

Supporting information

1. The optimized geometries of 34 thioesters in the gas phase

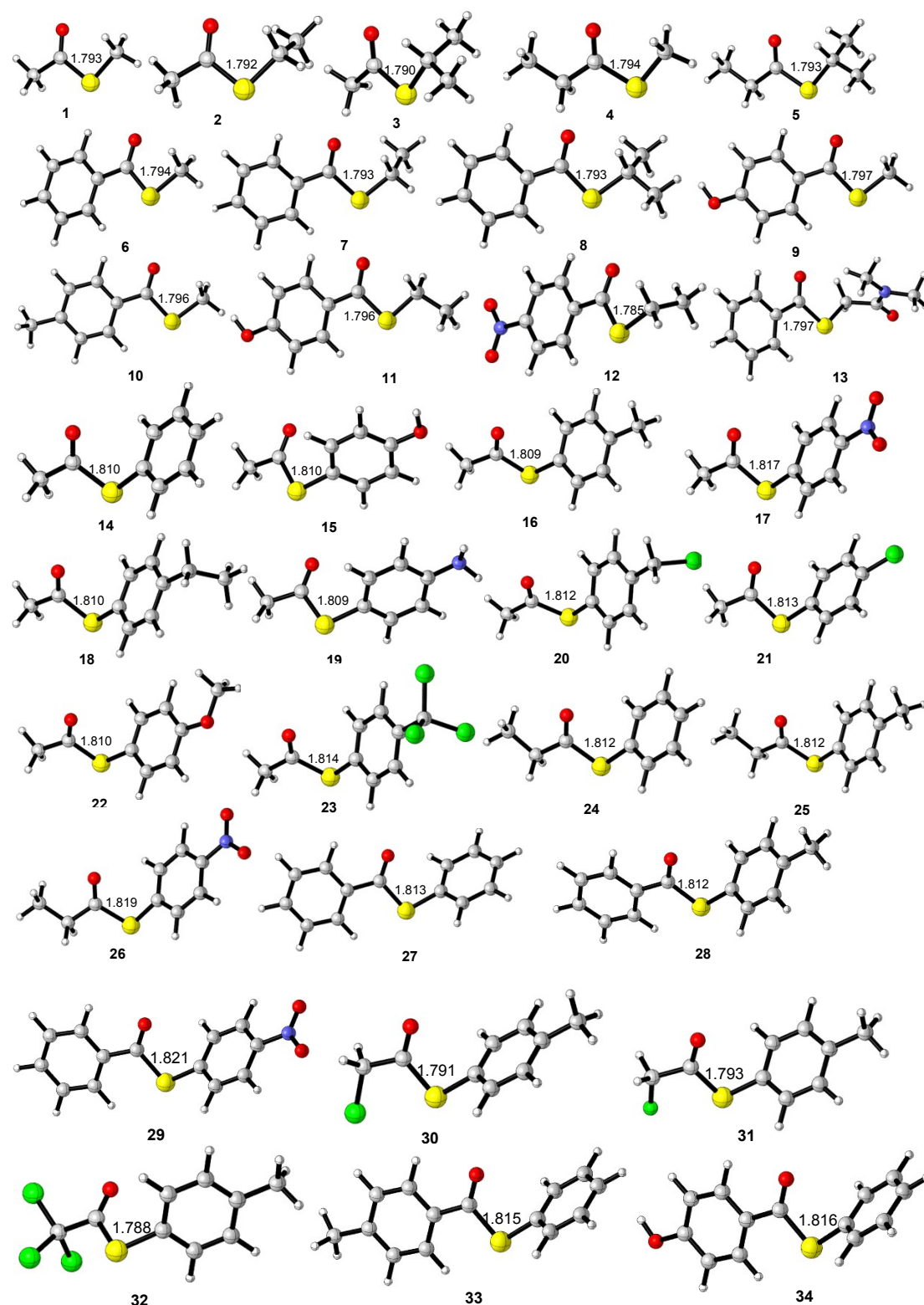


Figure S1. The optimized geometries of 34 thioesters.

2. The linear plot between $\Delta G^\ddagger$ and the C-S BDE of the substrates.

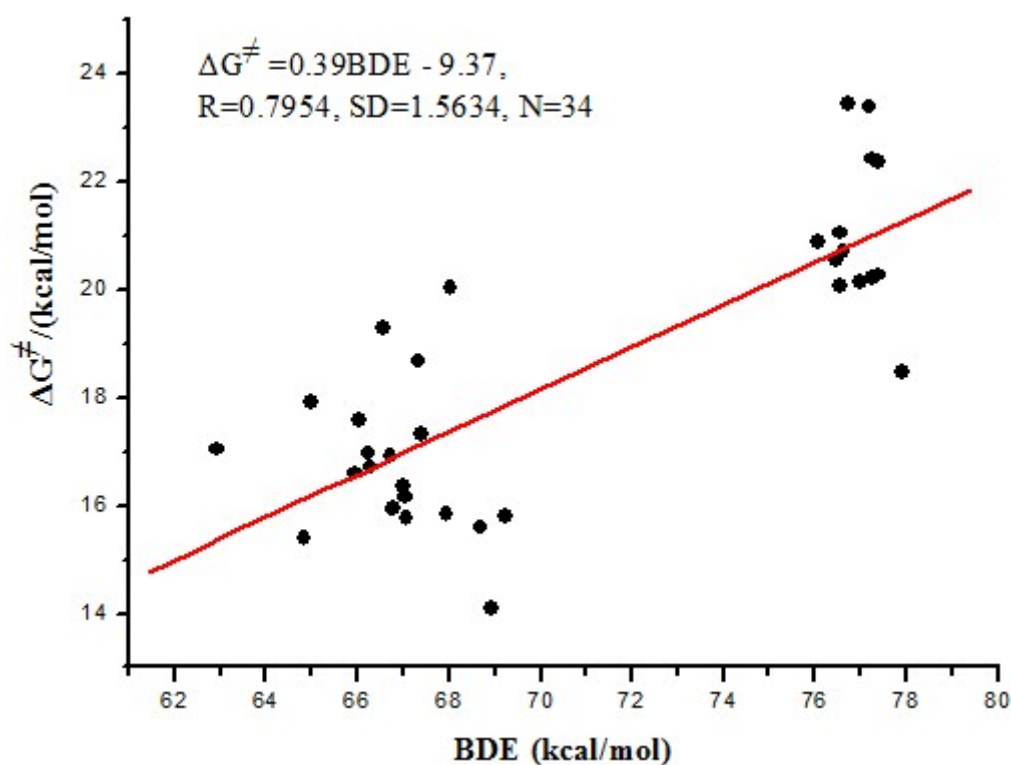


Figure S2. The correlation between $\Delta G^\ddagger$ and BDE.

3. The bond lengths of C-S, Pd-S and Pd-C in the transition states and the Cartesian coordinates of the 34 transition states.

Table S1. The bond lengths ($\text{\AA}$) of C-S, Pd-S and Pd-C in the transition states.

Transition state	1-TS	2-TS	3-TS	4-TS	5-TS	6-TS	7-TS	8-TS	9-TS
C-S	2.125	2.120	2.047	2.141	2.108	2.057	2.039	2.195	2.065
Pd-S	2.472	2.470	2.514	2.461	2.496	2.479	2.480	2.464	2.478
Pd-C	2.113	2.115	2.142	2.118	2.112	2.127	2.137	2.066	2.128
	10-TS	11-TS	12-TS	13-TS	14-TS	15-TS	16-TS	17-TS	18-TS
C-S	2.069	2.054	2.052	1.960	2.040	2.070	2.051	1.955	2.048
Pd-S	2.477	2.478	2.475	2.512	2.510	2.497	2.505	2.584	2.507
Pd-C	2.123	2.132	2.113	2.218	2.172	2.150	2.165	2.269	2.167
	19-TS	20-TS	21-TS	22-TS	23-TS	24-TS	25-TS	26-TS	27-TS
C-S	2.084	2.001	2.007	2.082	1.973	2.164	2.062	2.033	1.916
Pd-S	2.488	2.526	2.527	2.495	2.543	2.495	2.501	2.536	2.562
Pd-C	2.143	2.213	2.201	2.151	2.253	2.106	2.181	2.183	2.297

	28-TS	29-TS	30-TS	31-TS	32-TS	33-TS	34-TS
C-S	1.922	1.920	2.147	2.237	2.061	1.929	1.947
Pd-S	2.556	2.573	2.497	2.501	2.480	2.566	2.546
Pd-C	2.276	2.353	2.070	2.034	2.068	2.268	2.299

The cartesian coordinates of the 34 transition states.

1-TS

C	2.66929900	-3.14774900	-1.10444100
C	-2.62404600	-2.18250200	-0.09806100
C	-1.70071400	-1.13727600	-0.16370600
C	-0.83250900	-1.07071800	-1.26250600
C	-0.88458300	-2.02676600	-2.26841500
C	-1.80231400	-3.07327900	-2.18878700
H	-3.39334300	-3.95454200	-1.03860700
H	-3.32191700	-2.24481600	0.73095300
H	-0.10229000	-0.26585800	-1.32997600
H	-0.19477500	-1.96540900	-3.10432800
H	-1.83662200	-3.82824200	-2.96869100
P	-1.51829900	0.15707800	1.13315200
C	-2.96254900	-0.12097500	2.22678200
C	-4.00947300	0.79398100	2.34844600
C	-2.94125200	-1.24794200	3.06046800
C	-5.01929800	0.58309300	3.28734300
H	-4.03016300	1.68069200	1.72233100
C	-3.95914900	-1.46807000	3.98011000
H	-2.10918300	-1.94766900	2.99589500
C	-4.99900800	-0.54589300	4.09998600
H	-5.82164300	1.30799200	3.38318000
H	-3.93309200	-2.34702300	4.61675400
H	-5.78520600	-0.70517300	4.83123200
C	-1.94422000	1.67317500	0.19238500
C	-1.35595600	2.88265100	0.57917000
C	-2.84113300	1.65182600	-0.88305700
C	-1.66346600	4.05604800	-0.10896700
H	-0.67975100	2.90998000	1.43116400
C	-3.14334100	2.82606000	-1.56460100
H	-3.29677900	0.71391400	-1.19032500
C	-2.55238800	4.02894400	-1.17932800
H	-1.20619700	4.99120000	0.19905500
H	-3.83692800	2.80223500	-2.39960300
H	-2.78775700	4.94366500	-1.71512500
P	2.34685400	-0.73630600	0.79267300
C	1.98451800	-2.27576100	-0.14106700
C	1.03676100	-3.14366900	0.41539500
C	2.58130800	-2.60976300	-1.35869100
C	0.70270200	-4.33184500	-0.22669300
H	0.54136400	-2.86548900	1.34463900
C	2.24033800	-3.79535400	-2.00599200
H	3.30542500	-1.93844800	-1.81100400
C	1.30431700	-4.65749800	-1.44043800
H	-0.04383600	-4.99020400	0.20670400
H	2.70710200	-4.04427800	-2.95447900
H	1.03621900	-5.57807100	-1.95030800

