2.42491500	3.40061800	-0.52614100
C	-0.32415400	2.68281800	0.63737700
C	-0.43731100	2.59676000	-1.80141600
H	-3.14215300	3.23267400	-1.33259900
H	-2.97070100	3.40519700	0.42015800
H	-2.00547000	4.40702400	-0.66063800
H	0.53948200	2.01361200	0.62158600
H	0.04318800	3.71288300	0.53565500
H	-0.79017900	2.59623900	1.61714700
H	-0.00405200	3.60443200	-1.76105400
H	0.39535400	1.88913700	-1.85662500
H	-1.02206800	2.53414700	-2.72136800
C	-2.51603400	0.01592600	-2.10392900
C	-3.26699400	-1.31316300	-1.93723500
C	-3.44797100	1.02543600	-2.78328700
C	-1.33542100	-0.29850400	-3.03861200
H	-2.65775200	-2.05459100	-1.41168000
H	-4.21986100	-1.20358700	-1.41571300
H	-3.48877800	-1.71132800	-2.93623700
H	-2.92916100	1.94103400	-3.07637800
H	-3.84772600	0.57360600	-3.70148000
H	-4.29880600	1.30095500	-2.15576800
H	-1.73325700	-0.66006400	-3.99650200
H	-0.70263000	0.56280100	-3.25108500
H	-0.70904000	-1.08684400	-2.61327300
H	2.81653500	0.28382000	-3.89768000
H	1.31373300	-0.13645800	-1.98333700
H	5.27235000	-0.06085800	-3.65369000
H	6.18934900	-0.82999000	-1.47106400
H	4.67972000	-1.25751800	0.43095200
H	0.79481800	-2.32855500	-1.51371700
H	-1.07099300	-3.94863100	-1.53147400
H	-1.75297300	-5.07553800	0.56466000
H	-0.64445000	-4.47939700	2.71663800

H	1.08931200	-2.74252800	2.78774300
H	3.60585000	1.13673100	1.04574200
H	3.46119100	2.94341100	2.71137900
H	1.64187100	2.93495700	4.41187700
H	-0.01013000	1.07536400	4.43269500
H	0.14597800	-0.73776600	2.78695800

TS_{2/3}^{BPh}

Ni	0.11219600	0.00658900	-0.47896800
B	2.10700700	0.00311300	0.19669900
C	3.52916100	-0.12261400	-0.52896600
C	3.75065100	-1.00529900	-1.60051300
C	4.63983800	0.59909300	-0.06059300
C	5.00841000	-1.15837900	-2.18239000
C	5.90727000	0.44763100	-0.62697500
C	6.09654400	-0.43029100	-1.69506000
C	1.73133400	1.41688000	0.83916700
C	0.94603600	1.58535700	1.99523200
C	2.10547900	2.60105600	0.16002000
C	0.57178600	2.85070900	2.46036500
C	1.72573200	3.86150800	0.60384200
C	0.95593700	3.99379500	1.76642400
C	1.61074600	-1.33975700	0.91797000
C	1.07072300	-2.42407700	0.19351000
C	1.76173800	-1.52261200	2.30900400
C	0.67496700	-3.60793100	0.82262900
C	1.38956000	-2.70641100	2.94065100
C	0.82760700	-3.75073000	2.19965300
C	0.66084900	0.69703100	-2.28649300
H	0.02608800	0.12604800	-2.96186800
H	0.31670800	1.72664100	-2.17426700
H	1.66869600	0.73150000	-2.71601700
H	1.42523900	0.09552400	-1.17142000
P	-2.14061000	-0.01696600	-0.36319400
C	-2.77534400	-0.30896800	1.42297600
C	-1.88613200	-1.38377100	2.06784600
C	-2.56422100	0.96181100	2.25748000
C	-4.24500600	-0.72684900	1.55458400
H	-1.95590800	-2.35794100	1.58782100
H	-0.83417700	-1.09001800	2.06049700
H	-2.19178500	-1.50830400	3.11535700
H	-3.27947100	1.75250600	2.02307300
H	-2.70195200	0.70450600	3.31598400

H	-1.55482700	1.35827600	2.14090100
H	-4.49170800	-0.78616100	2.62353300
H	-4.93186200	-0.00940400	1.10030600
H	-4.44491700	-1.71122200	1.12648800
C	-2.83770600	1.66405600	-0.95977800
C	-4.29815600	1.95397100	-0.59135200
C	-1.93901200	2.76726900	-0.37043000
C	-2.71634200	1.76847900	-2.48842500
H	-4.98772600	1.20535000	-0.98816800
H	-4.45613400	2.02743300	0.48602800
H	-4.58019900	2.92357600	-1.02416900
H	-0.87815800	2.57408600	-0.55538500
H	-2.20038200	3.72434400	-0.84146800
H	-2.06085000	2.88837200	0.70527800
H	-2.97244000	2.79521900	-2.78103000
H	-1.70255700	1.57275800	-2.84123500
H	-3.40497900	1.10457300	-3.01512000
C	-2.87838700	-1.40549000	-1.45915200
C	-2.65016100	-2.76562000	-0.78304300
C	-4.36792600	-1.26646400	-1.79574400
C	-2.07407100	-1.47044700	-2.76773700
H	-1.60843800	-2.89014100	-0.47581300
H	-3.29289400	-2.92998800	0.08340900
H	-2.88041300	-3.55445600	-1.51140900
H	-4.57305900	-0.40413400	-2.43402400
H	-4.68641300	-2.15993900	-2.35004900
H	-4.99742600	-1.19017000	-0.90745500
H	-2.49138500	-2.26979500	-3.39470600
H	-2.10682700	-0.54772800	-3.34768400
H	-1.02649800	-1.71294000	-2.56524800
H	5.14175400	-1.84557200	-3.01534700
H	2.91773400	-1.58678900	-1.99280500
H	7.08042400	-0.54694000	-2.14343300
H	6.74730000	1.01756400	-0.23520800
H	4.50984500	1.29065600	0.76934300
H	0.98036600	-2.35167200	-0.88921700
H	0.25771100	-4.42115000	0.23302200
H	0.52558700	-4.67169800	2.69253000
H	1.53673300	-2.81831700	4.01259900
H	2.21246700	-0.73002400	2.90140000
H	2.70151700	2.51711400	-0.74615100
H	2.02880200	4.74677700	0.04874300
H	0.66159000	4.97860900	2.12140900
H	-0.02944700	2.93748900	3.36303600

H	0.62548700	0.71239700	2.55525500
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3^{BPh}

Ni	0.22040400	-0.13187000	-0.56773300
P	2.40830000	0.01103500	-0.30762200
C	2.44470500	1.71573800	0.55051700
C	3.53139400	0.07344000	-1.84904900
C	3.04528100	-1.33284000	0.87592500
C	2.27588000	2.84201200	-0.48115900
H	1.40936600	2.67357800	-1.12829000
H	2.09656800	3.77601600	0.06625800
H	3.15867800	2.99690000	-1.10376600
C	1.17078900	1.76084200	1.41025800
H	0.26129100	1.63166200	0.79906700
H	1.14781600	1.02530700	2.21067600
H	1.07073100	2.75729500	1.86064400
C	3.67142500	2.01143600	1.41659400
H	4.60167800	1.99093600	0.84397900
H	3.56573700	3.01888500	1.84109900
H	3.77052800	1.31743300	2.25370200
C	2.78290200	0.79764400	-2.98068300
H	2.56191700	1.83981500	-2.75456000
H	3.41574700	0.78292000	-3.87763500
H	1.84379000	0.29647000	-3.22128100
C	4.86614700	0.78560600	-1.58598200
H	5.47230300	0.73378700	-2.49996100
H	4.73912700	1.84228100	-1.34511000
H	5.44108900	0.31838900	-0.78351800
C	3.84936400	-1.33599200	-2.37421400
H	2.94973500	-1.91007500	-2.60599600
H	4.41228900	-1.22423400	-3.30967100
H	4.47272800	-1.91723400	-1.69287200
C	4.56291800	-1.36537200	1.08459900
H	4.79313600	-2.13019000	1.83809900
H	5.11131300	-1.63279900	0.17871300
H	4.95314700	-0.41337000	1.45360600
C	2.36082600	-1.16038100	2.23713700
H	2.58326000	-2.04480300	2.84704500
H	2.71645000	-0.28881600	2.79061000
H	1.27481200	-1.10419400	2.13936500
C	2.55293300	-2.68678700	0.33349500
H	2.96822300	-2.94707400	-0.64020100
H	2.85210600	-3.47121300	1.04081700
H	1.46159600	-2.70016600	0.26123400

B	-2.04034600	0.03307500	-0.10837700
C	-3.20352800	-0.78892900	-0.86340800
C	-3.39685900	-0.66668200	-2.24940100
C	-4.11509300	-1.59726400	-0.16537900
C	-4.43934000	-1.31651000	-2.91107300
C	-5.16870000	-2.24734900	-0.81179400
C	-5.33412700	-2.11188200	-2.19136100
C	-1.45542100	-0.75756800	1.18514800
C	-1.31087700	-0.14579200	2.44437500
C	-1.20401000	-2.14714200	1.13580300
C	-0.96892000	-0.86921100	3.58898400
C	-0.85279800	-2.88015600	2.26752200
C	-0.74173800	-2.24317400	3.50621700
C	-2.46392700	1.56608300	0.16477800
C	-1.87554000	2.65285600	-0.49984300
C	-3.48831400	1.86662900	1.08031000
C	-2.26488800	3.97274900	-0.25667700
C	-3.88967700	3.17775700	1.33412400
C	-3.27405100	4.24152800	0.66789800
H	-1.20765600	0.18395000	-1.10353800
C	0.15529900	-1.31644100	-2.04147800
H	-0.73528900	-1.92752200	-1.86739900
H	0.02114000	-0.74938500	-2.96728800
H	1.04232300	-1.94635300	-2.10330100
H	-4.55504300	-1.20399100	-3.98740200
H	-2.71093600	-0.04490100	-2.82435100
H	-1.09336500	2.46107500	-1.23456700
H	-1.78302200	4.78918700	-0.79138300
H	-3.58389300	5.26560400	0.86327500
H	-4.68554300	3.37273500	2.05035900
H	-3.98402100	1.05056100	1.60411800
H	-6.14947100	-2.62102500	-2.70037400
H	-5.85943300	-2.86325400	-0.23892300
H	-3.99604700	-1.72472000	0.90924400
H	-1.32420700	-2.66864600	0.18925700
H	-0.67293700	-3.94993000	2.18604100
H	-0.47629900	-2.81147500	4.39457400
H	-0.88297000	-0.35907900	4.54620600
H	-1.49489500	0.92203200	2.53305000

1^{BCF}

Ni	-0.87551100	-0.28877500	0.28316100
P	-2.24019200	0.22263900	-1.44321100
C	-3.72638200	-0.95273200	-1.17836400

C	-1.53154700	-0.08279600	-3.19265400
C	-2.81760800	2.03345200	-1.32331400
C	-3.32963200	-2.37771300	-1.59622000
H	-2.40849900	-2.70186200	-1.10125100
H	-4.12805600	-3.06011100	-1.27770000
H	-3.21010700	-2.50149900	-2.67334000
C	-3.99373100	-1.04153900	0.33456100
H	-3.12925100	-1.46619700	0.85754700
H	-4.23782600	-0.08750800	0.79933900
H	-4.84063300	-1.71981600	0.50199900
C	-5.02071100	-0.55347400	-1.89456200
H	-4.89319700	-0.44759700	-2.97358900
H	-5.77128900	-1.33699100	-1.72555400
H	-5.43703100	0.37860800	-1.50506500
C	-0.59003900	-1.29652000	-3.11088700
H	-1.06648300	-2.20162400	-2.73587100
H	-0.20889900	-1.51310600	-4.11738900
H	0.27180700	-1.07188500	-2.47545200
C	-2.59318300	-0.30956200	-4.27639000
H	-2.08275800	-0.40614400	-5.24366800
H	-3.17193500	-1.22247500	-4.12738900
H	-3.28918000	0.52914500	-4.35636400
C	-0.65259800	1.09329500	-3.64089900
H	0.10830600	1.34108400	-2.90214200
H	-0.12910000	0.78958600	-4.55669900
H	-1.22479400	1.99060100	-3.88159000
C	-3.62017100	2.54266400	-2.52649800
H	-3.93283600	3.57539900	-2.32341600
H	-3.03732800	2.56014800	-3.44909400
H	-4.52397600	1.95569800	-2.70487700
C	-3.67599000	2.20871000	-0.06314500
H	-3.86608900	3.28057700	0.07476200
H	-4.64817000	1.71694000	-0.13879700
H	-3.16501800	1.85246000	0.83341300
C	-1.56838600	2.91067400	-1.11948200
H	-0.92968900	2.96155800	-2.00034700
H	-1.89639900	3.93356900	-0.89342600
H	-0.96829100	2.55768900	-0.27653900
B	1.25676700	-0.10235400	0.83866700
C	1.74193800	1.37748000	0.59511600
C	2.02614000	1.85847200	-0.68292400
C	1.93414500	2.29216200	1.63342600
C	2.40117500	3.16837300	-0.94271500
C	2.31892700	3.60990700	1.41878000

C	2.54050200	4.05495300	0.11986900
C	0.21118700	-0.44037100	1.92226400
C	0.12481500	-1.68914100	2.60995300
C	-0.91949200	0.45448800	2.08235300
C	-0.94788200	-2.04876600	3.37729100
C	-2.01105700	0.07105100	2.92087300
C	-2.04131600	-1.15921000	3.51369000
C	2.04355700	-1.26593200	0.09717800
C	1.42965600	-2.41817500	-0.39652500
C	3.42122600	-1.19555100	-0.13165300
C	2.09776400	-3.41697800	-1.08808800
C	4.13444900	-2.17737000	-0.80987900
C	3.46679700	-3.29419000	-1.29911800
F	-3.08982500	-1.54027700	4.24664500
F	-0.98830800	-3.21716100	4.02990600
F	1.16367300	-2.53794200	2.55839000
F	-3.02015200	0.93120200	3.11309800
F	-0.77722900	1.81850900	2.00673000
F	1.77904200	1.90994700	2.90924700
F	2.48277800	4.45234700	2.44425300
F	2.90014600	5.31924600	-0.10477000
F	2.63101300	3.58379200	-2.19410100
F	1.93926200	1.03178800	-1.74238400
F	4.13306100	-0.15408200	0.32847500
F	5.45228600	-2.05896500	-0.99574200
F	4.13238200	-4.24130200	-1.95888300
F	1.44282700	-4.48625900	-1.55215900
F	0.10068500	-2.60665900	-0.22352800

2^{BCF}

Ni	0.95544300	0.02722500	0.35282100
B	-1.18554300	0.38012200	0.81973000
C	-2.08526400	-0.84040100	0.37686500
C	-2.41568700	-1.08210300	-0.95566600
C	-2.67951900	-1.69900100	1.30442300
C	-3.24329300	-2.11830500	-1.36381400
C	-3.52528500	-2.73911900	0.93965700
C	-3.80434400	-2.95413300	-0.40509500
C	-0.15625300	0.23510900	1.96073800
C	0.26914900	1.28070200	2.83497100
C	0.63538300	-0.97781800	1.99179300
C	1.36618500	1.17700000	3.64544100
C	1.75162300	-1.08034200	2.87550400
C	2.13167800	-0.01507500	3.64407800

C	-1.57842100	1.81140900	0.25316900
C	-0.64824000	2.82405800	0.00658000
C	-2.89882100	2.14991900	-0.06550300
C	-0.96683600	4.05839400	-0.53811400
C	-3.26599000	3.37802300	-0.60463500
C	-2.29236400	4.33850700	-0.85084100
F	3.20814300	-0.08621300	4.42948200
F	1.73125100	2.16897900	4.46692200
F	-0.46121500	2.40324700	2.91623600
F	2.42281100	-2.23695800	2.94656300
F	0.08347700	-2.19591300	1.69682500
F	-2.47685800	-1.51986600	2.61884100
F	-4.06848800	-3.53796300	1.86448300
F	-4.60231000	-3.95700100	-0.77361300
F	-3.50826900	-2.31715700	-2.66070400
F	-1.93591400	-0.27433200	-1.91966500
F	-3.90105200	1.28780200	0.16757400
F	-4.54498500	3.64439200	-0.88430400
F	-2.62530200	5.51761000	-1.37368300
F	-0.01818700	4.97253800	-0.76621700
F	0.65875200	2.62625400	0.28903000
C	-1.21251200	-5.13335900	-0.37694200
H	-0.38657300	-5.84753400	-0.40534600
H	-1.01887900	-4.38680900	0.39510400
H	-2.14235800	-5.66064500	-0.15366900
H	-1.29679900	-4.63731100	-1.34631500
P	2.28629200	-0.38228400	-1.43048300
C	4.05456800	-0.26296600	-0.70962400
C	4.07993500	0.92776200	0.26700600
C	4.35276600	-1.50471800	0.14227900
C	5.17596700	-0.10527100	-1.74258300
H	3.88483200	1.88946800	-0.20553700
H	3.34839500	0.79417100	1.07328400
H	5.07339900	0.97977100	0.73126700
H	4.49075300	-2.40976800	-0.45191100
H	5.28859900	-1.32810700	0.68759700
H	3.57396400	-1.68993700	0.88516600
H	6.13923300	-0.11168800	-1.21543200
H	5.19313500	-0.92256600	-2.46722100
H	5.11662000	0.83716200	-2.29049800
C	2.01969400	-2.12265800	-2.15832500
C	3.19560400	-2.66937300	-2.97601500
C	1.71089800	-3.07693900	-0.99409800
C	0.76000700	-2.12877900	-3.03597900

H	3.47273300	-2.01761100	-3.80729300
H	4.08467900	-2.84350800	-2.36621800
H	2.90166800	-3.63845100	-3.40027600
H	0.80622000	-2.76780600	-0.46688500
H	1.53421300	-4.07857900	-1.40563200
H	2.51524900	-3.15861500	-0.26413300
H	0.51643500	-3.17222400	-3.27244100
H	-0.09923700	-1.70135800	-2.51441900
H	0.89275700	-1.60601400	-3.98520300
C	2.10648600	0.91483300	-2.82384700
C	2.66389700	2.26866400	-2.35930900
C	2.79108000	0.53548700	-4.14269600
C	0.60780800	1.13901200	-3.08490500
H	2.22546500	2.59177500	-1.41292600
H	3.75122500	2.27520000	-2.26678600
H	2.40060700	3.01963700	-3.11495200
H	2.34014100	-0.34179600	-4.61080000
H	2.67559700	1.37097200	-4.84581800
H	3.86108600	0.35079800	-4.02570700
H	0.50179100	1.95097100	-3.81614600
H	0.10327900	0.26396600	-3.49022600
H	0.07661100	1.43786300	-2.17803000

TS_{2/3}^{BCF}

Ni	0.84308300	0.01564600	-0.70918600
B	-1.16251200	-0.07650400	-0.04237000
C	-2.49612800	-0.63103600	-0.76676300
C	-3.08300400	0.11138800	-1.79456800
C	-3.21441200	-1.76501500	-0.38533300
C	-4.26608700	-0.24267600	-2.43005800
C	-4.40336900	-2.15630800	-0.99277100
C	-4.93223700	-1.39365200	-2.02659400
C	-0.33848600	-1.11975500	0.85712500
C	0.01229200	-0.92768500	2.20395300
C	-0.02199500	-2.39851200	0.35352900
C	0.59070700	-1.91494500	2.99315400
C	0.57331000	-3.39839900	1.10462600
C	0.87654900	-3.15680500	2.44191400
C	-1.48710200	1.37876800	0.58425800
C	-0.95296400	2.59064400	0.16665800
C	-2.45707000	1.47597200	1.58269900
C	-1.32111200	3.81920600	0.70603500
C	-2.85761400	2.67708900	2.15140600

C	-2.27968400	3.86316500	1.70934000
F	1.46273700	-4.09961600	3.17619600
F	0.89970200	-1.67035700	4.27033600
F	-0.23221400	0.23539100	2.82418600
F	0.85436400	-4.58838000	0.56506700
F	-0.35691400	-2.72120400	-0.90648000
F	-2.79654900	-2.53894200	0.63254200
F	-5.04764400	-3.25532200	-0.58373400
F	-6.07027200	-1.75826000	-2.62081300
F	-4.76742100	0.50884000	-3.41718700
F	-2.49202900	1.24836100	-2.21534200
F	-3.04052400	0.35577300	2.04803700
F	-3.78290000	2.70806400	3.11751400
F	-2.64655300	5.03128700	2.24222200
F	-0.76372200	4.95390500	0.26343900
F	-0.03226500	2.62822000	-0.81924100
C	0.25431200	-0.16904800	-2.62622200
H	0.68805300	0.69720400	-3.11715800
H	0.84656400	-1.07354100	-2.77030400
H	-0.73565700	-0.35840800	-3.04990200
H	-0.47029300	0.04245900	-1.44744200
P	3.10125100	0.33365400	-0.74847200
C	3.69876600	0.34993800	1.06500300
C	2.71410400	1.22084600	1.86866600
C	3.57770700	-1.07978900	1.60698400
C	5.12440700	0.84620500	1.32811000
H	2.89035800	2.28820100	1.74072900
H	1.67202900	1.02505400	1.59888200
H	2.82342400	0.99402200	2.93636600
H	4.36548900	-1.73861800	1.23690600
H	3.66020400	-1.05527100	2.70041600
H	2.61249900	-1.52200400	1.35495000
H	5.33521500	0.73893900	2.40070700
H	5.87865800	0.27105200	0.78706800
H	5.25468600	1.90188000	1.08125400
C	3.97306900	-1.09649900	-1.67621900
C	5.46056000	-1.28125200	-1.35196000
C	3.22748500	-2.40360400	-1.35274100
C	3.83468000	-0.89289300	-3.19404100
H	6.04990800	-0.38312800	-1.54646300
H	5.62868900	-1.58453100	-0.31650000
H	5.85898900	-2.08192000	-1.98925400
H	2.16285600	-2.33063000	-1.59073200
H	3.65144800	-3.20968600	-1.96534200

H	3.31885100	-2.70554100	-0.30996000
H	4.19972700	-1.79945900	-3.69329600
H	2.79670200	-0.74828000	-3.50338300
H	4.42854000	-0.05815300	-3.56974700
C	3.63927300	1.98838300	-1.54379100
C	3.29200500	3.15310300	-0.60314200
C	5.13243000	2.07886200	-1.88558500
C	2.81186800	2.23024400	-2.81667700
H	2.25950300	3.10323800	-0.25034300
H	3.96198300	3.21861100	0.25582000
H	3.40085400	4.08833000	-1.16719100
H	5.42313200	1.40219600	-2.69169300
H	5.34686700	3.09940100	-2.22967700
H	5.77520200	1.88213200	-1.02523100
H	3.16991300	3.15332500	-3.29084700
H	2.89176000	1.43205800	-3.55486300
H	1.75761000	2.37518400	-2.57028100

3^{BCF}

Ni	1.14321700	0.12354500	-0.76184700
P	3.31953200	0.29599000	-0.74862100
C	3.34315300	1.85512700	0.34345900
C	4.28414800	0.62305300	-2.35599300
C	4.08360500	-1.17989700	0.17225200
C	3.05363400	3.11191000	-0.49146600
H	2.14857300	3.00496300	-1.09545000
H	2.88368000	3.94380600	0.20347900
H	3.88274800	3.39867300	-1.13989600
C	2.12197900	1.68109900	1.26356000
H	1.18203700	1.55530300	0.68708100
H	2.21297200	0.85904400	1.96898700
H	1.95433900	2.59983700	1.83911500
C	4.60591200	2.08783200	1.17455600
H	5.48946300	2.22924600	0.54711300
H	4.47209400	3.00126200	1.76891300
H	4.80994800	1.27434100	1.87309300
C	3.40460100	1.45748600	-3.30204600
H	3.14374100	2.43538400	-2.90029400
H	3.96284800	1.62236700	-4.23235800
H	2.47947800	0.93559200	-3.55350300
C	5.60414700	1.36353200	-2.09177900
H	6.13226000	1.47650200	-3.04718200
H	5.45333000	2.36598200	-1.68855400
H	6.26423600	0.81736600	-1.41442400