C	3.85970200	-1.17233200	1.73340400
C	4.24557200	-2.49343800	1.97684000
C	4.57149900	-0.12796900	2.34080600
C	5.32343400	-2.76592700	2.81790800
H	3.70554700	-3.31264000	1.51048500
C	5.64885400	-0.40487300	3.17519300
H	4.27046800	0.90220400	2.16991900
C	6.02450000	-1.72507400	3.41955400
H	5.61478700	-3.79604000	2.99996200
H	6.18848600	0.41260400	3.64330000
H	6.86156500	-1.94076700	4.07646100
C	2.98753700	0.43087500	-0.46924600
C	4.27698700	0.33735600	-1.00727200
C	2.14469200	1.46294800	-0.89557000
C	4.70061500	1.23951400	-1.97771500
H	4.95205000	-0.43758800	-0.65206300
C	2.56866200	2.36428700	-1.86987900
H	1.15834300	1.57331400	-0.44762400
C	3.84457900	2.25010600	-2.41414100
H	5.70165200	1.15832600	-2.39021200
H	1.90447600	3.16114500	-2.18997100
H	4.17959900	2.95536000	-3.16860100
Pd	0.57863100	0.34677400	2.28942200
C	-0.95240600	0.75906500	4.92239400
H	-0.78018300	1.19760300	5.91034600
H	-0.71610900	-0.30641600	4.94490800
H	-2.00744300	0.88540400	4.66031300
C	-0.13040500	1.51874600	3.89802400
O	-0.35614600	2.67566300	3.60730800
S	1.94409500	1.15737800	4.18341900
C	2.25040900	-0.46622800	4.96469100
H	2.68894000	-1.17062600	4.25255900
H	2.95118200	-0.31410800	5.78923700
H	1.32739000	-0.88763200	5.37032400

2-TS

C	-2.61456900	-3.24265200	-1.23101300
C	-2.59743500	-2.27270400	-0.22806500
C	-1.68808100	-1.21475500	-0.28591300
C	-0.80653000	-1.14019700	-1.37339200
C	-0.83077900	-2.10064700	-2.37586300
C	-1.73399200	-3.16017800	-2.30383800
H	-3.32739500	-4.05988900	-1.17175000
H	-3.30546600	-2.34167600	0.59192900
H	-0.08726400	-0.32502100	-1.43414300
H	-0.13131500	-2.03212000	-3.20311600
H	-1.74603800	-3.91920800	-3.08048700
P	-1.53591700	0.08965400	1.00434000
C	-2.98379100	-0.20018100	2.08992300
C	-4.03904500	0.70624300	2.20373400
C	-2.95596600	-1.32339200	2.92843200
C	-5.05055100	0.49079000	3.13968900
H	-4.06471500	1.59025400	1.57400900
C	-3.97537400	-1.54806800	3.84536200
H	-2.11758200	-2.01606600	2.87013700
C	-5.02347600	-0.63430400	3.95747400
H	-5.85944700	1.20919800	3.22930400
H	-3.94423200	-2.42397200	4.48597900

H	-5.81087300	-0.79702900	4.68668000
C	-1.97659400	1.59279600	0.04955000
C	-1.40257700	2.81237400	0.42559900
C	-2.87182600	1.55108000	-1.02673300
C	-1.72283200	3.97579800	-0.27380800
H	-0.72796300	2.85545700	1.27820700
C	-3.18693800	2.71536700	-1.71932600
H	-3.31613700	0.60507600	-1.32584900
C	-2.61037100	3.92854000	-1.34454600
H	-1.27668700	4.91896400	0.02601600
H	-3.87954100	2.67589900	-2.55455900
H	-2.85589900	4.83546500	-1.88895300
P	2.34347600	-0.77621500	0.70164700
C	2.00920800	-2.32814000	-0.22246300
C	1.06328300	-3.20056400	0.33020900
C	2.62258300	-2.66616900	-1.43066100
C	0.74672000	-4.39633000	-0.30657100
H	0.55538400	-2.92053500	1.25207200
C	2.29921000	-3.85953200	-2.07272100
H	3.34529200	-1.99170200	-1.88035900
C	1.36445500	-4.72562700	-1.51121700
H	0.00119900	-5.05790400	0.12363600
H	2.77874400	-4.11142900	-3.01400600
H	1.10999100	-5.65223100	-2.01712800
C	3.84623000	-1.18847800	1.66848600
C	4.22357500	-2.50366100	1.95343800
C	4.54920000	-0.13045300	2.26275400
C	5.28237300	-2.75750400	2.82420400
H	3.69019700	-3.33316000	1.49761300
C	5.61003200	-0.38886000	3.12402800
H	4.25567000	0.89587600	2.05909100
C	5.97455600	-1.70357500	3.41307100
H	5.56565500	-3.78344600	3.03940900
H	6.14526000	0.43913800	3.57928600
H	6.79625200	-1.90375400	4.09382900
C	2.98932100	0.38693000	-0.56119000
C	4.28340000	0.29744700	-1.08882500
C	2.14472200	1.41280900	-0.99875200
C	4.70984500	1.19697400	-2.06047400
H	4.95989500	-0.47203300	-0.72453900
C	2.57155100	2.31159800	-1.97420700
H	1.15463800	1.52021200	-0.55832200
C	3.85200300	2.20105800	-2.50834600
H	5.71437200	1.11893000	-2.46501600
H	1.90584800	3.10348700	-2.30330500
H	4.18915500	2.90420400	-3.26381100
Pd	0.55126600	0.31094400	2.17098600
C	-0.99438900	0.72962400	4.79027700
H	-0.82984400	1.17321300	5.77737800
H	-0.74650500	-0.33315300	4.81744100
H	-2.04979100	0.84437400	4.52410200
C	-0.17688000	1.49424500	3.76572500
O	-0.42124500	2.64394700	3.46170100
S	1.89752700	1.16556700	4.05709500
C	2.24178200	-0.44025100	4.87510200
H	2.65496400	-1.13796200	4.13947100
H	1.30339800	-0.86041400	5.24984200
C	3.22705200	-0.23735000	6.02089400

H	3.44448500	-1.19227000	6.51132400
H	4.16863200	0.17444900	5.64605800
H	2.82256100	0.45509800	6.76470700

3-TS

C	-2.59073600	-3.21969000	-1.03950500
C	-2.56947300	-2.21237900	-0.07482200
C	-1.65975700	-1.15763100	-0.17428700
C	-0.78135400	-1.12440800	-1.26607500
C	-0.81020800	-2.12226300	-2.23175700
C	-1.71291700	-3.17855300	-2.11680400
H	-3.30379800	-4.03355400	-0.94681100
H	-3.27282100	-2.25200700	0.75084000
H	-0.06021400	-0.31390300	-1.35754500
H	-0.11685800	-2.08319800	-3.06597400
H	-1.72721700	-3.96630300	-2.86427000
P	-1.50791100	0.18073600	1.08260500
C	-2.96633300	-0.11330000	2.15793900
C	-4.09651900	0.70622500	2.16723500
C	-2.88734600	-1.17415200	3.07011400
C	-5.12645900	0.47032000	3.07803000
H	-4.16985200	1.53763300	1.47243700
C	-3.92308000	-1.42170200	3.96260400
H	-1.99667400	-1.80136100	3.08456900
C	-5.04398200	-0.59139600	3.97308100
H	-5.99585300	1.12044400	3.08480000
H	-3.84964700	-2.24900200	4.66184300
H	-5.84652600	-0.77057800	4.68169100
C	-1.96910600	1.66305500	0.10517700
C	-1.43994300	2.89870300	0.49567700
C	-2.83581800	1.59717500	-0.99293000
C	-1.78121900	4.05458600	-0.20598500
H	-0.77142600	2.95895700	1.35274200
C	-3.17096200	2.75407500	-1.68911400
H	-3.24321600	0.63886900	-1.30493300
C	-2.64332000	3.98363800	-1.29623500
H	-1.36887000	5.00942600	0.10500000
H	-3.84189900	2.69657000	-2.54086000
H	-2.90484100	4.88448600	-1.84325000
P	2.39942200	-0.63883100	0.75036800
C	2.01940900	-2.24237000	-0.05723600
C	1.08071100	-3.05254900	0.59295500
C	2.58599400	-2.68432300	-1.25544700
C	0.72134100	-4.28685700	0.06349900
H	0.61310800	-2.69155500	1.50843900
C	2.22175600	-3.91901300	-1.78905300
H	3.30363800	-2.06107300	-1.78189300
C	1.29236300	-4.72064900	-1.13119300
H	-0.01962400	-4.89799000	0.56944300
H	2.66309000	-4.25350700	-2.72337100
H	1.00419300	-5.67829300	-1.55469600
C	3.93676400	-1.00508800	1.68251600
C	4.43034200	-2.29849400	1.87368400
C	4.55810400	0.06925900	2.33598100
C	5.52439000	-2.51491400	2.71095300
H	3.95782100	-3.13993900	1.37510100
C	5.65389700	-0.15031600	3.16281800
H	4.16592700	1.07552200	2.21261800

C	6.13507700	-1.44500300	3.35800900
H	5.89909100	-3.52383000	2.85500800
H	6.12393200	0.68914500	3.66614600
H	6.98301400	-1.61767000	4.01381700
C	3.00386900	0.44337500	-0.60152800
C	4.28091900	0.31996100	-1.16198800
C	2.14969500	1.45026100	-1.06415000
C	4.68131400	1.16756300	-2.19005600
H	4.96545800	-0.43242700	-0.77750200
C	2.55055200	2.29666500	-2.09563500
H	1.17434000	1.58479300	-0.59852100
C	3.81427500	2.15271700	-2.66134000
H	5.67331600	1.06511300	-2.61932400
H	1.87900600	3.07520500	-2.44409500
H	4.13110300	2.81615300	-3.46026100
Pd	0.60111900	0.41382900	2.20870900
C	-1.12160200	1.20980500	4.71667500
H	-1.01354800	1.68972900	5.69467200
H	-1.13210100	0.12832900	4.83670100
H	-2.06734400	1.53255700	4.26890000
C	-0.00565100	1.69418900	3.81555900
O	0.05921000	2.84713600	3.42889000
S	1.87526100	1.03677400	4.28498500
C	2.16112000	-0.69651200	4.86910700
H	2.67372900	-1.20318900	4.04366200
C	3.11137500	-0.62176700	6.06175100
H	3.38466100	-1.63303900	6.38537500
H	4.02897500	-0.08737100	5.80041000
H	2.63495200	-0.10303500	6.90042600
C	0.90099300	-1.47796100	5.21479200
H	0.36006100	-1.00690400	6.04225300
H	0.22995000	-1.55016200	4.35134800
H	1.17560200	-2.49378400	5.52228000

4-TS

C	-2.53750100	-3.26022600	-1.26076300
C	-2.55332200	-2.30208100	-0.24664600
C	-1.68172900	-1.21173200	-0.29436600
C	-0.80252000	-1.09588000	-1.37944100
C	-0.79132300	-2.04727400	-2.39094400
C	-1.65916300	-3.13637200	-2.33176100
H	-3.22072900	-4.10298500	-1.21097700
H	-3.25537900	-2.40574700	0.57522800
H	-0.11282000	-0.25519000	-1.43177100
H	-0.09249200	-1.94773700	-3.21557000
H	-1.64299000	-3.88799200	-3.11548800
P	-1.57183800	0.07248900	1.02083800
C	-3.05913200	-0.25991800	2.03967900
C	-4.22641200	0.50425800	1.97787400
C	-2.97449500	-1.30258900	2.97120400
C	-5.28585500	0.23530200	2.84357400
H	-4.30268700	1.32184600	1.26716700
C	-4.03714400	-1.57960100	3.82373400
H	-2.05935800	-1.89004600	3.03260400
C	-5.19375800	-0.80291000	3.76572900
H	-6.18344600	0.84435600	2.79940700
H	-3.95700200	-2.38786300	4.54420100
H	-6.01783200	-1.00424300	4.44308000