C	4.61995700	-0.67835400	-3.10258600
H	3.73373000	-1.26885400	-3.34434100
H	5.09158400	-0.40059500	-4.05339700
H	5.32951500	-1.31061000	-2.56653800
C	5.61410000	-1.16569100	0.25444600
H	5.93600100	-2.01943900	0.86456700
H	6.09224200	-1.27086800	-0.72140800
H	5.99728900	-0.25904100	0.72986000
C	3.51701200	-1.24009500	1.59619300
H	3.82280100	-2.19183800	2.04725500
H	3.88356800	-0.44260600	2.24505000
H	2.42575500	-1.22017300	1.59097500
C	3.59741100	-2.46205100	-0.52716900
H	3.95411900	-2.56253100	-1.55203100
H	3.96934000	-3.32585700	0.03783300
H	2.50505500	-2.51441600	-0.53987200
B	-1.17783400	-0.00751100	-0.05889500
C	-2.31092600	-0.80660000	-0.90647200
C	-2.61677500	-0.38311400	-2.19999400
C	-3.09208100	-1.86102500	-0.43737500
C	-3.59675200	-0.96609400	-2.99400100
C	-4.08419800	-2.47421300	-1.19638200
C	-4.33757800	-2.02644800	-2.48658900
C	-0.43859900	-0.88578300	1.10005700
C	-0.17373500	-0.41446900	2.39103000
C	-0.10059800	-2.23399600	0.91010300
C	0.35556800	-1.19985000	3.41112000
C	0.42723000	-3.05222800	1.89958400
C	0.65560900	-2.53275300	3.16783900
C	-1.82264000	1.40339000	0.42347700
C	-1.42517000	2.64680300	-0.05625500
C	-2.90054800	1.43214800	1.30647800
C	-2.03151200	3.84308500	0.31615800
C	-3.53888900	2.59862700	1.70531300
C	-3.09805900	3.81939700	1.20430400
F	1.18282700	-3.29532700	4.12719600
F	0.59245500	-0.67451100	4.61898000
F	-0.41848900	0.86599500	2.72535900
F	0.72924800	-4.32947300	1.64009600
F	-0.30776000	-2.82440000	-0.27965600
F	-2.91800100	-2.34954500	0.80438300
F	-4.79834000	-3.48974800	-0.69440800
F	-5.28691900	-2.60381100	-3.22870800
F	-3.83704500	-0.51575200	-4.23251900

F	-1.95237900	0.65960900	-2.73884700
F	-3.35567700	0.27933800	1.83046600
F	-4.56409700	2.56456300	2.56529500
F	-3.69530300	4.95603400	1.57402400
F	-1.59719800	5.01213700	-0.17448200
F	-0.39549000	2.75583900	-0.92549100
H	-0.41390100	0.36161800	-0.99830300
C	0.97581900	-0.85555300	-2.36422700
H	0.20550900	-1.60162100	-2.15848400
H	0.61797600	-0.14141300	-3.11182400
H	1.88833700	-1.34317300	-2.70071500

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Ni	-1.43614600	0.38981500	0.73720400
P	-0.99455900	2.58326200	0.39789200
C	-2.55158900	3.47174000	1.05983900
C	-0.72139900	3.07762100	-1.42449100
C	0.52038400	3.11910600	1.41454700
C	-3.70254100	3.33851900	0.05097600
H	-3.88607200	2.29604600	-0.22300000
H	-4.61659900	3.71649700	0.52689000
H	-3.54966700	3.91919900	-0.86014300
C	-3.01867400	2.70963100	2.31363300
H	-3.27662200	1.67278000	2.06575900
H	-2.28482000	2.69244100	3.11874800
H	-3.92691000	3.18964700	2.70118000
C	-2.36065100	4.95334600	1.40121600
H	-2.01533700	5.53808000	0.54574900
H	-3.32658700	5.36888300	1.71781300
H	-1.65970600	5.10541100	2.22484700
C	-1.65644600	2.21773400	-2.29133900
H	-2.71233500	2.32519300	-2.04596800
H	-1.52648500	2.51188400	-3.34102500
H	-1.38655900	1.16065700	-2.21253000
C	-0.95126500	4.56439600	-1.72144000
H	-0.69705700	4.74916200	-2.77352400
H	-1.98945400	4.87262200	-1.58274100
H	-0.31641000	5.21286800	-1.11326300
C	0.70214800	2.71605100	-1.86858800
H	0.95206900	1.67913300	-1.64306000
H	0.75550900	2.83200800	-2.95808400
H	1.46768300	3.36644600	-1.44531700
C	1.05620700	4.52057400	1.10213700
H	1.89838800	4.72688200	1.77598200

H	1.43623200	4.60597300	0.08285700
H	0.30904900	5.30187700	1.26048600
C	0.19851900	3.03644300	2.91216900
H	1.13244400	3.18749000	3.46838600
H	-0.50409200	3.80235900	3.24691500
H	-0.18791500	2.05384900	3.19141700
C	1.61737100	2.07717500	1.15587400
H	1.99223200	2.09142600	0.13701400
H	2.46883600	2.28478700	1.81626000
H	1.25725800	1.06788200	1.36952100
B	-1.04249800	-1.62203300	-0.13430400
C	0.49344900	-1.95646200	-0.28325000
C	1.26893600	-1.43890200	-1.31994400
C	1.11023500	-2.94609400	0.48643900
C	2.56255800	-1.85850700	-1.59112500
C	2.39445300	-3.41205800	0.23322100
C	3.12644600	-2.86282000	-0.81280000
C	-1.72177800	-1.48437100	1.24189800
C	-3.08307300	-1.80618700	1.53182500
C	-1.01187200	-0.74333100	2.26498500
C	-3.70186800	-1.45033000	2.69787100
C	-1.66523900	-0.42430600	3.49472200
C	-2.98293900	-0.73019100	3.68410000
C	-1.92203000	-1.74670500	-1.45502500
C	-3.03033000	-0.93954600	-1.71745700
C	-1.63145400	-2.67410700	-2.46207100
C	-3.77973400	-0.99815400	-2.88192000
C	-2.36041200	-2.77605800	-3.64203400
C	-3.43865200	-1.92668100	-3.85903500
F	-3.61480000	-0.37621200	4.80559300
F	-4.97309600	-1.78576500	2.95240000
F	-3.78306900	-2.54327900	0.65526200
F	-0.97250600	0.18885000	4.46419600
F	0.34806700	-0.85830200	2.40382900
F	0.43816000	-3.54685600	1.48163100
F	2.91987500	-4.39939900	0.96409700
F	4.35294500	-3.30791100	-1.08448300
F	3.25393600	-1.34285400	-2.61437200
F	0.74191600	-0.51877800	-2.15077500
F	-0.62430400	-3.54991600	-2.31626400
F	-2.03677600	-3.68505500	-4.56645600
F	-4.14282200	-2.00540700	-4.98740700
F	-4.81667100	-0.17569400	-3.07245700
F	-3.42623000	-0.01872300	-0.80914600

C	4.42899000	1.17283700	-0.46166100
C	4.53664600	0.26164800	0.33743900
C	4.25615500	2.27926100	-1.34180600
C	4.06830800	2.08580200	-2.72159100
C	4.23966900	3.58838900	-0.82507900
C	3.86684200	3.17847000	-3.56014600
H	4.07109600	1.07660600	-3.12004700
C	4.03566500	4.67465500	-1.67064500
H	4.38037500	3.73765800	0.24124600
C	3.84744800	4.47405900	-3.03997500
H	3.71799900	3.01679900	-4.62456400
H	4.02177800	5.68070100	-1.25930200
H	3.68543600	5.32362700	-3.69809500
C	4.63286000	-0.78800000	1.29595500
C	5.72362100	-1.67466400	1.28892900
C	3.62542200	-0.94694100	2.26444900
C	5.80168700	-2.69357600	2.23404000
H	6.49759900	-1.55951200	0.53600600
C	3.70972100	-1.96983000	3.20288200
H	2.77858400	-0.27158200	2.26511100
C	4.79810500	-2.84424400	3.19269300
H	6.64615300	-3.37739800	2.21728300
H	2.91767000	-2.08910600	3.93722500
H	4.85817600	-3.64750400	3.92204200

3

Ni	-0.67112500	0.93024800	0.56793000
P	-0.11692800	2.80783900	-0.56278100
C	0.20051800	4.07194700	0.83785800
C	-1.46481700	3.51564200	-1.71898000
C	1.47640300	2.55070400	-1.56866400
C	-1.14088000	4.53261500	1.43025900
H	-1.76479700	3.68346800	1.72769700
H	-0.92986400	5.11470100	2.33665800
H	-1.71821500	5.17367700	0.76258000
C	0.91021900	3.33167500	1.98521400
H	0.26699300	2.54485400	2.39607400
H	1.86029000	2.88199900	1.70107400
H	1.10743100	4.04616900	2.79534700
C	1.03003600	5.29848100	0.44369800
H	0.59319500	5.85675600	-0.38663400
H	1.08489300	5.97655300	1.30584000
H	2.05588500	5.03350700	0.17734900
C	-2.83268800	3.20562600	-1.08854800

H	-2.95854100	3.60751400	-0.08379600
H	-3.61843900	3.63799000	-1.72175900
H	-2.99868100	2.12496600	-1.05092500
C	-1.33951300	5.01892100	-1.99650700
H	-2.11671200	5.30225300	-2.71859500
H	-1.48896700	5.63387600	-1.10764200
H	-0.37374700	5.28006600	-2.43614900
C	-1.45887100	2.78840200	-3.07100500
H	-1.50485700	1.70631500	-2.95398700
H	-2.35785700	3.09609700	-3.62092600
H	-0.59949100	3.04438700	-3.69278100
C	1.85494600	3.70727900	-2.50134600
H	2.80805100	3.45940500	-2.98664400
H	1.12295200	3.87200500	-3.29404500
H	1.99605200	4.64839400	-1.96524600
C	2.65003800	2.30345200	-0.61378900
H	3.52268700	2.02386000	-1.21369700
H	2.93127900	3.18769800	-0.03921900
H	2.45615000	1.47784500	0.07327100
C	1.31541000	1.25596300	-2.38499500
H	0.58529900	1.33803600	-3.18964000
H	2.28393400	1.01672700	-2.84100600
H	1.03421000	0.41556900	-1.74533100
B	-1.70127700	-0.99902400	0.21479900
C	-1.14430100	-1.73076800	-1.06564600
C	-1.47549200	-1.32747300	-2.35717800
C	-0.34574600	-2.87366200	-0.97865700
C	-1.01395700	-1.96452600	-3.49986600
C	0.11960900	-3.55402000	-2.09672600
C	-0.20781700	-3.08946200	-3.36570200
C	-0.82870700	-0.81772200	1.47292800
C	-1.31573900	-0.79882300	2.81383200
C	0.54772700	-0.40640500	1.28005700
C	-0.55033600	-0.41701400	3.87953800
C	1.33025200	-0.02183400	2.41245400
C	0.78426200	0.00377400	3.66391100
C	-3.26175800	-0.70520000	0.27094500
C	-3.81113600	0.41569100	0.89676500
C	-4.19892400	-1.55448300	-0.32678500
C	-5.16620900	0.70799200	0.91661300
C	-5.56713300	-1.30722900	-0.32302100
C	-6.05554400	-0.16339600	0.29742900
F	1.50326800	0.41612100	4.71215600
F	-1.01975700	-0.44294600	5.13403700

F	-2.56159900	-1.23432600	3.06376900
F	2.60508400	0.34637800	2.24015300
F	1.30259500	-0.90326600	0.25006600
F	-0.03514200	-3.38812100	0.21791000
F	0.87227000	-4.65283800	-1.97189700
F	0.24383200	-3.72359300	-4.44896900
F	-1.34005900	-1.51686500	-4.71876400
F	-2.29830900	-0.27656900	-2.53616600
F	-3.80455900	-2.69023400	-0.92479700
F	-6.41611800	-2.15820700	-0.90679200
F	-7.36300500	0.09353200	0.30424800
F	-5.62125200	1.81210700	1.51804000
F	-3.00709100	1.30664600	1.52207600
C	4.94165500	-0.86050400	0.30284200
C	4.38152500	-1.84992900	0.73640200
C	5.51832500	0.34299700	-0.18285800
C	5.86834100	0.48035800	-1.53875500
C	5.70032300	1.43708200	0.68439200
C	6.37125700	1.68782500	-2.01466400
H	5.73069200	-0.36238500	-2.20855900
C	6.20628500	2.63907300	0.20048900
H	5.42583200	1.33350600	1.72983800
C	6.53879500	2.77200400	-1.14977600
H	6.63213600	1.78397600	-3.06549800
H	6.33628200	3.47868200	0.87858000
H	6.92896000	3.71418900	-1.52555500
C	3.66836900	-2.96059800	1.26180300
C	3.39544400	-4.08545800	0.46318100
C	3.19844900	-2.93106300	2.58882900
C	2.66631900	-5.15072500	0.98129900
H	3.74995900	-4.10739700	-0.56268200
C	2.46490500	-3.99839900	3.09606100
H	3.41704100	-2.06699300	3.20853200
C	2.19660400	-5.11110900	2.29531900
H	2.45209000	-6.01000800	0.35199000
H	2.10138100	-3.96217700	4.11985300
H	1.61959300	-5.94191500	2.69270100
C	3.08946400	-1.94312200	-2.96786200
H	3.09647100	-1.63960000	-1.91973300
H	3.99689100	-1.58567900	-3.45958700
H	2.21872400	-1.51395700	-3.46683300
H	3.04973500	-3.03220300	-3.03559400