C	-1.98648500	1.59320300	0.08228500
C	-1.45264900	2.80848900	0.52717000
C	-2.81133900	1.57294800	-1.04992900
C	-1.74471800	3.98779800	-0.15707200
H	-0.82452300	2.83450700	1.41535100
C	-3.09866700	2.75359400	-1.72731500
H	-3.22124500	0.63092700	-1.40502000
C	-2.56349000	3.96190900	-1.28229800
H	-1.32922300	4.92663600	0.19548000
H	-3.73649200	2.73067500	-2.60562100
H	-2.78619000	4.88157000	-1.81505600
P	2.29606700	-0.81588000	0.71663100
C	1.96922900	-2.36207900	-0.22163600
C	1.02652300	-3.24145300	0.32500900
C	2.59035000	-2.69458600	-1.42734800
C	0.72116400	-4.43859400	-0.31482100
H	0.51368800	-2.96733100	1.24580600
C	2.27783800	-3.88897300	-2.07267800
H	3.31034600	-2.01516400	-1.87346200
C	1.34685500	-4.76255500	-1.51666100
H	-0.02137900	-5.10586900	0.11174600
H	2.76354100	-4.13630300	-3.01200400
H	1.10168600	-5.69068200	-2.02437000
C	3.81068400	-1.23487900	1.66362600
C	4.17365800	-2.55298100	1.95657400
C	4.54501400	-0.18238500	2.22765100
C	5.24997500	-2.81362800	2.80283300
H	3.61711900	-3.37942800	1.52330000
C	5.62088300	-0.44763100	3.06829000
H	4.26570100	0.84587400	2.01551700
C	5.97310000	-1.76395700	3.36188300
H	5.52317800	-3.84148600	3.02195600
H	6.17857900	0.37697100	3.50160200
H	6.80941400	-1.96998400	4.02284300
C	2.93332300	0.36411500	-0.53592700
C	4.21718000	0.26852600	-1.08744500
C	2.09526800	1.40863900	-0.94077500
C	4.63742500	1.17709400	-2.05310200
H	4.89125700	-0.51319700	-0.74543400
C	2.51586700	2.31725300	-1.91006400
H	1.11533400	1.52310600	-0.47972300
C	3.78421700	2.19815600	-2.47050400
H	5.63356400	1.09272700	-2.47669100
H	1.85491100	3.12308900	-2.21388100
H	4.11613800	2.90796600	-3.22207500
Pd	0.51037400	0.27568300	2.22637300
C	-0.92155100	0.65401200	4.93499100
H	-0.31732900	0.67681100	5.84901800
H	-1.00343300	-0.39526200	4.63051900
C	-0.16948100	1.44220100	3.85830100
O	-0.44162600	2.59001400	3.57684400
S	1.93900800	1.12042400	4.04347900
C	2.24669900	-0.47995100	4.86987000
H	2.67555200	-1.20702200	4.17511200
H	2.95393100	-0.30938500	5.68527800
H	1.32203500	-0.88432200	5.29033700
C	-2.29494600	1.26361900	5.19901300
H	-2.82837000	0.68387300	5.95815900

H	-2.18768900	2.29281300	5.54868700
H	-2.90326600	1.28098700	4.29095600

5-TS

C	-2.42901700	-3.17897500	-1.18388800
C	-2.45560900	-2.22817700	-0.16330400
C	-1.61846400	-1.11142300	-0.22177500
C	-0.75944400	-0.96358700	-1.31808700
C	-0.73590100	-1.90953700	-2.33484000
C	-1.57202100	-3.02275100	-2.26827200
H	-3.08431400	-4.04331200	-1.12825800
H	-3.13701200	-2.35679700	0.67274400
H	-0.09507800	-0.10264300	-1.37367500
H	-0.05145200	-1.78748100	-3.16851000
H	-1.54574500	-3.76980000	-3.05602700
P	-1.55468100	0.19353300	1.07586400
C	-2.97062800	-0.26501900	2.15472900
C	-4.25570600	0.26635900	2.01666900
C	-2.72298100	-1.18652600	3.17917300
C	-5.26983900	-0.11161000	2.89358200
H	-4.46234900	0.99146300	1.23505300
C	-3.73927700	-1.57358500	4.04718700
H	-1.72065000	-1.59599600	3.29615200
C	-5.01511100	-1.03011500	3.90859000
H	-6.26121400	0.31715800	2.78395800
H	-3.53298100	-2.28876700	4.83759100
H	-5.80696000	-1.31950500	4.59255700
C	-2.16431300	1.64771600	0.13311600
C	-1.71696700	2.91943900	0.50758100
C	-3.06038700	1.51834100	-0.93635400
C	-2.17629500	4.04721900	-0.17255600
H	-1.00970200	3.03133600	1.32684300
C	-3.51521300	2.64682700	-1.60978500
H	-3.39740200	0.53117600	-1.24273400
C	-3.07374100	3.91332900	-1.22707900
H	-1.82417900	5.02995500	0.12506600
H	-4.21158800	2.53858100	-2.43575200
H	-3.42660200	4.79327400	-1.75669000
P	2.33106100	-0.83036200	0.74885800
C	1.99180300	-2.36322100	-0.20816600
C	1.05877300	-3.25128000	0.34108800
C	2.59891600	-2.68274600	-1.42449300
C	0.75635700	-4.44739300	-0.30224600
H	0.55478400	-2.98890400	1.27009700
C	2.28722500	-3.87495400	-2.07428700
H	3.30799800	-1.99570600	-1.87575200
C	1.37183200	-4.76075000	-1.51218300
H	0.02450000	-5.12321100	0.12943600
H	2.76322500	-4.11149700	-3.02134900
H	1.12970200	-5.68874700	-2.02153600
C	3.81895700	-1.29641600	1.71929900
C	4.12279300	-2.62421600	2.03469600
C	4.58706400	-0.26773200	2.28231000
C	5.17046600	-2.91807200	2.90576400
H	3.54159600	-3.43321500	1.60094500
C	5.63620100	-0.56648300	3.14540100
H	4.35459200	0.76842600	2.05309700
C	5.92579900	-1.89220800	3.46594000

H	5.39692200	-3.95345300	3.14217300
H	6.22207300	0.24025900	3.57588900
H	6.74003200	-2.12294800	4.14601600
C	3.02630100	0.34729800	-0.47617600
C	4.30643700	0.20402900	-1.02701700
C	2.24551600	1.44677600	-0.84857100
C	4.77763300	1.12068400	-1.96105300
H	4.93883100	-0.62110800	-0.70826500
C	2.71808100	2.36496800	-1.78467300
H	1.27210400	1.59653600	-0.38363700
C	3.98057900	2.19841600	-2.34574000
H	5.77019500	0.99960900	-2.38406000
H	2.10365100	3.21569600	-2.06179500
H	4.35246200	2.91560000	-3.07103500
Pd	0.58034500	0.44245600	2.17367100
C	-0.96504800	1.59007400	4.61923100
H	-0.58855600	1.85981700	5.61275100
H	-1.15567500	0.51469300	4.61792400
C	0.12417500	1.92460100	3.60718900
O	0.25549200	3.03501400	3.13178000
S	2.03818200	1.16961200	4.06415600
C	2.24520700	-0.46563100	4.90081500
H	2.67369100	-1.14081500	4.15127100
C	3.25984800	-0.27545000	6.02584800
H	3.47901100	-1.23960000	6.49975100
H	4.19711000	0.13816700	5.64373600
H	2.86536500	0.40691700	6.78636100
C	0.95046100	-1.07321300	5.42471600
H	0.47742600	-0.41703200	6.16299300
H	0.23952100	-1.25044300	4.61073600
H	1.16390100	-2.03366900	5.90881900
C	-2.23178300	2.37840300	4.29613100
H	-2.55084300	2.20393000	3.26387800
H	-3.05046600	2.07541100	4.95552400
H	-2.05415200	3.44980900	4.41201600

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C	-3.01132700	-3.02794300	-0.98834700
C	-2.91281500	-2.01477700	-0.03478700
C	-1.82648600	-1.13764700	-0.04498300
C	-0.85613800	-1.27751900	-1.04706100
C	-0.96034400	-2.27953500	-2.00383900
C	-2.03575800	-3.16666100	-1.96941900
H	-3.86107900	-3.70350800	-0.96445300
H	-3.69224500	-1.90708500	0.71196400
H	-0.00982700	-0.59390900	-1.08059700
H	-0.19230500	-2.37748300	-2.76464100
H	-2.11400100	-3.95752400	-2.70929500
P	-1.56075100	0.19058300	1.20108000
C	-3.06693100	0.15357500	2.24099000
C	-3.90221800	1.26322300	2.37695700
C	-3.32135000	-0.98997700	3.01135100
C	-4.98909800	1.22028100	3.24896800
H	-3.70378400	2.16609000	1.80779900
C	-4.41774500	-1.03806600	3.86350400
H	-2.65282400	-1.84607700	2.94779800
C	-5.25481300	0.07034700	3.98451500
H	-5.63042300	2.09084900	3.34718100

H	-4.60279700	-1.93130800	4.45224300
H	-6.10503100	0.03916300	4.65915900
C	-1.75011400	1.71073800	0.18250500
C	-1.19435600	2.90318000	0.66711400
C	-2.40631100	1.70858300	-1.05233300
C	-1.29123600	4.07173400	-0.08535600
H	-0.70796300	2.91665400	1.64112900
C	-2.49357100	2.87880800	-1.80222500
H	-2.84120200	0.78932000	-1.43386000
C	-1.93300200	4.06001500	-1.32183100
H	-0.86123000	4.99179300	0.29815000
H	-3.00055800	2.86622000	-2.76236800
H	-1.99934300	4.97132700	-1.90875500
P	2.37323100	-0.52463400	0.88131300
C	2.03835900	-2.18430400	0.17174600
C	1.16171000	-3.00283400	0.89421200
C	2.55088600	-2.64332300	-1.04490600
C	0.80863800	-4.26024300	0.41667800
H	0.72998900	-2.62998200	1.82206300
C	2.19062000	-3.90016100	-1.52694400
H	3.21700700	-2.01303000	-1.62750700
C	1.31998500	-4.70819400	-0.79929500
H	0.11827200	-4.87944100	0.98087500
H	2.58677400	-4.24632600	-2.47705300
H	1.03266400	-5.68213100	-1.18380100
C	3.93185200	-0.76175500	1.81790000
C	4.49260300	-2.01586800	2.07218600
C	4.50659000	0.37743700	2.40011700
C	5.60988400	-2.12979200	2.89924200
H	4.05679200	-2.90652300	1.62816400
C	5.62520200	0.25990800	3.21644100
H	4.06171400	1.35462700	2.22746600
C	6.17616800	-0.99571100	3.47277000
H	6.03784000	-3.10912400	3.09121000
H	6.06006800	1.14873900	3.66337400
H	7.04384200	-1.08684900	4.11896800
C	2.90546700	0.49962700	-0.54186200
C	4.18070200	0.40595300	-1.11187600
C	1.99293300	1.42870600	-1.05393000
C	4.52508200	1.20903500	-2.19456100
H	4.90579300	-0.28902600	-0.69486400
C	2.33823200	2.22982600	-2.14041600
H	1.01491200	1.54007000	-0.58857800
C	3.60225800	2.11786100	-2.71239200
H	5.51591000	1.13067400	-2.63154500
H	1.62053200	2.94743900	-2.52583700
H	3.87551600	2.74564700	-3.55496800
Pd	0.54887300	0.38630500	2.36064500
C	-0.34547300	1.29344400	4.06420500
O	-0.85795100	2.38308100	3.85505100
S	1.69336000	1.42344300	4.29968500
C	2.41975800	-0.03019900	5.13471600
H	2.74210400	-0.79368100	4.42158000
H	3.29685100	0.32964700	5.67833300
H	1.71400200	-0.45534000	5.85193800
C	-0.98742800	0.27834800	4.97199100
C	-0.62734000	-1.07170800	4.99130800
C	-2.03824000	0.72041100	5.77901700

C	-1.29607200	-1.96487900	5.82362600
H	0.16596800	-1.42512800	4.33549400
C	-2.69968700	-0.17061500	6.61630900
H	-2.32526300	1.76543800	5.72162900
C	-2.32832300	-1.51400700	6.64401700
H	-1.01061500	-3.01275500	5.83217700
H	-3.51651900	0.17948000	7.24070000
H	-2.84643600	-2.20983900	7.29758500

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C	-3.01325400	-3.02320700	-0.99293500
C	-2.91212500	-2.01161700	-0.03794100
C	-1.82388500	-1.13679800	-0.04703700
C	-0.85444500	-1.27738300	-1.04990600
C	-0.96129400	-2.27764600	-2.00822900
C	-2.03851000	-3.16261100	-1.97469400
H	-3.86451900	-3.69690000	-0.96965900
H	-3.69128800	-1.90331400	0.70897600
H	-0.00665000	-0.59562500	-1.08291700
H	-0.19391400	-2.37584800	-2.76965900
H	-2.11882300	-3.95216300	-2.71575000
P	-1.55402300	0.18982200	1.20044900
C	-3.06017200	0.15401900	2.24078700
C	-3.89082400	1.26643400	2.38252200
C	-3.31850600	-0.99156000	3.00678000
C	-4.97695900	1.22419400	3.25546000
H	-3.68913200	2.17101000	1.81727400
C	-4.41386000	-1.03872700	3.86031300
H	-2.65380200	-1.85022000	2.93839700
C	-5.24646800	0.07239000	3.98672200
H	-5.61464800	2.09694400	3.35799900
H	-4.60184500	-1.93373500	4.44544000
H	-6.09607400	0.04179800	4.66217500
C	-1.74507700	1.71035200	0.18224500
C	-1.18456200	2.90182800	0.66352200
C	-2.40795900	1.70932400	-1.04905400
C	-1.28332200	4.07050400	-0.08855200
H	-0.69323700	2.91449300	1.63501900
C	-2.49724500	2.87957800	-1.79860800
H	-2.84666200	0.79078300	-1.42799100
C	-1.93190700	4.05984600	-1.32146300
H	-0.84966500	4.98985300	0.29256000
H	-3.00960500	2.86781200	-2.75590400
H	-1.99990800	4.97123700	-1.90808900
P	2.37984800	-0.53047600	0.87952600
C	2.03542300	-2.18988100	0.17282100
C	1.15747800	-3.00426300	0.89825800
C	2.54393500	-2.65265200	-1.04415500
C	0.79867800	-4.26102500	0.42301400
H	0.72965700	-2.62879200	1.82678800
C	2.17816400	-3.90874300	-1.52377700
H	3.21113300	-2.02563300	-1.62900200
C	1.30581000	-4.71248500	-0.79337500
H	0.10720600	-4.87693800	0.98944400
H	2.57119500	-4.25761900	-2.47418800
H	1.01393800	-5.68578500	-1.17603600
C	3.95078800	-0.77240800	1.79459600
C	4.50923700	-2.02830000	2.04398200

C	4.54495600	0.36649600	2.35811800
C	5.64348200	-2.14495600	2.84746300
H	4.05894900	-2.91858700	1.61402600
C	5.68501600	0.24658100	3.14410700
H	4.10310700	1.34584700	2.18865800
C	6.23252400	-1.01136700	3.39789500
H	6.06829000	-3.12616300	3.03682300
H	6.14051500	1.13574500	3.56990300
H	7.11569100	-1.10353000	4.02256000
C	2.90279300	0.49082100	-0.55001100
C	4.17289100	0.39292700	-1.13083400
C	1.98878500	1.42184000	-1.05589500
C	4.51043700	1.19333700	-2.21762900
H	4.89975800	-0.30323700	-0.71894400
C	2.32713100	2.22031600	-2.14658200
H	1.01494600	1.53671900	-0.58277100
C	3.58589500	2.10397700	-2.72914800
H	5.49738200	1.11143700	-2.66270000
H	1.60809000	2.93923200	-2.52707900
H	3.85383000	2.72969300	-3.57496900
Pd	0.56211100	0.38488700	2.35902100
C	-0.33802000	1.29977600	4.06781500
O	-0.86378500	2.38173700	3.84883700
S	1.68281400	1.44748300	4.29992800
C	2.44181900	0.01873800	5.16408000
H	2.85330600	-0.67811700	4.42637100
H	1.66866500	-0.49617900	5.74082800
C	-0.98171800	0.27705300	4.96673200
C	-0.62861400	-1.07512400	4.97205200
C	-2.02839700	0.71593900	5.78080700
C	-1.29792600	-1.97270600	5.79923600
H	0.15966700	-1.42669900	4.30877800
C	-2.69045500	-0.17956100	6.61295900
H	-2.31182600	1.76245000	5.73352600
C	-2.32461400	-1.52463900	6.62798700
H	-1.01749500	-3.02197100	5.79670300
H	-3.50349900	0.16872500	7.24326100
H	-2.84312600	-2.22386700	7.27758500
C	3.53955000	0.52573400	6.09303000
H	3.12726000	1.20357700	6.84574700
H	4.01842300	-0.31630300	6.60362300
H	4.30853100	1.06349800	5.53159300

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C	-3.08585000	-3.01820600	-0.98893900
C	-2.96460600	-1.99482000	-0.04916100
C	-1.82426200	-1.18832700	-0.02759100
C	-0.82349400	-1.40784000	-0.98368600
C	-0.95055500	-2.41940800	-1.92773600
C	-2.08035400	-3.23658500	-1.92452400
H	-3.97649000	-3.63917300	-0.99064700
H	-3.76670900	-1.82394400	0.66097200
H	0.05855700	-0.77230200	-1.00253800
H	-0.16145400	-2.57404100	-2.65671100
H	-2.17864900	-4.03374400	-2.65499300
P	-1.53469800	0.15703400	1.19226800
C	-3.06363700	0.21832600	2.19822600
C	-3.81568800	1.38681300	2.32770600

C	-3.40316900	-0.89964900	2.97231000
C	-4.89807000	1.43045100	3.20452000
H	-3.55340400	2.26922500	1.75282800
C	-4.48936400	-0.85809700	3.83798800
H	-2.80461700	-1.80526000	2.90611000
C	-5.23914600	0.31092100	3.95627900
H	-5.47263200	2.34674600	3.29867500
H	-4.73518900	-1.73047700	4.43522500
H	-6.08045200	0.34998500	4.64149800
C	-1.61685600	1.66669200	0.14556900
C	-1.08385700	2.85586900	0.66490600
C	-2.13444600	1.65375900	-1.15287600
C	-1.06809700	4.00970700	-0.11485600
H	-0.69328200	2.87579500	1.68112200
C	-2.10551400	2.80952400	-1.93099200
H	-2.54945200	0.73863400	-1.56449600
C	-1.57011500	3.98706300	-1.41487400
H	-0.65500200	4.92612500	0.29482500
H	-2.50366600	2.78728400	-2.94093000
H	-1.54780000	4.88643900	-2.02303300
P	2.42046100	-0.45266600	0.86157000
C	2.14045900	-2.15653600	0.23265800
C	1.35928500	-2.99683400	1.03525600
C	2.60024500	-2.62908200	-1.00001200
C	1.04513600	-4.28610000	0.61778300
H	0.97662900	-2.62071600	1.98321000
C	2.28070300	-3.91856100	-1.42032600
H	3.19471000	-1.98478800	-1.64160200
C	1.50094300	-4.74628200	-0.61535600
H	0.42967900	-4.92331600	1.24498500
H	2.63758400	-4.27500400	-2.38211300
H	1.24468100	-5.74654600	-0.95081300
C	4.06554600	-0.55044600	1.66331300
C	4.80586500	-1.72877100	1.77808300
C	4.56194000	0.63220900	2.22822200
C	6.02876400	-1.72333800	2.44917900
H	4.42928900	-2.65233600	1.34748400
C	5.78887100	0.63701000	2.88031200
H	3.97422700	1.54513500	2.17252200
C	6.52234300	-0.54338700	2.99737200
H	6.59568300	-2.64508900	2.53889900
H	6.16324300	1.55842100	3.31538400
H	7.47378100	-0.54293600	3.52029200
C	2.80803500	0.52758000	-0.64371400
C	4.05866500	0.47755200	-1.27215900
C	1.81770500	1.36606400	-1.16504900
C	4.29962000	1.22927100	-2.41758000
H	4.84712200	-0.14321500	-0.85320400
C	2.05927900	2.11741900	-2.31378400
H	0.85677800	1.44918800	-0.66321200
C	3.29866300	2.04660300	-2.94220200
H	5.27239100	1.18329100	-2.89782500
H	1.27829900	2.76478700	-2.70089600
H	3.49294100	2.63591000	-3.83324000
Pd	0.54664400	0.29332300	2.46809400
C	-0.45074900	1.15465300	4.05871100
O	-0.85519600	2.28363300	3.84527100
S	1.70165000	1.10637300	4.48725900

C	2.11930000	-0.34652400	5.54674700
H	1.52359200	-1.19864800	5.21291100
C	-1.16353500	0.22610600	5.00486900
C	-0.98432600	-1.15814600	4.99128700
C	-2.07546600	0.79240300	5.89806400
C	-1.68132200	-1.96665500	5.88359600
H	-0.31393700	-1.59952900	4.25636300
C	-2.77435800	-0.01541300	6.78895700
H	-2.22130400	1.86760400	5.87308000
C	-2.57316500	-1.39499100	6.78950200
H	-1.53361200	-3.04251900	5.86886500
H	-3.48049600	0.42957100	7.48377700
H	-3.11602400	-2.02441300	7.48859800
C	3.59702200	-0.69402100	5.38722700
H	4.22764700	0.16666200	5.63493000
H	3.86010400	-1.51635000	6.06399700
H	3.82683200	-0.99785000	4.36259000
C	1.76589300	-0.03169000	6.99733800
H	0.69773400	0.17646000	7.10850600
H	2.02568400	-0.87945700	7.64279200
H	2.32395800	0.84623100	7.34049400

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C	2.99709200	-3.02271400	-0.98945500
C	-2.90021500	-2.01222200	-0.03292500
C	-1.81735100	-1.13071800	-0.04256500
C	-0.84873100	-1.26392200	-1.04714500
C	-0.95089400	-2.26370900	-2.00654600
C	-2.02297200	-3.15487100	-1.97286900
H	-3.84442300	-3.70137100	-0.96599900
H	-3.67833900	-1.90993000	0.71597700
H	-0.00471500	-0.57744600	-1.07986700
H	-0.18344300	-2.35713700	-2.76855800
H	-2.09969400	-3.94384500	-2.71494600
P	-1.55564200	0.19494300	1.20793700
C	-3.05866400	0.13634500	2.25173300
C	-3.91358100	1.23054500	2.38933700
C	-3.29194300	-1.01211800	3.02165300
C	-4.99904300	1.16651300	3.26245500
H	-3.73209200	2.13748300	1.82077400
C	-4.38470700	-1.08074500	3.87696900
H	-2.60756100	-1.85551300	2.95484400
C	-5.24242400	0.01216400	3.99839400
H	-5.65639700	2.02489000	3.36206100
H	-4.55177200	-1.97448900	4.47138900
H	-6.08894900	-0.03429200	4.67668800
C	-1.76425700	1.71641600	0.19547100
C	-1.20609900	2.90950700	0.67520200
C	-2.43761400	1.71461800	-1.03027300
C	-1.31767200	4.07950600	-0.07303700
H	-0.70612900	2.92236700	1.64225900
C	-2.53991600	2.88626600	-1.77574600
H	-2.87406900	0.79438300	-1.40780100
C	-1.97684800	4.06838500	-1.30023700
H	-0.88564200	5.00021400	0.30662700
H	-3.06030100	2.87430500	-2.72868000
H	-2.05481700	4.98090800	-1.88387700
P	2.37770000	-0.53360100	0.88327000