TS_{3/4}

Ni	1.19764800	0.11060100	-0.19149200
B	-0.44735000	-1.09477300	0.38131400
C	-2.03994400	-0.89084500	0.19231600
C	-2.71967600	0.02787200	0.99698400
C	-2.86534800	-1.69136800	-0.59733000
C	-4.10071000	0.16212400	1.02382900
C	-4.25306700	-1.59922400	-0.59180700
C	-4.87823200	-0.66837900	0.22660200
C	0.34677600	-1.88311000	-0.76477500
C	1.20644400	-2.97380500	-0.55004700
C	0.14474600	-1.56763900	-2.12489400
C	1.78435000	-3.70950000	-1.57901200
C	0.71382700	-2.26935300	-3.17384100
C	1.53747100	-3.35831200	-2.89875000
C	-0.18268600	-1.52134300	1.91920400
C	0.45193400	-0.75094900	2.88486500
C	-0.71069900	-2.72722400	2.38137300
C	0.58203600	-1.14087100	4.21419200
C	-0.60571500	-3.15943100	3.69619000
C	0.05094600	-2.35643900	4.62359000
F	2.10942700	-4.03348300	-3.89388900
F	2.59224300	-4.73953000	-1.30753400
F	1.48836200	-3.39921300	0.69036600
F	0.48395200	-1.91477900	-4.44250200
F	-0.68630700	-0.56754800	-2.46039100
F	-2.34642900	-2.64687300	-1.39143000
F	-4.99142800	-2.41421200	-1.35474200
F	-6.20950900	-0.58784800	0.26541500
F	-4.68745500	1.06560000	1.81785600
F	-2.02296200	0.82393500	1.83401900
F	-1.34844700	-3.54210800	1.52020400
F	-1.12073100	-4.33373300	4.07988200
F	0.16631000	-2.75035600	5.89472900
F	1.20922900	-0.35355700	5.09860400
F	0.97757500	0.44955300	2.56593400
C	-0.01765200	1.69745900	-0.33907400
H	0.44733100	2.44735400	0.29141000
H	0.20839500	1.83578000	-1.39664000
H	-1.09970100	1.77850700	-0.23158200
H	-0.22835600	0.43637600	0.18675300
P	3.28162700	0.94508000	-0.56861000
C	4.49322100	-0.52878900	-0.66824700
C	4.16251900	-1.48557800	0.49333800

C	4.19079700	-1.28318600	-1.96917500
C	5.99178200	-0.21167200	-0.62628800
H	4.58167100	-1.15756100	1.44389700
H	3.08554700	-1.61051400	0.63469900
H	4.58175500	-2.47514400	0.27296100
H	4.56933500	-0.76641600	-2.85315100
H	4.67575300	-2.26638500	-1.93382200
H	3.11838200	-1.44355000	-2.09667000
H	6.54750400	-1.15031400	-0.75557100
H	6.30474100	0.46671800	-1.42254600
H	6.30249400	0.21395300	0.33040100
C	3.33319400	1.90290600	-2.22756100
C	4.72813400	2.08162900	-2.83987100
C	2.44167300	1.16150500	-3.24031800
C	2.71244600	3.29889600	-2.04695900
H	5.42317500	2.58619000	-2.16583300
H	5.17519800	1.13426200	-3.14870000
H	4.63514400	2.70091200	-3.74209100
H	1.42650700	1.01903900	-2.86119300
H	2.37472400	1.76420700	-4.15534900
H	2.83261700	0.18435700	-3.52244500
H	2.60980700	3.75488200	-3.04006600
H	1.71633500	3.26489900	-1.60118600
H	3.33508600	3.96688700	-1.44954300
C	3.90387600	2.10725200	0.81775900
C	4.23788000	1.27864600	2.06806400
C	5.13906100	2.93970700	0.44916600
C	2.76947000	3.05356700	1.23987100
H	3.43267300	0.58842700	2.33125600
H	5.17078200	0.72054500	1.96880700
H	4.36483300	1.97083100	2.91037200
H	4.92579800	3.69527000	-0.30989500
H	5.47639600	3.47355000	1.34771600
H	5.97332100	2.32889100	0.09883700
H	3.16016900	3.74484700	1.99775100
H	2.36994100	3.65975200	0.42820100
H	1.94610400	2.50132400	1.69655600
C	-2.54924700	3.80153100	-0.20647500
C	-3.32122900	3.11213900	-0.84650100
C	-1.55647300	4.51127500	0.52710800
C	-1.48031900	4.39099800	1.92562500
C	-0.58607000	5.27093800	-0.15179800
C	-0.45079100	5.01428400	2.62537800
H	-2.22016300	3.79138400	2.44698900

C	0.43749300	5.89283400	0.55648600
H	-0.64051600	5.35525300	-1.23336700
C	0.51005600	5.76504300	1.94533700
H	-0.39432600	4.90715200	3.70541500
H	1.18547200	6.47338400	0.02258600
H	1.31545500	6.24487800	2.49495800
C	-4.11717500	2.22393100	-1.62422300
C	-5.51927500	2.21776400	-1.53306000
C	-3.47807300	1.31463700	-2.48709600
C	-6.26226400	1.31882800	-2.29301400
H	-6.01254800	2.91189200	-0.85911700
C	-4.22876500	0.41611700	-3.23724900
H	-2.39515400	1.31407500	-2.54809800
C	-5.62206600	0.41600300	-3.14409500
H	-7.34556300	1.31361300	-2.21028800
H	-3.72416800	-0.29332100	-3.88767200
H	-6.20616200	-0.29318800	-3.72395300

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Ni	1.33948800	0.20555100	-0.25736200
B	-0.71405700	-1.03059300	0.39661500
C	-2.27059700	-0.69291700	0.05432200
C	-2.84804700	0.42909400	0.64906800
C	-3.15709900	-1.47818700	-0.67923000
C	-4.18813100	0.77258000	0.53228600
C	-4.50426200	-1.16658100	-0.83460600
C	-5.02732000	-0.03550300	-0.22298800
C	-0.00577900	-2.13814500	-0.56718400
C	0.68582600	-3.27031600	-0.12639700
C	-0.10113000	-2.04085800	-1.96129400
C	1.22836100	-4.22747000	-0.97942600
C	0.44333000	-2.95790000	-2.84837400
C	1.11576400	-4.06929000	-2.35281200
C	-0.65240500	-1.33859500	1.99129000
C	-0.02980200	-0.52488300	2.92966500
C	-1.35141400	-2.41976600	2.52556300
C	-0.06376200	-0.76399000	4.30003100
C	-1.41629000	-2.70000400	3.88350200
C	-0.76160300	-1.86277800	4.78194000
F	1.65592500	-4.96127900	-3.18591700
F	1.89346000	-5.27811400	-0.48365300
F	0.90020000	-3.49230900	1.18413600
F	0.31788200	-2.78962100	-4.17010300
F	-0.78478600	-1.02495600	-2.51733100

F	-2.74962000	-2.61861100	-1.27018900
F	-5.30528400	-1.95399000	-1.56555100
F	-6.32314200	0.26235500	-0.34884200
F	-4.67584000	1.85815700	1.14464400
F	-2.09035600	1.23192800	1.42286100
F	-1.99576000	-3.26284500	1.69756000
F	-2.09219900	-3.76241700	4.33768100
F	-0.80722400	-2.11273300	6.09384900
F	0.56614900	0.05619300	5.15342900
F	0.65725900	0.57448400	2.54298700
C	0.64848300	1.50710100	-1.42251500
H	1.34867500	2.25135200	-1.79080100
H	0.23743500	0.93050200	-2.25386300
H	-0.14988100	2.00180100	-0.86713700
H	-0.19829800	0.11554500	0.26406500
P	3.42200100	0.63430700	-0.69052900
C	4.08590900	-0.90108200	0.21652900
C	3.09447600	-1.09256700	1.37964200
C	3.93850800	-2.14645900	-0.66729400
C	5.51999000	-0.83814700	0.74285100
H	3.11075500	-0.29458000	2.11779400
H	2.05153200	-1.21097500	1.02143800
H	3.30296600	-2.03904100	1.89335100
H	4.66921100	-2.19250600	-1.47580400
H	4.09063000	-3.03274900	-0.03932000
H	2.93805300	-2.21988800	-1.09732500
H	5.75343300	-1.79105900	1.23596200
H	6.24523600	-0.69806100	-0.06323000
H	5.66812400	-0.04695500	1.47994400
C	4.00391200	0.62462400	-2.50282100
C	5.48143000	0.22855900	-2.64047100
C	3.11904600	-0.35945600	-3.28639900
C	3.82815200	1.99805600	-3.17021800
H	6.14704700	0.91449900	-2.11176400
H	5.68723700	-0.78365300	-2.29051500
H	5.74962000	0.26262300	-3.70415700
H	2.06192300	-0.09409900	-3.20611000
H	3.39971700	-0.31106100	-4.34598500
H	3.23659100	-1.39385900	-2.96625100
H	4.10873600	1.89048700	-4.22543200
H	2.79426800	2.34876200	-3.14620200
H	4.47499100	2.76649900	-2.74347100
C	4.01775900	2.21275300	0.18563700
C	3.77599000	2.08288400	1.69720400

C	5.49855800	2.52751300	-0.06214400
C	3.15809700	3.40627000	-0.26319000
H	2.73413800	1.83839400	1.92050000
H	4.42935800	1.35446900	2.18143900
H	3.98267100	3.05818400	2.15410300
H	5.69672500	2.80611800	-1.09967600
H	5.77654700	3.38761000	0.56047300
H	6.16034600	1.70046000	0.20461200
H	3.52650000	4.29952300	0.25465100
H	3.20423900	3.60724800	-1.33296200
H	2.11348800	3.27468900	0.02421800
C	-1.50222700	4.03573000	-0.32556000
C	-2.35232600	3.52310700	-1.02952600
C	-0.48189300	4.55501600	0.52356500
C	-0.06574800	3.81786400	1.64809000
C	0.13289700	5.78961600	0.24886300
C	0.92979100	4.31555200	2.48307300
H	-0.52939700	2.86115200	1.85492800
C	1.13228900	6.27651200	1.08744500
H	-0.18196900	6.35783700	-0.62172300
C	1.53110700	5.54478900	2.20813700
H	1.23776200	3.73708500	3.34992800
H	1.59996400	7.23253200	0.86628800
H	2.30868700	5.93057900	2.86242600
C	-3.31086300	2.84960100	-1.84146000
C	-4.63735800	3.30590000	-1.92734000
C	-2.93888600	1.68527200	-2.53743000
C	-5.56832500	2.60590000	-2.69001800
H	-4.92985600	4.19715500	-1.38014700
C	-3.87548800	0.99214800	-3.29624000
H	-1.92067300	1.32422900	-2.45869800
C	-5.19268500	1.44890000	-3.37525700
H	-6.59492000	2.95861300	-2.74017800
H	-3.57820400	0.08574100	-3.81690200
H	-5.92616900	0.89887500	-3.95855500

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Ni	2.59295300	-0.06835300	1.05374700
B	-1.99969000	0.08781400	-0.45232300
C	-2.78306400	1.07380600	0.58437200
C	-2.65344100	0.88479800	1.96118800
C	-3.46126200	2.24335000	0.24457900
C	-3.11566900	1.76555700	2.92779800
C	-3.92976900	3.16868100	1.17590300