C	2.03751500	-2.19114700	0.17053900
C	1.15248400	-3.00507100	0.88791400
C	2.55418000	-2.65305200	-1.04326900
C	0.79563400	-4.26075900	0.40862100
H	0.71700300	-2.62911700	1.81280000
C	2.19007300	-3.90798700	-1.52730200
H	3.22660400	-2.02630600	-1.62243500
C	1.31150300	-4.71160600	-0.80434200
H	0.09832700	-4.87614900	0.96849100
H	2.58948200	-4.25616500	-2.47530600
H	1.02124600	-5.68406100	-1.19040500
C	3.93700500	-0.77761100	1.81673000
C	4.48423100	-2.03533600	2.08243500
C	4.52511400	0.36065600	2.38737900
C	5.60119900	-2.15378100	2.90919400
H	4.03844200	-2.92524300	1.64684800
C	5.64338800	0.23843300	3.20353100
H	4.09079000	1.34099600	2.20609700
C	6.18082900	-1.02061900	3.47119000
H	6.01889000	-3.13587400	3.10966300
H	6.08840400	1.12663300	3.64165400
H	7.04838200	-1.11519300	4.11707700
C	2.91188900	0.49244600	-0.53800200
C	4.18490700	0.39403100	-1.11225400
C	2.00333800	1.42902100	-1.04341900
C	4.53047800	1.19923300	-2.19295300
H	4.90766400	-0.30594600	-0.69958900
C	2.34971000	2.23231600	-2.12796400
H	1.02764400	1.54432500	-0.57408200
C	3.61118400	2.11517400	-2.70451900
H	5.51956600	1.11709200	-2.63317500
H	1.63491900	2.95549700	-2.50837300
H	3.88533000	2.74452900	-3.54563100
Pd	0.56076000	0.39473400	2.36324200
C	-0.32339300	1.31368700	4.06710100
O	-0.83197400	2.40458800	3.85755900
S	1.72664700	1.44225500	4.28274700
C	2.45100000	-0.00411300	5.13097000
H	2.76744700	-0.77794600	4.42614500
H	3.33190700	0.35723500	5.66743400
H	1.74621400	-0.41703500	5.85650500
C	-0.96385500	0.30266800	4.97218800
C	-0.60482600	-1.04532000	5.00387900
C	-2.03457600	0.73575900	5.76267800
C	-1.29087100	-1.94483300	5.81369600
H	0.20198600	-1.40352300	4.36775900
C	-2.71747300	-0.14846400	6.58122200
H	-2.32530800	1.77967400	5.70359200
C	-2.34833300	-1.49516000	6.60411600
H	-1.01068100	-2.99615600	5.82593500
H	-3.55545600	0.17150000	7.19170100
O	-3.07172800	-2.33000700	7.40016300
H	-2.68983400	-3.21810500	7.35816500

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C	-3.00217300	-3.01387600	-0.99942100
C	-2.90411500	-2.00438300	-0.04200200
C	-1.81710000	-1.12792300	-0.04718700

C	-0.84593600	-1.26452600	-1.04880500
C	-0.94936300	-2.26319300	-2.00925200
C	-2.02526600	-3.14982600	-1.97953900
H	-3.85244600	-3.68891000	-0.97905900
H	-3.68437800	-1.89933800	0.70420800
H	0.00093800	-0.58155300	-1.07864700
H	-0.18004800	-2.35912500	-2.76903100
H	-2.10283600	-3.93818900	-2.72215900
P	-1.55369000	0.19742300	1.20312800
C	-3.05529800	0.14067200	2.24917000
C	-3.90040200	1.24110700	2.39874000
C	-3.29673200	-1.01261500	3.00901700
C	-4.98491000	1.17849000	3.27282200
H	-3.71198600	2.15166500	1.83832400
C	-4.39058200	-1.08033200	3.86295500
H	-2.62019400	-1.86149200	2.93459600
C	-5.23851100	0.01843100	3.99663600
H	-5.63437800	2.04171600	3.38181900
H	-4.56670600	-1.98279400	4.44119400
H	-6.08711900	-0.02770000	4.67255500
C	-1.76149800	1.71911500	0.19065100
C	-1.20122400	2.91184600	0.66880900
C	-2.43531800	1.71701200	-1.03483000
C	-1.31125100	4.08117200	-0.08070800
H	-0.70089900	2.92497700	1.63565300
C	-2.53604900	2.88798300	-1.78157700
H	-2.87310600	0.79698900	-1.41132700
C	-1.97089200	4.06972200	-1.30765800
H	-0.87748800	5.00158900	0.29768700
H	-3.05667400	2.87570500	-2.73437600
H	-2.04745600	4.98166000	-1.89239600
P	2.37898500	-0.52821400	0.88365500
C	2.03784700	-2.18831700	0.17785700
C	1.15617200	-3.00081900	0.90104900
C	2.55040300	-2.65311000	-1.03657100
C	0.79809400	-4.25790400	0.42625400
H	0.72479000	-2.62361900	1.82733500
C	2.18508000	-3.90948100	-1.51593100
H	3.22040100	-2.02748200	-1.61972400
C	1.30939700	-4.71147300	-0.78765800
H	0.10395600	-4.87242400	0.99094900
H	2.58126100	-4.26002300	-2.46441800
H	1.01814900	-5.68507600	-1.17002800
C	3.93833900	-0.76805100	1.81795300
C	4.49058500	-2.02406400	2.08123000
C	4.52159400	0.37156500	2.39077800
C	5.60797000	-2.13946100	2.90787500
H	4.04807600	-2.91503900	1.64452400
C	5.64026200	0.25240400	3.20680300
H	4.08286800	1.35036800	2.21182600
C	6.18281400	-1.00496900	3.47205600
H	6.02932000	-3.12025300	3.10693600
H	6.08140500	1.14154900	3.64689600
H	7.05049100	-1.09722200	4.11810600
C	2.91215800	0.49246400	-0.54187400
C	4.18491400	0.39184200	-1.11631200
C	2.00321000	1.42678100	-1.05071100
C	4.52983200	1.19269600	-2.20046800

H	4.90786500	-0.30655400	-0.70130500
C	2.34895800	2.22576800	-2.13863300
H	1.02759500	1.54363900	-0.58161200
C	3.61019400	2.10646600	-2.71528100
H	5.51868900	1.10883800	-2.64088500
H	1.63387500	2.94729900	-2.52161600
H	3.88386800	2.73244900	-3.55905800
Pd	0.55911300	0.39748400	2.36158700
C	-0.33339600	1.31015100	4.05751700
O	-0.84038400	2.40206000	3.84974700
S	1.71865100	1.43495300	4.28916500
C	2.44121800	-0.01815400	5.12802800
H	2.76495000	-0.78313700	4.41701900
H	3.31696200	0.34044600	5.67471500
H	1.73223500	-0.44175300	5.84313800
C	-0.97389000	0.29935800	4.96762900
C	-0.61970100	-1.05021100	4.99385300
C	-2.03293800	0.73807600	5.76748200
C	-1.30381900	-1.94174900	5.81605400
H	0.17805900	-1.41028000	4.34698500
C	-2.70392500	-0.15405100	6.59107900
H	-2.32217200	1.78260200	5.71059700
C	-2.35068500	-1.50749200	6.63041500
H	-1.02267800	-2.99220900	5.82202500
H	-3.53258700	0.19610900	7.20290700
C	-3.09359400	-2.46496800	7.52660400
H	-2.86858900	-2.27313400	8.58144200
H	-4.17672000	-2.36010600	7.40228900
H	-2.82543900	-3.50277200	7.31127600

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C	-2.99604600	-3.01185800	-0.99924000
C	-2.89740400	-2.00347900	-0.04068800
C	-1.81290500	-1.12393200	-0.04814500
C	-0.84465500	-1.25675400	-1.05310700
C	-0.94868500	-2.25427700	-2.01466400
C	-2.02219500	-3.14373500	-1.98287000
H	-3.84427700	-3.68938800	-0.97670300
H	-3.67556800	-1.90201900	0.70818400
H	0.00067200	-0.57191600	-1.08457700
H	-0.18133700	-2.34736200	-2.77678700
H	-2.10007200	-3.93128300	-2.72632900
P	-1.54817800	0.19986900	1.20413000
C	-3.05122900	0.13880200	2.24851800
C	-3.90466100	1.23336100	2.39291900
C	-3.28661800	-1.01406800	3.01084600
C	-4.99186400	1.16425800	3.26334100
H	-3.72120400	2.14400000	1.83095600
C	-4.38118300	-1.08822800	3.86354200
H	-2.60469800	-1.85876300	2.93886700
C	-5.23851000	0.00440100	3.98988800
H	-5.64930000	2.02215900	3.36680800
H	-4.54873500	-1.98925600	4.44703900
H	-6.09016200	-0.04616800	4.66186700
C	-1.76110700	1.72216500	0.19341700
C	-1.19824500	2.91444500	0.66938400
C	-2.44230700	1.72120000	-1.02805500
C	-1.31296000	4.08455700	-0.07826700

H	-0.69228000	2.92653300	1.63328200
C	-2.54793100	2.89289700	-1.77288900
H	-2.88210700	0.80136100	-1.40272300
C	-1.98012600	4.07428700	-1.30113000
H	-0.87704700	5.00467000	0.29841900
H	-3.07435900	2.88155200	-2.72250000
H	-2.06050000	4.98684300	-1.88441100
P	2.38128300	-0.53858500	0.88406400
C	2.02822600	-2.19626800	0.17761200
C	1.14262600	-3.00395400	0.90126100
C	2.53860900	-2.66447800	-1.03645200
C	0.77837400	-4.25969600	0.42731500
H	0.71375900	-2.62441400	1.82770500
C	2.16716800	-3.91924900	-1.51504100
H	3.21176100	-2.04266400	-1.61999800
C	1.28754300	-4.71649500	-0.78624200
H	0.08148100	-4.87053700	0.99258700
H	2.56174500	-4.27233900	-2.46325400
H	0.99168100	-5.68899500	-1.16786200
C	3.95069700	-0.78883600	1.79902200
C	4.48918800	-2.04954300	2.06718000
C	4.56150400	0.34862900	2.34735300
C	5.62001100	-2.17243000	2.87441500
H	4.02586200	-2.93875600	1.64902400
C	5.69812800	0.22205700	3.13729300
H	4.13511500	1.33218200	2.16356800
C	6.22555100	-1.04041700	3.41003300
H	6.02910700	-3.15734400	3.07862600
H	6.16636400	1.10997600	3.55171200
H	7.10583200	-1.13746800	4.03804500
C	2.90893800	0.48178500	-0.54447000
C	4.17612200	0.37461300	-1.13012800
C	2.00184300	1.42292400	-1.04391700
C	4.51679600	1.17518700	-2.21580900
H	4.89858700	-0.32853100	-0.72239900
C	2.34315200	2.22164000	-2.13350700
H	1.03104900	1.54513300	-0.56630200
C	3.59853200	2.09550000	-2.72132200
H	5.50140900	1.08597600	-2.66462100
H	1.62914700	2.94807800	-2.50921200
H	3.86885900	2.72116100	-3.56642100
Pd	0.57109500	0.39986100	2.36272100
C	-0.32072200	1.32501800	4.06382200
O	-0.83843500	2.41131000	3.84783100
S	1.71705700	1.46579800	4.28350800
C	2.46793200	0.03970300	5.15782300
H	2.87568800	-0.66599200	4.42635300
H	1.69188000	-0.46597200	5.73919400
C	-0.96385700	0.31021300	4.96388900
C	-0.62106400	-1.04579100	4.98111000
C	-2.02127300	0.74775300	5.76370000
C	-1.30772100	-1.94575300	5.78486900
H	0.17702500	-1.40531200	4.33413300
C	-2.70619400	-0.14036500	6.58100600
H	-2.30380800	1.79446000	5.71596500
C	-2.35368700	-1.49065300	6.58855200
H	-1.05678100	-3.00114400	5.80059500
H	-3.53708000	0.20534200	7.19296800