C	-3.75101400	2.93464200	2.53063400
C	-2.19976300	0.45467000	-2.02951900
C	-2.99805000	-0.25545500	-2.92308600
C	-1.49198900	1.50507400	-2.60974100
C	-3.06374700	0.01698700	-4.28794900
C	-1.52097400	1.81686700	-3.96192100
C	-2.31224400	1.05767300	-4.81585000
C	-2.19535500	-1.51014000	-0.21263500
C	-1.24931500	-2.38990400	-0.73441700
C	-3.25059200	-2.13137000	0.44826500
C	-1.32695700	-3.77258000	-0.63281500
C	-3.35660400	-3.50979500	0.60647600
C	-2.38860100	-4.34014300	0.05775900
F	-2.35629400	1.33454100	-6.12556700
F	-3.84556000	-0.71324700	-5.09737000
F	-3.78394400	-1.26382400	-2.49246800
F	-0.80053100	2.84018800	-4.45179700
F	-0.73726100	2.32012800	-1.83574000
F	-3.70472300	2.56175600	-1.04497900
F	-4.55113800	4.28876500	0.77284100
F	-4.18960300	3.81484000	3.44076100
F	-2.94989000	1.50593400	4.23483300
F	-2.03047000	-0.21836400	2.42974100
F	-4.26542900	-1.40051000	0.95452300
F	-4.38782500	-4.04939900	1.27687200
F	-2.47798400	-5.67056300	0.19350900
F	-0.39425800	-4.56100800	-1.19247600
F	-0.18456400	-1.90951900	-1.41750400
C	0.99107100	-0.99485700	1.86140200
C	0.79499400	0.22895900	1.98415600
C	0.78957000	-2.41193400	1.94951700
C	1.67333100	-3.31793900	1.34564500
C	-0.31829500	-2.89341900	2.66889700
C	1.45101800	-4.68661300	1.45382200
H	2.52876700	-2.94315700	0.79276200
C	-0.53321900	-4.26318700	2.76933500
H	-1.00476200	-2.19026300	3.12529200
C	0.34800700	-5.16212200	2.16431300
H	2.13205800	-5.38289900	0.97282000
H	-1.39875400	-4.63076500	3.31344300
H	0.16737500	-6.23084400	2.23648600
C	0.45002800	1.57826000	2.29652400
C	0.10977700	2.48558300	1.27984800
C	0.39877600	1.98082300	3.64290400

C	-0.29218800	3.77473900	1.60923500
H	0.10947900	2.15400300	0.24958900
C	-0.00500800	3.27278100	3.96067200
H	0.64763900	1.26842900	4.42382600
C	-0.35422700	4.16908200	2.94700500
H	-0.57985700	4.46363200	0.82024600
H	-0.06606100	3.57652000	5.00180200
H	-0.68739400	5.17126400	3.20247400
P	4.19721700	0.39740500	-0.41096900
C	3.19341600	0.06138800	-1.99499100
C	5.76134300	-0.68873500	-0.39292600
C	4.66692400	2.23587500	-0.29681300
C	3.06220200	-1.45053600	-2.23493000
H	2.65910700	-1.97079700	-1.36107900
H	2.34178900	-1.59822000	-3.04796900
H	3.99536100	-1.92860600	-2.53650200
C	1.76864300	0.55940200	-1.70366200
H	1.31097500	0.06412800	-0.83237900
H	1.69815100	1.63411800	-1.56366700
H	1.11888300	0.29154500	-2.54431400
C	3.71750800	0.73565300	-3.26546700
H	4.73490600	0.42898700	-3.51892900
H	3.06640000	0.44958900	-4.10150500
H	3.69182100	1.82544600	-3.19862500
C	5.34845300	-2.10103000	0.05588200
H	4.63554900	-2.57505000	-0.61844700
H	6.24460400	-2.73370900	0.08391300
H	4.91634100	-2.08859000	1.06020300
C	6.44295400	-0.75549300	-1.76756400
H	7.34831700	-1.36864400	-1.67442100
H	5.81707000	-1.22065900	-2.52995600
H	6.74877900	0.22951500	-2.12838900
C	6.81053900	-0.19739600	0.61764600
H	6.43144400	-0.15823100	1.64087000
H	7.63680100	-0.91912400	0.61093200
H	7.23321000	0.77528100	0.36148400
C	5.81270800	2.63964600	-1.23307200
H	5.96717900	3.72257400	-1.14421900
H	6.75818800	2.15791400	-0.97619000
H	5.59173700	2.42412500	-2.28084800
C	3.44419800	3.11203800	-0.60641800
H	3.70828700	4.15123000	-0.37431000
H	3.14747800	3.08263500	-1.65635900
H	2.58367500	2.85005700	0.01697800

C	5.04245400	2.54509900	1.16274900
H	5.89520800	1.97367100	1.52902300
H	5.30611500	3.60799700	1.23005300
H	4.19477000	2.36815700	1.83113700
C	3.65988100	-0.23637400	2.59966700
H	3.53455900	-1.27447700	2.92414500
H	3.20595600	0.44641300	3.32413000
H	4.70886700	0.00424700	2.45570800
H	-0.82592800	0.29435700	-0.21909600

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Ni	-2.46601000	1.03550700	0.59548100
B	1.82908900	-0.52565000	-0.46766800
C	2.81316000	-0.61940000	0.83001000
C	2.83155400	0.43228100	1.74654300
C	3.57675600	-1.71636400	1.22478900
C	3.51287500	0.41930600	2.95402900
C	4.25718400	-1.79064500	2.43937700
C	4.22246500	-0.71754700	3.31734100
C	1.82676400	-1.84804600	-1.41835800
C	2.30533300	-1.91620000	-2.72412800
C	1.24487300	-3.02956500	-0.96196200
C	2.19161500	-3.04702800	-3.53132600
C	1.11100000	-4.18169700	-1.72279300
C	1.58404600	-4.18928000	-3.03000400
C	1.95638800	0.84942600	-1.32540900
C	0.85905000	1.30207100	-2.05280100
C	3.07571100	1.67214100	-1.40407100
C	0.85105200	2.46786000	-2.80718200
C	3.10774500	2.86460000	-2.11936700
C	1.98557800	3.26673700	-2.83163800
F	1.46084900	-5.28575200	-3.78981300
F	2.66582500	-3.04448500	-4.78669300
F	2.93514100	-0.86368200	-3.28657800
F	0.52899600	-5.28238100	-1.21705900
F	0.78645100	-3.10314000	0.30822600
F	3.71295400	-2.79792000	0.42879900
F	4.95363100	-2.89107800	2.76586600
F	4.87238500	-0.77003100	4.48850400
F	3.49269500	1.48487900	3.77236200
F	2.16016100	1.56860900	1.46419600
F	4.22105900	1.32664700	-0.77862700
F	4.21073300	3.63066000	-2.13591400
F	2.00269000	4.40309100	-3.54238100

F	-0.23663500	2.82659200	-3.51173300
F	-0.28606800	0.57963800	-2.07541100
C	-1.18958700	2.31680400	1.01701800
C	-0.92314300	1.18076800	1.61731000
C	-0.57158500	3.48016300	0.39652600
C	-1.16753800	4.08781000	-0.71798100
C	0.62315900	4.00291200	0.91116800
C	-0.57135100	5.19296300	-1.31616300
H	-2.08190100	3.67343000	-1.13293300
C	1.22035400	5.10308900	0.30289300
H	1.08249800	3.53911900	1.77584300
C	0.62576700	5.70109100	-0.80939500
H	-1.02850400	5.64371400	-2.19222200
H	2.15540200	5.49136000	0.69711300
H	1.09949300	6.55391500	-1.28707400
C	-0.33771800	0.40831500	2.65638900
C	-0.11650100	-0.97183300	2.49355500
C	0.06747500	1.04282700	3.85044400
C	0.50973800	-1.70030000	3.49550700
H	-0.38451500	-1.44046600	1.55622600
C	0.68617800	0.30534200	4.84978000
H	-0.09608300	2.11021200	3.96701900
C	0.91362500	-1.06397800	4.67135300
H	0.70637100	-2.75804400	3.34868900
H	1.01385500	0.79717400	5.76085900
H	1.42031200	-1.63129900	5.44731600
P	-4.02534700	-0.58073300	0.14755200
C	-4.53256300	-1.49906300	1.74075800
C	-3.37345500	-1.82270000	-1.13584700
C	-5.55007500	0.32366900	-0.57257000
C	-3.45910700	-2.52656600	2.12724700
H	-2.46702400	-2.07452200	2.19548100
H	-3.70785300	-2.91517300	3.12298300
H	-3.41583900	-3.38046600	1.44934700
C	-4.55198100	-0.47478700	2.88893100
H	-3.55324400	-0.05368900	3.04760200
H	-5.25445000	0.34511700	2.73622700
H	-4.84390300	-0.99031500	3.81285600
C	-5.88148400	-2.22285900	1.65539200
H	-5.90907100	-2.95237100	0.84245100
H	-6.04466800	-2.76880500	2.59369200
H	-6.72388300	-1.53957600	1.53102100
C	-1.93706800	-2.19198600	-0.73857400
H	-1.87318700	-2.74579800	0.19588700

H	-1.51942900	-2.83305300	-1.52379700
H	-1.29413200	-1.30933100	-0.66630100
C	-4.20663300	-3.10047100	-1.28718100
H	-3.76434400	-3.71003000	-2.08563700
H	-4.20424100	-3.71062000	-0.38125500
H	-5.24443600	-2.89985200	-1.56249000
C	-3.26208900	-1.13319800	-2.50410000
H	-2.70787000	-0.19165200	-2.44413000
H	-2.69790400	-1.79654000	-3.17112700
H	-4.23136400	-0.95361200	-2.97384600
C	-6.55341000	-0.57847800	-1.30043500
H	-7.40957500	0.03250400	-1.61563600
H	-6.13094200	-1.02784400	-2.20153100
H	-6.93693000	-1.37945800	-0.66500400
C	-6.28756900	1.07752800	0.54427100
H	-7.06525100	1.69809400	0.08152600
H	-6.78447800	0.41508900	1.25455600
H	-5.62441700	1.74845100	1.09751300
C	-5.04832300	1.40202900	-1.55125300
H	-4.56059100	0.99574100	-2.43548700
H	-5.90731800	1.99570900	-1.88931700
H	-4.34678800	2.09297700	-1.07051800
C	-3.03856500	2.74918500	1.51819100
H	-3.58177800	2.17446400	2.27184100
H	-3.67001200	3.09738000	0.69717100
H	-2.56873500	3.60252600	2.00396400
H	0.71375200	-0.47579700	0.01131700

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Ni	1.70128100	-0.66696800	-0.12317000
B	-1.52012800	0.61939500	-0.17091300
C	-2.96882200	0.66877800	0.56499600
C	-3.22871800	0.14203000	1.82396500
C	-4.04728900	1.32596200	-0.02472200
C	-4.46447500	0.23698900	2.45868100
C	-5.29728900	1.44943500	0.56676100
C	-5.50880600	0.89598700	1.82506500
C	-1.06388500	2.16751700	-0.42498300
C	-0.90299100	2.82065100	-1.64439500
C	-0.83966200	2.97279300	0.69239000
C	-0.51444100	4.15313600	-1.76015600
C	-0.45918000	4.30695300	0.62758000
C	-0.28789500	4.90423300	-0.61505800
C	-1.47647700	-0.34061600	-1.48581400

C	-0.28886400	-0.46880400	-2.19018800
C	-2.49107800	-1.17384600	-1.95763300
C	-0.07121500	-1.30745800	-3.27003700
C	-2.32907400	-2.05451100	-3.02494900
C	-1.11190800	-2.12670500	-3.68783000
F	0.09599400	6.18356600	-0.70560800
F	-0.35846300	4.71925500	-2.96591900
F	-1.13064700	2.17917500	-2.80858600
F	-0.23910200	5.01779200	1.74476500
F	-0.99460600	2.45780500	1.93060100
F	-3.90564000	1.86409900	-1.25327200
F	-6.29994400	2.08495600	-0.05707100
F	-6.70418300	1.00007000	2.41817700
F	-4.65384700	-0.29568700	3.67637100
F	-2.26484800	-0.50217400	2.51490000
F	-3.71073000	-1.17711900	-1.39330300
F	-3.34267900	-2.82877900	-3.42808800
F	-0.94062100	-2.96890800	-4.71246400
F	1.11079000	-1.34289400	-3.90649800
F	0.79474200	0.30143400	-1.80498700
C	0.99582900	-2.82216300	-0.11516400
C	1.32974700	-2.01629600	0.95206100
C	-0.34189700	-3.45088300	-0.20496200
C	-0.58020700	-4.51723600	-1.08772200
C	-1.42079000	-2.95832500	0.54906600
C	-1.85017400	-5.08149500	-1.19715000
H	0.22403200	-4.91601000	-1.69775700
C	-2.68328000	-3.52752400	0.44652600
H	-1.27748300	-2.10037900	1.19315200
C	-2.90611500	-4.59234500	-0.42918600
H	-2.01402500	-5.90075800	-1.89225100
H	-3.50319200	-3.11549700	1.02804700
H	-3.89875600	-5.02354700	-0.52609800
C	1.00027300	-2.11667600	2.35301900
C	0.61979900	-1.00099000	3.11914800
C	1.09381800	-3.37626000	2.97834900
C	0.33582300	-1.14105500	4.47101000
H	0.51087300	-0.03948500	2.63327000
C	0.82278800	-3.51038500	4.33492700
H	1.38043500	-4.23870900	2.38261600
C	0.44362300	-2.39271200	5.08392300
H	0.01874400	-0.27630300	5.04712400
H	0.89947900	-4.48495100	4.80941200
H	0.22431000	-2.49873500	6.14304300

P	3.67224400	0.28690900	0.21263800
C	4.72983000	-0.61840900	1.51670100
C	3.30876700	2.06432600	0.80231900
C	4.66752500	0.36970600	-1.42359800
C	4.14083100	-0.39602400	2.91675100
H	3.08148200	-0.65220600	2.96410900
H	4.66819500	-1.05861000	3.61447200
H	4.27791600	0.62522700	3.27717600
C	4.66727900	-2.13299900	1.26009800
H	3.64321000	-2.50520000	1.34092500
H	5.06537500	-2.43010500	0.29029600
H	5.26673700	-2.63522200	2.02992200
C	6.19952500	-0.17366900	1.54108100
H	6.31259600	0.90045700	1.70005000
H	6.69501300	-0.68287400	2.37762700
H	6.74201300	-0.44632200	0.63422600
C	2.17292700	1.98342500	1.83202400
H	2.43883200	1.43448900	2.73408900
H	1.89897000	3.00172600	2.13286200
H	1.28529500	1.51933500	1.39392400
C	4.49611200	2.81086100	1.42102400
H	4.16925900	3.83053300	1.66248900
H	4.83491100	2.35431300	2.35363400
H	5.34991400	2.89185700	0.74596600
C	2.74992000	2.89011800	-0.36656000
H	1.88005100	2.41375900	-0.82836300
H	2.41248700	3.85211800	0.03589100
H	3.48799600	3.10742100	-1.13993000
C	5.75604200	1.45201100	-1.42937400
H	6.31123100	1.37302100	-2.37303600
H	5.34447600	2.46158500	-1.38464800
H	6.47478300	1.33618300	-0.61597300
C	5.33228900	-0.97804500	-1.74124300
H	5.75269000	-0.91159400	-2.75256600
H	6.15257600	-1.22961000	-1.06758600
H	4.61537800	-1.80315800	-1.74909600
C	3.68987700	0.62725300	-2.58204500
H	3.07893200	1.52010500	-2.45812700
H	4.27443000	0.75219100	-3.50257900
H	3.02243900	-0.22347300	-2.73435800
C	2.00548300	-3.19495600	-1.17592400
H	2.90352400	-2.58246200	-1.09585900
H	1.60273900	-3.10827500	-2.18713000
H	2.31240400	-4.23901900	-1.02803400

H	-0.68655900	0.13867700	0.58899800
7			
Ni	-0.98684200	-0.64462600	-0.05871700
B	1.84342900	-0.12599200	0.00053400
C	2.17238100	-0.03442800	1.58359100
C	1.40688500	-0.70802000	2.52753700
C	3.21640200	0.71747500	2.11892400
C	1.59938800	-0.62518100	3.89924400
C	3.45580100	0.83119800	3.48501100
C	2.63474000	0.16323100	4.38551500
C	2.27935900	-1.53101900	-0.68496100
C	1.86622000	-1.86212800	-1.97720800
C	3.02782900	-2.52663300	-0.05546300
C	2.13982000	-3.06811600	-2.60402600
C	3.32268500	-3.75676400	-0.64234300
C	2.87372100	-4.03406600	-1.92510000
C	2.22457700	1.22633400	-0.80068400
C	1.74593800	2.45199600	-0.33186700
C	3.00011100	1.31252000	-1.95524900
C	1.97602800	3.66807900	-0.96091100
C	3.23226000	2.50455400	-2.63587000
C	2.70993900	3.69148500	-2.14096500
F	3.14393200	-5.20779500	-2.50128500
F	1.70198400	-3.31306600	-3.84606800
F	1.14072900	-0.98100800	-2.69039600
F	4.03830800	-4.67163200	0.02256700
F	3.52845200	-2.35269700	1.18086900
F	4.07398500	1.36937800	1.31278500
F	4.46869100	1.57723100	3.94112700
F	2.84558500	0.26653300	5.70055800
F	0.80495100	-1.29207000	4.74754200
F	0.40406500	-1.52147700	2.11624200
F	3.60680000	0.22623100	-2.47138400
F	3.97228400	2.51870300	-3.75225600
F	2.93907700	4.84675500	-2.77110400
F	1.53380300	4.81561000	-0.43460300
F	1.06180600	2.49909800	0.82714000
C	-1.46060800	1.86809600	-1.23722700
C	-1.59417800	1.11305800	-0.12655300
C	-1.85862100	3.30389200	-1.26691500
C	-1.50569300	4.19696800	-0.24543600
C	-2.61958300	3.79345500	-2.34060500
C	-1.90736300	5.52919800	-0.28901900

H	-0.90866000	3.84318000	0.58631700
C	-3.03153900	5.12486600	-2.38137500
H	-2.91262800	3.12440000	-3.14546900
C	-2.67654800	6.00032100	-1.35427300
H	-1.61115700	6.20326600	0.51087700
H	-3.62931900	5.47768400	-3.21835200
H	-2.99005600	7.04059600	-1.38741900
C	-2.13795900	1.56920400	1.16003600
C	-3.40127400	2.17671300	1.25024300
C	-1.40099600	1.39161500	2.34175800
C	-3.91702000	2.57058300	2.48073800
H	-3.96637000	2.35949600	0.34130100
C	-1.91358800	1.78683000	3.57455800
H	-0.40940800	0.95807500	2.28376200
C	-3.17966900	2.37021000	3.65072200
H	-4.89733400	3.03851200	2.52823400
H	-1.32272100	1.63943800	4.47509800
H	-3.58558200	2.67474800	4.61183600
P	-2.87628500	-1.82174300	-0.22293000
C	-3.64722300	-2.30628800	1.45681600
C	-1.94712100	-3.32696000	-0.93011800
C	-4.26309500	-1.30802600	-1.41830300
C	-2.61205400	-3.03023500	2.33039000
H	-1.69539500	-2.44799400	2.44768300
H	-3.04772300	-3.15074200	3.33000500
H	-2.36242200	-4.03017400	1.97033800
C	-4.01825500	-1.03374500	2.23282000
H	-3.13439800	-0.43658200	2.45956800
H	-4.73477900	-0.39503800	1.72173400
H	-4.46930700	-1.34033600	3.18523700
C	-4.88753700	-3.20047800	1.32672500
H	-4.70101000	-4.11197300	0.75522900
H	-5.19489100	-3.50232900	2.33637600
H	-5.73498400	-2.67859900	0.87810200
C	-0.60644400	-3.34159000	-0.17688600
H	-0.68663000	-3.57780700	0.88054200
H	0.06590300	-4.07586700	-0.63820200
H	-0.05186900	-2.38735300	-0.26963500
C	-2.62502200	-4.69201400	-0.79473100
H	-1.97232600	-5.44935700	-1.24877500
H	-2.78363900	-4.98406800	0.24491600
H	-3.58514800	-4.73098400	-1.31439200
C	-1.60379000	-3.09094500	-2.40796300
H	-1.09980900	-2.13383000	-2.56844300

H	-0.91331000	-3.88055000	-2.72809400
H	-2.47586100	-3.13992700	-3.06177700
C	-5.25262800	-0.36526200	-0.71991000
H	-5.92319700	0.04492200	-1.48547000
H	-5.87638200	-0.86659600	0.02205100
H	-4.74253600	0.47482900	-0.24494500
C	-3.65179800	-0.49529400	-2.56704900
H	-4.45144800	-0.25179600	-3.27833600
H	-3.23717100	0.43867600	-2.18746200
H	-2.87174300	-1.02198000	-3.11517200
C	-5.03777400	-2.50260900	-1.99218700
H	-5.47610400	-3.13935200	-1.22188900
H	-5.86116500	-2.11012000	-2.60281300
H	-4.42427100	-3.12573300	-2.64590800
C	-0.88142000	1.32918000	-2.51522700
H	-0.68722900	0.26060700	-2.43425800
H	-1.54375700	1.49092600	-3.37188900
H	0.06399800	1.83343100	-2.74428800
H	0.54876800	-0.05378800	-0.06365500

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Ni	0.90545300	0.22319600	0.14429800
B	-0.85154400	-1.27102400	-0.06871400
C	-2.19884300	-0.83584700	-0.83920900
C	-3.17179500	-0.09171800	-0.16669000
C	-2.58021000	-1.24159500	-2.12006300
C	-4.38017700	0.29787300	-0.72626500
C	-3.77033000	-0.85836400	-2.72748400
C	-4.67538000	-0.06851500	-2.03133800
C	0.36379200	-1.86255800	-0.92495900
C	1.08732500	-3.01312500	-0.55037900
C	0.66523000	-1.40341800	-2.22471100
C	1.97036600	-3.67710000	-1.39313800
C	1.53090100	-2.04745800	-3.09561400
C	2.18573300	-3.20047900	-2.68036800
C	-1.22931900	-2.03071700	1.30640800
C	-0.52882800	-1.91728500	2.50239400
C	-2.33315600	-2.88790400	1.37487200
C	-0.89771000	-2.52723000	3.69256000
C	-2.74073000	-3.52765600	2.54135500
C	-2.02559700	-3.33769500	3.71651500
F	3.04371300	-3.81490700	-3.48966400
F	2.61290000	-4.77219700	-0.97660200
F	0.91543900	-3.58020800	0.65073900

F	1.75253300	-1.56208700	-4.32039700
F	0.05328800	-0.31901100	-2.71208100
F	-1.82935300	-2.10862400	-2.82551100
F	-4.06401700	-1.26986500	-3.96681900
F	-5.81927600	0.31619300	-2.60168900
F	-5.24237600	1.05027700	-0.03015700
F	-2.96859300	0.28806300	1.11056100
F	-3.05515000	-3.17309500	0.27602800
F	-3.81008700	-4.33138300	2.53793800
F	-2.40358500	-3.93959200	4.84570100
F	-0.17167400	-2.35354900	4.80395900
F	0.61554400	-1.20540900	2.54087500
C	-0.40856100	1.71332300	0.30531100
C	-0.74188200	2.31958500	1.47811100
C	-1.28085700	3.69941300	1.52890400
C	-2.35343000	4.00903600	2.37905000
C	-0.71356400	4.73348300	0.76817800
C	-2.86790700	5.30335100	2.43693900
H	-2.80785400	3.22574700	2.97959200
C	-1.21664600	6.02902800	0.83546800
H	0.12690800	4.51408800	0.11788000
C	-2.30254200	6.31904600	1.66473500
H	-3.71291500	5.51772900	3.08647400
H	-0.76084300	6.81466500	0.23796700
H	-2.70066800	7.32928100	1.71264700
C	-0.86282000	2.27110600	-0.99873900
C	-0.00472000	2.40503100	-2.09185000
C	-2.19886400	2.67487100	-1.16224300
C	-0.44945900	2.91972200	-3.30788700
H	1.02225400	2.08702600	-1.98859300
C	-2.65660700	3.17588200	-2.37584500
H	-2.87743000	2.61221300	-0.31853500
C	-1.78207300	3.30173900	-3.45817600
H	0.24465300	3.00920200	-4.13998900
H	-3.69811600	3.47120400	-2.47585200
H	-2.13847100	3.69139800	-4.40823400
P	3.15139800	0.89742600	0.35942100
C	4.13814200	0.63510400	-1.26756500
C	3.97301500	-0.20897200	1.69733300
C	3.41196500	2.72580600	0.88340900
C	4.32855900	-0.87083000	-1.47985700
H	3.40396500	-1.41837400	-1.29463600
H	4.61871700	-1.04723600	-2.52312000
H	5.11298700	-1.29297400	-0.84997700