C	3.56825400	0.54611100	6.08410700
H	3.15950200	1.23164600	6.83181400
H	4.04214300	-0.29504400	6.60084700
H	4.34037100	1.07580800	5.51932700
O	-3.01158900	-2.41327800	7.34359100
H	-3.68662100	-1.96396500	7.87172100

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C	-2.96391200	-2.93528900	-1.06914900
C	-2.86545500	-1.95672100	-0.08051700
C	-1.77454800	-1.08474000	-0.05451500
C	-0.80208700	-1.19161000	-1.05767400
C	-0.90445500	-2.16146400	-2.04755000
C	-1.98285600	-3.04529100	-2.04835300
H	-3.81655100	-3.60748100	-1.07228000
H	-3.64825200	-1.87376500	0.66571500
H	0.04662100	-0.51068000	-1.06433600
H	-0.13173200	-2.23772600	-2.80612000
H	-2.05948800	-3.81158500	-2.81377600
P	-1.52265900	0.21174500	1.22848300
C	-2.98709500	0.04610800	2.31521900
C	-3.86659800	1.10350100	2.55288000
C	-3.16710100	-1.16026200	3.00718100
C	-4.92574400	0.94482400	3.44708600
H	-3.72529300	2.05224400	2.04390600
C	-4.23617500	-1.32369600	3.87882400
H	-2.46754000	-1.98002200	2.85279200
C	-5.11933000	-0.26682000	4.10198000
H	-5.60359600	1.77380800	3.62611800
H	-4.37180600	-2.26856200	4.39763700
H	-5.94563200	-0.38890600	4.79566000
C	-1.83028500	1.74947900	0.27111200
C	-1.22882400	2.93751400	0.70478700
C	-2.63127900	1.75932500	-0.87652900
C	-1.42491100	4.11742300	-0.01015200
H	-0.63264100	2.94112400	1.61437700
C	-2.81993800	2.94048700	-1.58774100
H	-3.09890200	0.84008400	-1.21867200
C	-2.21391000	4.11945300	-1.15769800
H	-0.95853100	5.03532000	0.33398700
H	-3.43855600	2.93924000	-2.47989900
H	-2.36026800	5.03971500	-1.71533300
P	2.40202500	-0.56984700	0.91629700
C	2.00708700	-2.22099000	0.21924300
C	1.09158900	-2.99867500	0.93843000
C	2.51819900	-2.71107800	-0.98560200
C	0.69671800	-4.24653300	0.46780100
H	0.66475800	-2.60248600	1.85902000
C	2.11657400	-3.95768900	-1.46078000
H	3.21510400	-2.11223500	-1.56505800
C	1.20613300	-4.72467900	-0.73746700
H	-0.02358100	-4.83402100	1.02843500
H	2.51174700	-4.32789400	-2.40207600
H	0.88676700	-5.69061200	-1.11652300
C	3.95703800	-0.85255900	1.84537500
C	4.44646800	-2.12578300	2.14555200
C	4.60822100	0.27442800	2.36775300
C	5.56980400	-2.27130800	2.95949600

H	3.95132100	-3.00662200	1.74657000
C	5.73826000	0.12450900	3.16303300
H	4.21961100	1.26869300	2.15778100
C	6.21685500	-1.15000800	3.46823700
H	5.94033800	-3.26552200	3.19007400
H	6.24074400	1.00372000	3.55528000
H	7.09187500	-1.26491900	4.10051900
C	2.96082200	0.43597900	-0.50952400
C	4.22063100	0.28432500	-1.10193900
C	2.08746200	1.41297800	-0.99905500
C	4.58457300	1.07628700	-2.18629300
H	4.91995200	-0.44539300	-0.70059700
C	2.45241600	2.20371600	-2.08673300
H	1.12439500	1.56746900	-0.51517000
C	3.69855000	2.03242100	-2.68257300
H	5.56276800	0.95307500	-2.64085000
H	1.76498800	2.95828400	-2.45613100
H	3.98699500	2.65110000	-3.52671500
Pd	0.60596400	0.42634900	2.37562600
C	-0.27895000	1.37624700	4.04239800
O	-0.80657300	2.45903500	3.82836200
S	1.75427900	1.51763900	4.27781000
C	2.53287400	0.12645100	5.18765700
H	2.91932700	-0.60964100	4.47498500
H	1.78002100	-0.35366400	5.81859900
C	-0.92154600	0.37324400	4.96901400
C	-0.52808800	-0.96719600	5.04611400
C	-2.02051500	0.81732800	5.70968700
C	-1.20997600	-1.85572400	5.86690000
H	0.29785200	-1.32214500	4.43448800
C	-2.71469300	-0.05794400	6.53222100
H	-2.32554700	1.85268100	5.60335000
C	-2.29298900	-1.38012900	6.59529200
H	-0.93157100	-2.89989600	5.93976400
H	-3.58099100	0.25501100	7.10231100
C	3.65968700	0.67750900	6.05482000
H	3.27121500	1.38964200	6.78817600
H	4.15580700	-0.14000900	6.58797000
H	4.40852000	1.18850000	5.44375000
N	-3.05265800	-2.32571800	7.42215800
O	-4.05806800	-1.91367400	7.97233100
O	-2.63832000	-3.46888700	7.49884100

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C	-2.97167700	-2.91834100	-1.14042300
C	-2.82946800	-1.98020100	-0.11773700
C	-1.75320400	-1.09082700	-0.11884400
C	-0.83286300	-1.14523600	-1.17445800
C	-0.98288100	-2.07022300	-2.19984900
C	-2.05085700	-2.96716300	-2.18037300
H	-3.81342400	-3.60425600	-1.12366900
H	-3.56858500	-1.94042700	0.67557500
H	0.01332700	-0.46066400	-1.19139200
H	-0.25468900	-2.10308200	-3.00428700
H	-2.16256200	-3.69908600	-2.97470800
P	-1.45631700	0.17399600	1.18840200
C	-2.88124200	-0.03668800	2.31846700
C	-3.79159600	0.98809100	2.57811400

C	-2.99094000	-1.24321500	3.02378300
C	-4.82014800	0.79297600	3.49998900
H	-3.69378100	1.94074700	2.06689200
C	-4.02556000	-1.44194400	3.92865900
H	-2.25818400	-2.03144200	2.85948500
C	-4.94621900	-0.42121800	4.16619200
H	-5.52523200	1.59578800	3.69328100
H	-4.09964000	-2.38257700	4.46596500
H	-5.74975900	-0.57026300	4.88130300
C	-1.83675000	1.71885300	0.26656000
C	-1.15238600	2.89302100	0.59900100
C	-2.78690500	1.74551400	-0.76125100
C	-1.41272700	4.07458700	-0.09318300
H	-0.43922000	2.88621100	1.41889900
C	-3.04363600	2.92694700	-1.44940800
H	-3.31984900	0.83678800	-1.02873300
C	-2.35400700	4.09240100	-1.11811200
H	-0.87770200	4.98042300	0.17428000
H	-3.77931300	2.93735900	-2.24805800
H	-2.55330400	5.01297100	-1.65856500
P	2.50421600	-0.68736600	0.89296500
C	1.96000000	-2.25106700	0.09356200
C	0.99725000	-3.00411000	0.77533500
C	2.41664200	-2.69940000	-1.14947700
C	0.50077200	-4.18358500	0.23079900
H	0.61306400	-2.63860200	1.72666800
C	1.92195400	-3.88283200	-1.69412500
H	3.15129900	-2.11712600	-1.69965700
C	0.96282000	-4.62346500	-1.00744500
H	-0.26219900	-4.74553300	0.76055100
H	2.28051600	-4.22177300	-2.66165000
H	0.56677200	-5.53637900	-1.44195900
C	4.07454000	-1.16466300	1.71852100
C	4.75044300	-2.36316000	1.46873200
C	4.59263100	-0.27234100	2.66618600
C	5.92904700	-2.65661500	2.15189400
H	4.35390500	-3.07124300	0.74652000
C	5.76530500	-0.57006600	3.35436800
H	4.07156100	0.65999000	2.87853800
C	6.43523700	-1.76398900	3.09362300
H	6.44691200	-3.59010400	1.95225800
H	6.12183400	0.12401700	4.10743600
H	7.34669900	-2.00379400	3.63281300
C	3.07963900	0.34789400	-0.51093300
C	4.33961100	0.20284900	-1.10193000
C	2.21167100	1.33646800	-0.98836100
C	4.71063800	1.01321900	-2.17122500
H	5.03450900	-0.53773900	-0.71346600
C	2.58225700	2.14374800	-2.06105900
H	1.24721500	1.48551500	-0.50528200
C	3.83092500	1.98019600	-2.65508100
H	5.69089400	0.89471200	-2.62284500
H	1.89830600	2.90647300	-2.42057200
H	4.12472300	2.61303800	-3.48688800
Pd	0.69106000	0.38517500	2.29217700
C	-0.27956400	1.43092200	3.99040500
O	-0.94853200	2.40761500	3.68202900
S	1.63913000	1.80432300	4.13528100

C	2.45721400	0.64106800	5.29407500
H	2.96077900	-0.15622400	4.74609800
H	1.71682000	0.20889600	5.96996100
C	-0.80482700	0.37856100	4.93197400
C	-0.27395500	-0.91134000	5.04106900
C	-1.91983500	0.72925600	5.69770400
C	-0.83812000	-1.82865400	5.92311300
H	0.57445500	-1.20186200	4.42352700
C	-2.47315300	-0.18482200	6.58799400
H	-2.34352400	1.71949600	5.56499800
C	-1.93145000	-1.46305800	6.70647900
H	-0.42017100	-2.82769800	6.00183600
H	-3.34062400	0.09512600	7.17836300
H	-2.36442300	-2.17714100	7.40072100
C	3.53678800	1.41829700	6.03494400
O	4.69768700	1.37027900	5.65162000
N	3.13819100	2.16785900	7.10138500
C	4.13553900	2.89217900	7.86595300
H	4.16029700	2.52951800	8.90071700
H	5.10757400	2.73714100	7.40193400
H	3.89880100	3.96194200	7.87660200
C	1.77908800	2.22628400	7.60972100
H	1.60131900	3.22968300	8.00747200
H	1.04675600	2.05607000	6.81943100
H	1.61772100	1.50202100	8.41893400