C	3.29036000	1.12136000	-2.45091600
H	2.33261900	0.60052700	-2.49235500
H	3.09891900	2.19444300	-2.43476400
H	3.82677900	0.89831300	-3.38199200
C	5.51354000	1.30740600	-1.35045100
H	6.17341200	1.02863300	-0.52696400
H	5.99608400	0.98262600	-2.28217600
H	5.44731300	2.39684900	-1.38856700
C	3.50292900	-1.66036100	1.50543900
H	3.93766700	-2.14255800	0.63147900
H	3.80691200	-2.24433300	2.38351600
H	2.41815400	-1.72630700	1.43486200
C	5.50682400	-0.20538800	1.73029900
H	5.82999900	-0.81415900	2.58551100
H	5.94779000	-0.65310000	0.83746800
H	5.93142400	0.79083800	1.86018000
C	3.46575200	0.23707100	3.07777700
H	2.37975600	0.35265900	3.10613800
H	3.73380400	-0.53373600	3.81102400
H	3.92836600	1.16933000	3.40758300
C	4.81610600	3.07906800	1.38971300
H	4.85809600	4.16635800	1.53913500
H	5.02981100	2.61821800	2.35693400
H	5.61384100	2.81313700	0.69609000
C	3.07117600	3.62940800	-0.31082700
H	3.04150200	4.66815300	0.04191500
H	3.81221200	3.58311900	-1.11086600
H	2.08641400	3.39858100	-0.72575000
C	2.40998900	3.09824000	1.98372500
H	2.55748800	2.55389300	2.91453200
H	2.52426000	4.16725000	2.20551700
H	1.38996300	2.93537200	1.64615300
C	-0.57820200	1.64647100	2.80796900
H	-0.18999100	2.34516600	3.55534400
H	0.10027500	0.80129300	2.73334100
H	-1.54247500	1.27602500	3.17650000
H	-0.62223900	0.41297500	0.37925600

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Ni	-1.49208800	-0.82043800	-0.15415800
B	-1.53997000	1.54835000	-0.49704600
C	-0.14386300	2.15106100	-0.89969200
C	0.80024700	2.50052800	0.06917400
C	0.16584700	2.54152800	-2.20502600

C	1.97669700	3.17666400	-0.21834200
C	1.34158400	3.20324500	-2.53594700
C	2.25343300	3.52126900	-1.53668200
C	-2.32052300	0.52861900	-1.31574600
C	-3.74863600	0.36976000	-1.27419300
C	-1.61460500	-0.49904600	-2.06802800
C	-4.41622000	-0.58594600	-1.98443900
C	-2.34478400	-1.40683800	-2.90390100
C	-3.70168200	-1.48548900	-2.82011700
C	-2.21734800	2.24080100	0.75872200
C	-2.66239000	1.51784300	1.85399200
C	-2.38054500	3.62173500	0.84663700
C	-3.23349400	2.08662800	2.98099800
C	-2.95509100	4.24261500	1.95060600
C	-3.38120500	3.46961900	3.02630700
F	-4.39073000	-2.38528700	-3.52764800
F	-5.75183900	-0.68231100	-1.94585000
F	-4.48835000	1.24565500	-0.57414500
F	-1.66986900	-2.17535000	-3.76817800
F	-0.36821000	-0.23386500	-2.57247600
F	-0.70900600	2.33537000	-3.19979600
F	1.59587300	3.55354000	-3.80054000
F	3.37922800	4.16581700	-1.83673400
F	2.84397700	3.49525300	0.74729100
F	0.58766900	2.16846200	1.35929800
F	-1.99783000	4.40896500	-0.17245300
F	-3.10288000	5.56988000	1.99017900
F	-3.92571000	4.05028900	4.09605300
F	-3.63088900	1.33283000	4.01153700
F	-2.52544000	0.16708300	1.84628600
C	3.44742300	0.37373400	0.89587100
C	4.35002800	0.02923400	1.83485200
C	5.68258100	-0.53078600	1.50480500
C	6.85200100	-0.03604600	2.09835500
C	5.78891600	-1.60516000	0.60827100
C	8.09714000	-0.57843800	1.77999600
H	6.79190700	0.79544600	2.79623000
C	7.02978300	-2.15358500	0.29590000
H	4.88584400	-2.00212200	0.15269700
C	8.19090300	-1.63829800	0.87698200
H	8.99530500	-0.17149900	2.23793500
H	7.09191100	-2.98480600	-0.40220600
H	9.16076200	-2.06299900	0.63104200
C	3.63262400	0.43139600	-0.56086700

C	2.58112200	0.05527700	-1.41072200
C	4.81370400	0.92271200	-1.14087900
C	2.71509100	0.13275700	-2.79486800
H	1.64138900	-0.28655400	-0.98540200
C	4.94449500	1.01240200	-2.52354200
H	5.62384700	1.25285700	-0.49787900
C	3.89852100	0.61128300	-3.35784100
H	1.88853200	-0.16510700	-3.43234000
H	5.86157100	1.40910500	-2.95187600
H	3.99819900	0.68783000	-4.43742400
P	-0.90301800	-2.85988400	0.67263600
C	-2.49357700	-3.60010500	1.44593700
C	0.41683500	-2.68545500	2.03898500
C	-0.24862800	-4.07391400	-0.64687800
C	-2.83261800	-2.88616800	2.76394100
H	-2.91469500	-1.80597800	2.64182000
H	-3.81236600	-3.24907900	3.10017600
H	-2.12166000	-3.09538500	3.56445700
C	-3.66326900	-3.29141100	0.49373000
H	-3.76642100	-2.21222700	0.33470600
H	-3.57158700	-3.76936300	-0.48112700
H	-4.59403500	-3.65054400	0.95177300
C	-2.44351800	-5.10679100	1.72744800
H	-1.62323800	-5.37925300	2.39541200
H	-3.38015100	-5.39880700	2.22054800
H	-2.36073300	-5.70652800	0.81946500
C	0.12592200	-1.37599900	2.79219600
H	-0.85318300	-1.35312000	3.27028000
H	0.88352300	-1.24576900	3.57570500
H	0.19975600	-0.51367900	2.11972900
C	0.49917100	-3.85238600	3.02998900
H	1.33381600	-3.66293100	3.71804600
H	-0.40001000	-3.96158200	3.63868900
H	0.69417000	-4.80589500	2.53393700
C	1.80078800	-2.50311100	1.40589100
H	1.80577400	-1.71806500	0.64846400
H	2.49964800	-2.19284900	2.19060400
H	2.19646000	-3.41941300	0.96522500
C	0.43242600	-5.33292800	-0.09556500
H	0.70535300	-5.97538900	-0.94323500
H	1.35319600	-5.11007300	0.44647200
H	-0.21878700	-5.91436800	0.55991800
C	-1.41169500	-4.51361800	-1.54711200
H	-0.99738400	-5.02739000	-2.42298700

H	-2.09122400	-5.20981000	-1.05275400
H	-1.99092000	-3.66510900	-1.91188500
C	0.74493600	-3.31887500	-1.54652000
H	1.66918000	-3.04948700	-1.03696400
H	1.01278800	-3.96895000	-2.38926900
H	0.31003000	-2.40683300	-1.95656700
C	4.00835200	0.12995100	3.29596600
H	2.98572400	0.48859500	3.43906200
H	4.11828400	-0.84206900	3.79256600
H	4.68259900	0.82290100	3.81332800
H	2.45518200	0.64646600	1.24844100

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Ni	0.82688900	-0.87461000	0.31043100
B	0.75933500	1.37782300	0.78869000
C	-0.68301300	1.99042900	0.59691400
C	-1.19427900	2.32206100	-0.65838300
C	-1.46311000	2.39037400	1.68518500
C	-2.39760300	2.98826800	-0.84221100
C	-2.66928600	3.06444800	1.54400700
C	-3.14098700	3.36262000	0.27059500
C	1.06897700	0.31284000	1.84745000
C	2.35071100	0.09203400	2.44986300
C	0.07768600	-0.72195300	2.09165900
C	2.63402900	-0.99498100	3.22737600
C	0.37444600	-1.80813300	2.97364700
C	1.63108300	-1.96719500	3.48080600
C	1.92380600	2.10085000	-0.01327900
C	2.97294900	1.41297400	-0.61844400
C	1.95443900	3.48711300	-0.19035600
C	3.96967900	2.01622400	-1.36867900
C	2.94020800	4.13931100	-0.92310600
C	3.95195700	3.39848100	-1.52332900
F	1.93991700	-3.02065100	4.24087400
F	3.83636000	-1.16005500	3.79396000
F	3.30974000	1.02029600	2.30499300
F	-0.59672900	-2.67680300	3.28356900
F	-1.25971300	-0.42909400	2.04761200
F	-1.03475700	2.17815400	2.93811700
F	-3.38258800	3.42695100	2.61542600
F	-4.30514000	3.99431200	0.11720500
F	-2.84463100	3.27518800	-2.07047400
F	-0.50036400	2.01488600	-1.76969200
F	1.01992800	4.26597100	0.37818000

F	2.92518500	5.46861000	-1.05512700
F	4.89876300	4.00648600	-2.23677400
F	4.93602200	1.28977200	-1.93954700
F	3.04805700	0.06713300	-0.49606400
P	0.48405700	-2.53221900	-1.18558800
C	-0.96026900	-3.68323600	-0.70806500
C	2.07995800	-3.58030700	-1.30431600
C	0.12395300	-1.72791400	-2.87306600
C	-0.53648300	-4.57853600	0.46545700
H	-0.13820800	-3.99479300	1.29819900
H	-1.42840300	-5.10047700	0.83407300
H	0.19267700	-5.34136100	0.18896900
C	-2.11598000	-2.82178800	-0.17820500
H	-1.80610300	-2.19834100	0.66150500
H	-2.55395700	-2.17414400	-0.93496500
H	-2.90800400	-3.49324100	0.17670300
C	-1.48384200	-4.56463800	-1.84795100
H	-0.70762100	-5.18472500	-2.30059100
H	-2.25070600	-5.23760300	-1.44213700
H	-1.95918100	-3.97709600	-2.63690700
C	2.62057200	-3.75921300	0.12708900
H	1.93890000	-4.28961100	0.79118400
H	3.55384900	-4.33559900	0.08090300
H	2.85232400	-2.79013600	0.58409000
C	1.90749800	-4.94775400	-1.97680000
H	2.89099800	-5.43203400	-2.03894900
H	1.25417900	-5.62088000	-1.41935500
H	1.52089900	-4.86020000	-2.99554600
C	3.17398800	-2.82178900	-2.07056200
H	3.35740600	-1.82807900	-1.65922500
H	4.10730700	-3.39139200	-1.97467300
H	2.96285100	-2.73107800	-3.13787600
C	0.26799600	-2.64538900	-4.09133300
H	-0.01467100	-2.08093700	-4.98992000
H	1.29475700	-2.98867700	-4.23681500
H	-0.38035000	-3.52229200	-4.03665800
C	-1.29758900	-1.14784300	-2.84485200
H	-1.42118000	-0.48818200	-3.71257700
H	-2.06889300	-1.91768800	-2.91074400
H	-1.47435900	-0.54555900	-1.94850900
C	1.07003200	-0.52422100	-3.02237500
H	2.12118700	-0.80007200	-3.08820200
H	0.80840100	0.01489700	-3.94196600
H	0.94631600	0.17619700	-2.19141500

C	-4.27158300	0.10056300	0.07186000
C	-5.06064900	-0.94384800	0.86159000
C	-6.56360000	-0.80012700	0.61158600
C	-6.88652100	-0.86786900	-0.88319500
C	-6.09074300	0.17342400	-1.67397600
C	-4.58909100	0.02779700	-1.42178200
H	-3.19607600	-0.01277900	0.24675200
H	-4.54767900	1.09576700	0.44387700
H	-4.83858300	-0.85677200	1.93184400
H	-4.74029700	-1.94874200	0.55480900
H	-6.90327100	0.16736000	1.00903900
H	-7.11695400	-1.57497100	1.15610300
H	-7.96221800	-0.73043600	-1.04738400
H	-6.63645200	-1.87112800	-1.25897100
H	-6.40952500	1.18030500	-1.36800800
H	-6.30829700	0.08706900	-2.74557200
H	-4.25551800	-0.94296800	-1.81569300
H	-4.03247800	0.79476800	-1.97230000

TS_{2/3}^{cyc}

Ni	0.91421700	-0.15528000	-0.64198200
B	-1.08773100	-0.00640600	0.25750700
C	-2.59807800	-0.44721500	-0.12944900
C	-3.32532700	0.32274000	-1.04482000
C	-3.35028300	-1.45153600	0.48712900
C	-4.65581500	0.09966100	-1.37332100
C	-4.68253700	-1.71603900	0.18118400
C	-5.34219300	-0.94225600	-0.76301300
C	-0.33201300	-0.90702200	1.38049600
C	0.17253200	-0.44526200	2.60681000
C	-0.17260200	-2.29257800	1.19382400
C	0.75341400	-1.27379400	3.56429700
C	0.41213800	-3.14650600	2.11440400
C	0.87833100	-2.63309000	3.32013900
C	-1.12913100	1.59830800	0.55209800
C	-0.55102900	2.62038100	-0.19176700
C	-1.92429600	2.03590400	1.61426000
C	-0.69474700	3.97104200	0.10875400
C	-2.10066800	3.37042000	1.95199600
C	-1.47050100	4.35179600	1.19441300
F	1.45813400	-3.43207800	4.21492000
F	1.20928300	-0.76142000	4.71296800
F	0.09892200	0.84670300	2.96015700

F	0.53104300	-4.45353000	1.85660800
F	-0.64302400	-2.86944100	0.07849900
F	-2.83674200	-2.21013200	1.47118300
F	-5.33824000	-2.70023300	0.80738000
F	-6.61817500	-1.18457400	-1.06856500
F	-5.27350200	0.86758400	-2.27852000
F	-2.73595200	1.35608200	-1.67654400
F	-2.56460600	1.13180200	2.37935300
F	-2.86044900	3.72131100	2.99622100
F	-1.61900700	5.64288100	1.50129600
F	-0.09982300	4.90331800	-0.64786600
F	0.17794300	2.34782500	-1.29613300
P	3.21217100	0.15029700	-0.64558500
C	3.95165200	0.46444900	-2.38636100
C	4.01725100	-1.42549600	0.07479600
C	3.67136400	1.64127300	0.46046300
C	3.92209800	-0.83715300	-3.20594300
H	2.93417300	-1.30359200	-3.24023200
H	4.20365200	-0.59706900	-4.23886000
H	4.63711100	-1.57715400	-2.84181000
C	3.07904600	1.49405000	-3.13163100
H	2.01211100	1.26712500	-3.08581300
H	3.21275100	2.50731000	-2.75577100
H	3.37392800	1.49682700	-4.18873800
C	5.39809400	0.97797200	-2.38756400
H	6.08787700	0.30496400	-1.87513100
H	5.73371100	1.06363300	-3.42981500
H	5.48977300	1.96948900	-1.94044100
C	3.28406800	-2.63456000	-0.53043500
H	3.38891500	-2.71869900	-1.61172600
H	3.68738000	-3.55243200	-0.08337800
H	2.21606100	-2.59085400	-0.29652200
C	5.52639300	-1.58194000	-0.13643400
H	5.86301400	-2.47847200	0.40100700
H	5.79000200	-1.72128700	-1.18715100
H	6.09526500	-0.73403800	0.25121200
C	3.71930500	-1.48299200	1.57809400
H	2.65664600	-1.32479300	1.77312300
H	3.97653400	-2.48365400	1.94744400
H	4.29313800	-0.76272700	2.16367500
C	5.11652400	1.66214100	0.97136700
H	5.27090000	2.59121500	1.53608100
H	5.33600600	0.83516500	1.64955700
H	5.84993500	1.64462400	0.16255700

C	3.39892000	2.95621000	-0.28590700
H	3.43971200	3.77466100	0.44404800
H	4.14568000	3.17439100	-1.05153500
H	2.40708800	2.97213300	-0.74288600
C	2.70617700	1.64177300	1.65392800
H	2.77888100	0.75152300	2.27674000
H	2.92765400	2.50772700	2.29107800
H	1.66935300	1.74296200	1.31969300
C	0.28686500	-0.76730200	-2.53219200
C	0.22852300	-2.28330500	-2.69662500
C	-1.17672800	-2.82836400	-2.93189100
C	-1.80840700	-2.15210600	-4.14572700
C	-1.91403700	-0.65089300	-3.89458700
C	-0.56379500	-0.01507700	-3.55970100
H	1.31369400	-0.44400800	-2.69646500
H	-0.49316200	-0.41334100	-1.24419600
H	0.70956300	-2.78715300	-1.85772700
H	0.83734100	-2.52420000	-3.58461500
H	-1.80058900	-2.64128200	-2.04940200
H	-1.13106600	-3.91526500	-3.06557100
H	-2.80218500	-2.56836800	-4.34771100
H	-1.19354500	-2.34728200	-5.03661900
H	-2.61299200	-0.50572200	-3.07018400
H	-2.34529700	-0.13543600	-4.76052100
H	0.03525300	0.00316400	-4.48449800
H	-0.69154800	1.02866400	-3.26230200

3^{eye}

Ni	1.15349400	0.58712100	0.14624500
B	-1.23401400	-0.21718600	0.00781200
C	-2.55079900	0.53670000	-0.60026300
C	-3.04090500	1.66767400	0.05414300
C	-3.31412500	0.13613400	-1.69668200
C	-4.15082900	2.39269900	-0.35993000
C	-4.43366300	0.82943200	-2.14881400
C	-4.85284100	1.97292800	-1.48258300
C	-0.55930800	-1.29691000	-1.01125400
C	-0.32560200	-2.64461000	-0.72482800
C	-0.29046400	-0.94318600	-2.33957100
C	0.11582500	-3.56894200	-1.66891400
C	0.14221800	-1.83031300	-3.31316000
C	0.34634400	-3.16298400	-2.97542900
C	-1.64524700	-0.79530700	1.46912000
C	-1.07730100	-0.40700200	2.67627500

C	-2.70692800	-1.69212600	1.58592500
C	-1.50326800	-0.87653300	3.91518100
C	-3.17061900	-2.18634300	2.79720900
C	-2.55987000	-1.77420500	3.97738300
F	0.78926300	-4.03122400	-3.88648500
F	0.33314900	-4.84293700	-1.32084400
F	-0.51815100	-3.14092600	0.51006000
F	0.37961800	-1.41546300	-4.56315100
F	-0.48998200	0.32254900	-2.74319300
F	-3.01582100	-0.98227500	-2.38395700
F	-5.11539100	0.39698700	-3.21713700
F	-5.92423100	2.64990600	-1.90468200
F	-4.55188800	3.47899500	0.31338600
F	-2.43676000	2.10452300	1.17798300
F	-3.32224900	-2.13726000	0.47429300
F	-4.18789300	-3.05516500	2.84358800
F	-2.98575900	-2.23769500	5.15598800
F	-0.90591600	-0.46753600	5.04327000
F	-0.04943400	0.47006900	2.70486700
P	3.34938800	0.26385500	0.23907400
C	3.88100700	-0.43870000	-1.45010600
C	3.40935700	-1.10680600	1.56485100
C	4.58545200	1.64367200	0.72020800
C	3.16750200	-1.77425300	-1.68173800
H	2.09726300	-1.68684400	-1.49211700
H	3.29436200	-2.05684200	-2.73378900
H	3.57002200	-2.58839000	-1.07621800
C	3.34060500	0.52293400	-2.52337900
H	2.25251900	0.61388400	-2.45123200
H	3.76665900	1.52473400	-2.46783300
H	3.57909500	0.11391400	-3.51334500
C	5.38388700	-0.66623000	-1.64558100
H	5.80215000	-1.34186700	-0.89517900
H	5.53427900	-1.13386200	-2.62736900
H	5.96458100	0.25748500	-1.63905600
C	2.12667500	-1.93272000	1.37630200
H	2.12048700	-2.52268400	0.46288800
H	2.01259700	-2.62554000	2.21895000
H	1.22715400	-1.29792100	1.38874400
C	4.62015600	-2.04319500	1.52412700
H	4.51456100	-2.78128400	2.33023300
H	4.68885100	-2.59916600	0.58685000
H	5.56451700	-1.51894500	1.68094900
C	3.30023700	-0.47805300	2.96213600

H	2.44069000	0.19415000	3.03935500
H	3.14707300	-1.28736000	3.68707700
H	4.20170400	0.05792900	3.26364300
C	5.91980900	1.06998300	1.22281800
H	6.61834000	1.90476800	1.36401300
H	5.82077700	0.57042700	2.18831100
H	6.37922200	0.37400000	0.51925800
C	4.89106100	2.57612300	-0.46487700
H	5.50103000	3.40495400	-0.08382900
H	5.46369800	2.09353400	-1.25782200
H	3.99128500	3.01500800	-0.90320500
C	3.99187700	2.53686200	1.82266300
H	3.60789100	1.98590200	2.67955000
H	4.78691900	3.20110900	2.18506700
H	3.19139700	3.16822100	1.43833400
C	1.16099200	2.46846800	-0.12855900
C	0.35702500	2.85900800	-1.35707700
C	0.36240600	4.39020200	-1.51324100
C	-0.16044300	5.07844100	-0.25364100
C	0.64010500	4.65473900	0.97717800
C	0.62726500	3.12436900	1.13572300
H	-0.47057100	0.77331500	0.20823500
H	0.76718000	2.39665400	-2.25884200
H	-0.67934000	2.51538500	-1.26591600
H	-0.23997200	4.66960000	-2.38628600
H	1.38901400	4.72881600	-1.71405200
H	-1.21519400	4.80773500	-0.10624900
H	-0.12757600	6.16814300	-0.37395200
H	0.23444000	5.12086600	1.88332600
H	1.67746600	5.00606000	0.87545600
H	-0.39950200	2.80190900	1.31489900
H	1.20451100	2.82946000	2.01665400
H	2.19931400	2.76683400	-0.29110300

Cyclohexane

C	-1.43705700	0.25265500	0.23076400
C	-0.49965000	1.37089700	-0.23101100
C	0.93736100	1.11813100	0.23125700
C	1.43703800	-0.25264700	-0.23116800
C	0.49974900	-1.37082400	0.23117200
C	-0.93729900	-1.11823300	-0.23107700
H	1.60110000	1.91014000	-0.13671900
H	-0.51929800	1.42541800	-1.32936300
H	-0.85375200	2.34145100	0.13758800

H	-1.49441700	0.26271700	1.32911400
H	-2.45461800	0.43154100	-0.13787800
H	1.49333600	-0.26251300	-1.32958600
H	2.45487900	-0.43158800	0.13655700
H	0.85363800	-2.34171300	-0.13676500
H	0.51950600	-1.42463400	1.32957500
H	-0.97442500	-1.16288200	-1.32942100
H	-1.60110400	-1.90984600	0.13761600
H	0.97430400	1.16203700	1.32965700

PhC≡CPh

C	-0.60885100	-0.00001000	-0.00016800
C	0.60887200	-0.00000100	-0.00014200
C	-2.03090000	0.00004800	-0.00012200
C	-2.74469700	-1.21350400	0.00007200
C	-2.74477500	1.21357300	-0.00010400
C	-4.13631200	-1.20849800	0.00017000
H	-2.19629300	-2.15102800	0.00010700
C	-4.13638100	1.20844900	-0.00001800
H	-2.19645500	2.15112200	-0.00022900
C	-4.83697800	-0.00004300	0.00012400
H	-4.67677100	-2.15146300	0.00029300
H	-4.67693400	2.15136100	-0.00005900
H	-5.92371000	-0.00003700	0.00019300
C	2.03092400	-0.00000300	-0.00010600
C	2.74474200	1.21353500	0.00003800
C	2.74472200	-1.21355300	-0.00014600
C	4.13635300	1.20848000	0.00017300
H	2.19638300	2.15107500	0.00005700
C	4.13632300	-1.20847400	-0.00001200
H	2.19634500	-2.15106700	-0.00027400
C	4.83696100	0.00000600	0.00014300
H	4.67686700	2.15141400	0.00030400
H	4.67684700	-2.15140000	-0.00003700
H	5.92369200	-0.00001000	0.00023100

cis-1,2-diphenylpropene

H	1.04265500	2.76563600	-0.00150600
C	0.60061600	1.76987200	0.03892600
C	-0.74628000	1.69785000	0.00547000
C	-1.49054500	0.41649500	-0.08725100
C	-2.51044800	0.10206300	0.82133600
C	-1.20353900	-0.49425700	-1.11483100
C	-3.20445200	-1.10420000	0.72449400

H	-2.74801700	0.79481000	1.62500500
C	-1.90158600	-1.69471900	-1.21865800
H	-0.42060400	-0.25396400	-1.82891000
C	-2.90170500	-2.00762300	-0.29510400
H	-3.98229100	-1.33806600	1.44724100
H	-1.66456100	-2.38828100	-2.02165800
H	-3.44447200	-2.94616200	-0.37312000
C	1.57300500	0.66971700	0.12006500
C	2.81847000	0.81589100	-0.51321200
C	1.33261500	-0.51124300	0.84340500
C	3.77609400	-0.19566100	-0.46249400
H	3.02946500	1.73242800	-1.06066000
C	2.29060600	-1.51978200	0.89991600
H	0.39164900	-0.63395600	1.37006900
C	3.51392000	-1.37213200	0.24115400
H	4.72861100	-0.06333700	-0.96978900
H	2.08398300	-2.42405000	1.46722700
H	4.25946500	-2.16187000	0.28622000
C	-1.58534500	2.94676200	0.00398800
H	-2.25183500	2.97466200	0.87450200
H	-0.96397700	3.84605100	0.02559300
H	-2.22862400	2.98191100	-0.88343000