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C	-2.26428200	-3.31857200	-0.84463100
C	-2.29714500	-2.28002700	0.08611300
C	-1.44145000	-1.18481200	-0.04854000
C	-0.56275600	-1.14314000	-1.13980000
C	-0.53848400	-2.17252200	-2.07207800
C	-1.38637500	-3.26881400	-1.92184200
H	-2.93416900	-4.16508500	-0.72538300
H	-2.99813700	-2.32723500	0.91372200
H	0.11907400	-0.30199600	-1.25428700
H	0.15765700	-2.12878100	-2.90383700
H	-1.35606500	-4.08224800	-2.64065800
P	-1.35208200	0.19776900	1.16462100
C	-2.77515800	-0.13751900	2.27360800
C	-3.95428200	0.60983800	2.25677700
C	-2.62631600	-1.15255800	3.22877000
C	-4.96629500	0.34561000	3.17913400
H	-4.08115000	1.40651300	1.53016900
C	-3.64347400	-1.42891500	4.13426500
H	-1.69560800	-1.71725900	3.26833400
C	-4.81605100	-0.67338300	4.11415500
H	-5.87386100	0.94110900	3.16458600
H	-3.51524500	-2.21832100	4.86833100
H	-5.60491400	-0.87459700	4.83220500
C	-1.90565000	1.62535300	0.15510200
C	-1.45564600	2.90042700	0.51663200
C	-2.77013400	1.47859200	-0.93606600
C	-1.87425300	4.01556000	-0.20813800
H	-0.78963100	3.01995000	1.36939000
C	-3.18217400	2.59548000	-1.65613000
H	-3.11638800	0.48879000	-1.22228800
C	-2.73370500	3.86470100	-1.29254600

H	-1.52381600	5.00211600	0.07868800
H	-3.85237200	2.47579500	-2.50201300
H	-3.05399900	4.73500000	-1.85757100
P	2.62063300	-0.54513700	0.77297200
C	2.31074400	-2.19997700	0.03726600
C	1.39343200	-3.01773900	0.70946600
C	2.89337900	-2.66534800	-1.14388500
C	1.07900200	-4.28221600	0.22482500
H	0.90355200	-2.64296300	1.60708600
C	2.56926300	-3.92805600	-1.63670700
H	3.59013800	-2.03797700	-1.69230800
C	1.66694900	-4.73834800	-0.95317700
H	0.35714600	-4.89908000	0.75109500
H	3.02303300	-4.27814200	-2.55925700
H	1.41300700	-5.71948500	-1.34338400
C	4.10111100	-0.81462000	1.82096600
C	4.38441200	-2.05912300	2.38919100
C	4.84692900	0.30233300	2.22009400
C	5.39204000	-2.18494800	3.34239800
H	3.80640800	-2.93290200	2.10082400
C	5.86132900	0.17097600	3.16252600
H	4.62291500	1.28094900	1.80235100
C	6.13198300	-1.07215900	3.73089400
H	5.59136200	-3.15536600	3.78672700
H	6.43024200	1.04539100	3.46348500
H	6.91131200	-1.17160900	4.48027000
C	3.25382800	0.48237400	-0.60631300
C	4.53792000	0.34190400	-1.14807500
C	2.40572500	1.47348900	-1.11160200
C	4.95022000	1.15807400	-2.19677200
H	5.21880600	-0.39718600	-0.73265800
C	2.81822700	2.28834700	-2.16400800
H	1.42489400	1.62018800	-0.66126800
C	4.08866300	2.12789300	-2.70893700
H	5.94701100	1.04297100	-2.61143800
H	2.15070500	3.05443200	-2.54576300
H	4.41470300	2.76608400	-3.52452100
Pd	0.77860200	0.53713500	2.17539300
C	-0.66593600	1.07950700	4.89893400
H	-0.59520600	1.64290600	5.83534400
H	-0.36430100	0.04567900	5.07329800
H	-1.70200700	1.10786500	4.54907400
C	0.19510400	1.77108500	3.86512300
O	0.00222200	2.90775700	3.48189800
S	2.18131600	1.36318800	4.08546000
C	2.46378800	-0.18378000	4.92104800
C	3.38854700	-0.18503900	5.97287100
C	1.86176700	-1.39477900	4.55534600
C	3.71053800	-1.36764400	6.63034800
H	3.86147000	0.74824000	6.26421300
C	2.17192600	-2.57207900	5.23003100
H	1.15385800	-1.41266600	3.72879100
C	3.10230400	-2.56644700	6.26513500
H	4.43721500	-1.34909600	7.43732400
H	1.69420900	-3.50049600	4.92943500
H	3.35112500	-3.48703000	6.78373500

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C	-2.36044600	-3.26991500	-0.97925000
C	-2.40670500	-2.25092100	-0.02741500
C	-1.55771700	-1.14733200	-0.13510000
C	-0.67401100	-1.07731400	-1.22056600
C	-0.63564600	-2.08736200	-2.17299100
C	-1.47596200	-3.19263700	-2.04954500
H	-3.02448700	-4.12379100	-0.88155100
H	-3.11220500	-2.32008200	0.79497300
H	0.00144000	-0.22871000	-1.31451200
H	0.06586500	-2.02198100	-2.99883500
H	-1.43435600	-3.99189200	-2.78355600
P	-1.47589100	0.21193000	1.10438200
C	-2.90285600	-0.14469700	2.20148900
C	-4.08183800	0.60315900	2.19245500
C	-2.75865600	-1.17649200	3.13919100
C	-5.09837100	0.32280100	3.10481200
H	-4.20494000	1.41300300	1.47990400
C	-3.78019800	-1.46820100	4.03503100
H	-1.82824700	-1.74202100	3.17397400
C	-4.95268300	-0.71239600	4.02252300
H	-6.00571700	0.91874500	3.09629400
H	-3.65539300	-2.27000300	4.75614700
H	-5.74501600	-0.92605700	4.73314800
C	-2.02705800	1.65700300	0.11867700
C	-1.57739300	2.92566500	0.50255900
C	-2.89019300	1.52915300	-0.97606900
C	-1.99518000	4.05315500	-0.20337600
H	-0.91288500	3.03059700	1.35837700
C	-3.30153200	2.65829700	-1.67702900
H	-3.23611700	0.54459100	-1.28020000
C	-2.85356300	3.92110600	-1.29104500
H	-1.64493600	5.03450700	0.10095700
H	-3.97062500	2.55339400	-2.52574000
H	-3.17347100	4.80095700	-1.84132400
P	2.49575900	-0.53143400	0.70794600
C	2.18137500	-2.17787900	-0.04495900
C	1.25561400	-2.99614500	0.61470300
C	2.77164700	-2.63812600	-1.22427400
C	0.93995600	-4.25628100	0.11941300
H	0.75999900	-2.62463900	1.51055200
C	2.44645600	-3.89626400	-1.72780900
H	3.47534400	-2.01026200	-1.76315100
C	1.53560300	-4.70736600	-1.05661000
H	0.21098700	-4.87329900	0.63565800
H	2.90626100	-4.24226000	-2.64892000
H	1.28106000	-5.68503900	-1.45508300
C	3.98102300	-0.81793600	1.74478300
C	4.27089600	-2.07204500	2.28785800
C	4.72977800	0.29252400	2.15605500
C	5.28913700	-2.21363500	3.22750500
H	3.69025100	-2.94103300	1.99056600
C	5.75424200	0.14556600	3.08513400
H	4.50074000	1.27796400	1.75760800
C	6.03252500	-1.10731200	3.62771800
H	5.49595200	-3.19252200	3.65019400
H	6.32545200	1.01512400	3.39563000
H	6.82004100	-1.21897000	4.36673900
C	3.13028400	0.50873900	-0.66178700

C	4.41216700	0.36645000	-1.20838000
C	2.28705400	1.51010700	-1.15471300
C	4.82621600	1.18970500	-2.25075300
H	5.09019800	-0.37975400	-0.80112200
C	2.70137800	2.33249100	-2.20056800
H	1.30857200	1.65888900	-0.70006400
C	3.96893300	2.16926400	-2.75133000
H	5.82114500	1.07261600	-2.66933000
H	2.03755600	3.10648200	-2.57273700
H	4.29627500	2.81301400	-3.56201600
Pd	0.65294100	0.53847300	2.12621900
C	-0.78887000	1.02443800	4.85479500
H	-0.72192000	1.57658100	5.79807200
H	-0.47379900	-0.00773500	5.01428700
H	-1.82632000	1.04472500	4.50818500
C	0.06041900	1.73920500	3.82699800
O	-0.13828400	2.88319100	3.47045500
S	2.06024700	1.33478000	4.03971400
C	2.35455000	-0.22837600	4.83879500
C	3.29187600	-0.25492600	5.87948100
C	1.75269500	-1.43420800	4.46156600
C	3.62500700	-1.45057100	6.50308800
H	3.76625200	0.67134600	6.19060700
C	2.07944300	-2.62355000	5.10642900
H	1.02798200	-1.44223200	3.64935300
C	3.02791600	-2.65702900	6.12792500
H	4.36261400	-1.44645500	7.30267200
H	1.59755100	-3.54721000	4.79278100
C	3.42100700	-3.95288600	6.78940300
H	4.36013900	-4.33755000	6.37453600
H	3.57049600	-3.82099500	7.86527800
H	.65679900	-4.72126300	6.64411900

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C	-2.23035600	-3.33141000	-0.87705200
C	-2.26961800	-2.29727000	0.05834300
C	-1.42075000	-1.19619300	-0.07214700
C	-0.54305200	-1.14408000	-1.16359800
C	-0.51214800	-2.16933600	-2.10017000
C	-1.35293100	-3.27154900	-1.95421200
H	-2.89450200	-4.18290500	-0.76123300
H	-2.96986300	-2.35262800	0.88610500
H	0.13290900	-0.29786700	-1.27495300
H	0.18392000	-2.11790300	-2.93155300
H	-1.31717800	-4.08201000	-2.67612200
P	-1.33775700	0.18198200	1.14593900
C	-2.75967000	-0.16058300	2.25349100
C	-3.93978500	0.58519500	2.23851100
C	-2.61029200	-1.17989800	3.20397100
C	-4.95259200	0.31510000	3.15818400
H	-4.06673600	1.38524000	1.51565300
C	-3.62827800	-1.46186800	4.10686600
H	-1.67894400	-1.74352500	3.24261100
C	-4.80196700	-0.70804400	4.08860000
H	-5.86097900	0.90936700	3.14524500
H	-3.49960700	-2.25432700	4.83752500
H	-5.59151400	-0.91386100	4.80460500
C	-1.89221700	1.61172200	0.14030000

C	-1.44073400	2.88622500	0.50189600
C	-2.75918300	1.46604200	-0.94911000
C	-1.86039200	4.00197600	-0.22139200
H	-0.77364600	3.00514700	1.35388700
C	-3.17240500	2.58357200	-1.66737400
H	-3.10629100	0.47653400	-1.23534100
C	-2.72239200	3.85230900	-1.30389900
H	-1.50900100	4.98818000	0.06545900
H	-3.84461400	2.46480200	-2.51177200
H	-3.04360900	4.72317400	-1.86753200
P	2.62607100	-0.56455700	0.75655000
C	2.32255700	-2.21546500	0.00962500
C	1.40841200	-3.04129400	0.67612500
C	2.90991200	-2.67191500	-1.17263600
C	1.10240200	-4.30550300	0.18520600
H	0.91470200	-2.67409200	1.57481600
C	2.59384600	-3.93402600	-1.67198600
H	3.60432000	-2.03826200	-1.71676400
C	1.69527900	-4.75281700	-0.99366100
H	0.38405500	-4.92934500	0.70798500
H	3.05157600	-4.27726400	-2.59516600
H	1.44864000	-5.73402000	-1.38835900
C	4.11113500	-0.83599800	1.79781500
C	4.39829100	-2.08282900	2.35879500
C	4.85753100	0.28006600	2.19836800
C	5.40878200	-2.21200700	3.30864800
H	3.82015700	-2.95616900	2.06945800
C	5.87543500	0.14543200	3.13644700
H	4.63118300	1.26019400	1.78580300
C	6.14882600	-1.09984600	3.69887000
H	5.60901700	-3.18458700	3.74834400
H	6.44488900	1.01902900	3.43879200
H	6.93127000	-1.20122800	4.44487500
C	3.25359600	0.47555700	-0.61612900
C	4.53659900	0.33983400	-1.16169800
C	2.40429100	1.47035300	-1.11201100
C	4.94626600	1.16337700	-2.20553700
H	5.21876500	-0.40152300	-0.75253400
C	2.81424000	2.29298900	-2.15940300
H	1.42437600	1.61387600	-0.65873300
C	4.08326200	2.13659700	-2.70874900
H	5.94214000	1.05140600	-2.62325600
H	2.14571000	3.06180900	-2.53385100
H	4.40720600	2.78061100	-3.52058700
Pd	0.78587000	0.52489600	2.17295600
C	-0.65301500	1.04160400	4.89138600
H	-0.57717400	1.60847100	5.82515200
H	-0.33085000	0.01332300	5.06255100
H	-1.69500300	1.05128300	4.55782100
C	0.18008700	1.74391400	3.84168500
O	-0.02207300	2.88395300	3.47598600
S	2.19931100	1.34380700	4.06115800
C	2.49249200	-0.20143600	4.89558700
C	3.40551600	-0.20421900	5.95537000
C	1.91072700	-1.42261600	4.52672300
C	3.74137600	-1.38344400	6.61084500
H	3.86852000	0.72918200	6.26157600
C	2.22530700	-2.60176600	5.18923100

H	1.20526800	-1.44964000	3.69833800
C	3.15278000	-2.58774800	6.22895900
H	4.46350100	-1.36481600	7.42461400
H	1.77687700	-3.54650500	4.89874100
O	3.44678100	-3.77556500	6.83044200
H	4.07336900	-3.61673300	7.55022100

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C	-2.32662100	-3.25413400	-1.00193200
C	-2.40279200	-2.23881400	-0.04751000
C	-1.55581100	-1.13143700	-0.12956300
C	-0.64470500	-1.05308600	-1.19153300
C	-0.57712100	-2.05851900	-2.14681100
C	-1.41458900	-3.16865100	-2.04826700
H	-2.98749900	-4.11246500	-0.92436000
H	-3.12801200	-2.31482800	0.75728500
H	0.03012700	-0.20160000	-1.26257800
H	0.14440300	-1.98602100	-2.95461000
H	-1.34947500	-3.96538000	-2.78323700
P	-1.50727900	0.23041300	1.10804400
C	-2.90317100	-0.17597900	2.23024400
C	-4.09721000	0.54792800	2.25608000
C	-2.71638800	-1.20890400	3.15972200
C	-5.08392200	0.24473500	3.19365600
H	-4.25676500	1.35625600	1.54905800
C	-3.70714000	-1.52239100	4.08237700
H	-1.78022000	-1.76636000	3.16076100
C	-4.89378800	-0.78895600	4.10459500
H	-6.00352600	0.82151500	3.20875200
H	-3.54989900	-2.32667100	4.79443200
H	-5.66298600	-1.02053000	4.83473400
C	-2.14194400	1.65220000	0.13862700
C	-1.75624200	2.93795900	0.53409100
C	-3.00940600	1.49221800	-0.94785400
C	-2.24260400	4.05094700	-0.14967700
H	-1.08246200	3.06635000	1.37937300
C	-3.48842500	2.60692700	-1.62885800
H	-3.30631100	0.49410300	-1.25956000
C	-3.10538400	3.88687700	-1.22972100
H	-1.94087600	5.04580800	0.16267900
H	-4.16080700	2.47738700	-2.47152500
H	-3.47901300	4.75547100	-1.76376900
P	2.56397300	-0.49596700	0.75866700
C	2.22097400	-2.15290100	0.04277800
C	1.26478600	-2.93260000	0.70569800
C	2.81885300	-2.65497300	-1.11544600
C	0.92621500	-4.19620500	0.23549500
H	0.76342000	-2.52640400	1.58287900
C	2.47058800	-3.91656900	-1.59460200
H	3.54661300	-2.05746700	-1.65680200
C	1.52941900	-4.68912200	-0.91966500
H	0.17436300	-4.78302800	0.75399600
H	2.93624100	-4.29558500	-2.49950000
H	1.25697700	-5.66950200	-1.29886200
C	4.02206800	-0.79597900	1.83341600
C	4.28806600	-2.05050700	2.39070600
C	4.79445800	0.30299600	2.23288000
C	5.31686300	-2.20651500	3.31716000

H	3.69050200	-2.91116000	2.10250400
C	5.82775300	0.14214800	3.15117000
H	4.58509400	1.28863700	1.82325700
C	6.09144500	-1.11303800	3.69605700
H	5.50934200	-3.18532800	3.74787200
H	6.42318300	1.00151600	3.44454000
H	6.89147800	-1.23772500	4.41949000
C	3.25576800	0.49074100	-0.62239400
C	4.54478100	0.30949400	-1.14010400
C	2.44088500	1.49318200	-1.15899400
C	4.99442600	1.09928600	-2.19390900
H	5.20065600	-0.44071200	-0.70459700
C	2.89046700	2.28076000	-2.21668400
H	1.45656700	1.66873900	-0.72696900
C	4.16596200	2.08131600	-2.73615900
H	5.99480600	0.95357500	-2.58984200
H	2.24844500	3.05614100	-2.62263300
H	4.52131000	2.69853500	-3.55563100
Pd	0.64895100	0.60064800	2.01859800
C	-0.82173300	1.22210400	4.76503800
H	-0.80470300	1.77411100	5.71114100
H	-0.58857100	0.17394900	4.95384500
H	-1.82117400	1.30247400	4.32849600
C	0.15105600	1.88782900	3.81958400
O	0.01276700	3.01586400	3.39290100
S	2.03693100	1.42191800	4.03696400
C	2.27305500	-0.17990200	4.76326300
C	3.32907500	-0.30370000	5.67703700
C	1.54038200	-1.32426100	4.40862600
C	3.66821300	-1.54074500	6.20457900
H	3.90188200	0.57560900	5.95314200
C	1.85506300	-2.56215300	4.94930000
H	0.73304900	-1.24176300	3.68491600
C	2.92371900	-2.65208800	5.83107100
H	4.49782700	-1.65738400	6.89125900
H	1.30630200	-3.45652500	4.67916700
N	3.29581600	-3.96545500	6.36132800
O	2.58491900	-4.91271800	6.07562900
O	4.29842100	-4.03176800	7.05043600

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C	-2.36876600	-3.31841100	-0.84116100
C	-2.38891400	-2.27791600	0.08757600
C	-1.53991500	-1.17980200	-0.06413600
C	-0.68013600	-1.13723000	-1.17045200
C	-0.66830900	-2.16898800	-2.10044400
C	-1.50990600	-3.26778800	-1.93352900
H	-3.03344400	-4.16699400	-0.70824900
H	-3.07509300	-2.32568900	0.92735600
H	-0.00320600	-0.29402600	-1.29882200
H	0.01394800	-2.12545700	-2.94364800
H	-1.48925600	-4.08260800	-2.65112800
P	-1.43766500	0.20408300	1.14680500
C	-2.84572100	-0.13521900	2.27379500
C	-4.02928400	0.60519600	2.26618000
C	-2.68259000	-1.14773800	3.22936500
C	-5.03161200	0.33687800	3.19774400
H	-4.16737800	1.39957000	1.53916800

C	-3.69018300	-1.42816400	4.14437300
H	-1.74865800	-1.70761200	3.26123300
C	-4.86726100	-0.67950200	4.13324200
H	-5.94272400	0.92704800	3.18984400
H	-3.55114600	-2.21558200	4.87862100
H	-5.64871800	-0.88400000	4.85844800
C	-2.01075500	1.63017600	0.14596300
C	-1.57032500	2.90776200	0.51074100
C	-2.88279300	1.48065800	-0.93872800
C	-2.00605900	4.02244500	-0.20432100
H	-0.89875000	3.02937900	1.35887000
C	-3.31165400	2.59726000	-1.64940300
H	-3.22237500	0.48913100	-1.22683500
C	-2.87286600	3.86888600	-1.28257500
H	-1.66325300	5.01090800	0.08511700
H	-3.98789000	2.47539000	-2.49013900
H	-3.20666000	4.73904800	-1.83998400
P	2.53079000	-0.50204600	0.68918800
C	2.21647200	-2.16114800	-0.03559500
C	1.32055400	-2.98464900	0.65819700
C	2.77491600	-2.62378900	-1.22957300
C	1.00238400	-4.25090700	0.18082300
H	0.85049200	-2.61403500	1.56799300
C	2.44752000	-3.88875400	-1.71436100
H	3.45484500	-1.99235000	-1.79414100
C	1.56557000	-4.70392000	-1.01043200
H	0.29713500	-4.87221000	0.72411600
H	2.88225100	-4.23659300	-2.64687200
H	1.30813700	-5.68651700	-1.39460700
C	4.03657400	-0.75858000	1.70416300
C	4.35286600	-2.00312900	2.25427600
C	4.77505300	0.36675800	2.09347700
C	5.38662700	-2.12115300	3.18010700
H	3.78050300	-2.88302300	1.97347300
C	5.81464600	0.24346100	3.00896600
H	4.52504700	1.34496900	1.68974900
C	6.11885500	-1.00002200	3.55916400
H	5.61229600	-3.09215500	3.61111600
H	6.37730400	1.12403900	3.30363400
H	6.91814300	-1.09298800	4.28816100
C	3.13060700	0.52294100	-0.70700400
C	4.40619900	0.38708200	-1.26950200
C	2.26756900	1.50522000	-1.20411900
C	4.79549500	1.19837900	-2.33055500
H	5.09833300	-0.34501400	-0.86047900
C	2.65703300	2.31530100	-2.26902000
H	1.29368000	1.64881900	-0.73810000
C	3.91893000	2.15900700	-2.83466200
H	5.78589000	1.08658400	-2.76115800
H	1.97829200	3.07443300	-2.64484900
H	4.22665100	2.79317900	-3.66041000
Pd	0.70409000	0.56087300	2.12848900
C	-0.69816700	1.06455000	4.88084600
H	-0.60842400	1.62142800	5.81947500
H	-0.38078800	0.03284800	5.03907000
H	-1.74346200	1.08495800	4.55887800
C	0.12910700	1.77262300	3.83052500
O	-0.08460000	2.91057300	3.46288500

S	2.13161800	1.38694200	4.01663700
C	2.45107300	-0.16784700	4.82306600
C	3.41129900	-0.18072600	5.84208400
C	1.85496900	-1.38190400	4.45929900
C	3.77546100	-1.37295900	6.45694500
H	3.88582400	0.75087500	6.13665600
C	2.21409100	-2.56641800	5.09352800
H	1.11667200	-1.39887400	3.65964600
C	3.18804000	-2.58635600	6.09242700
H	4.53686200	-1.36167500	7.23435900
H	1.74480600	-3.49918600	4.78570300
C	3.55908400	-3.87185600	6.78979000
H	4.60906000	-3.83100600	7.10194600
H	3.47034200	-4.70910000	6.08755800
C	2.67291100	-4.13517500	8.01228000
H	2.94728300	-5.07116800	8.50819100
H	2.76678300	-3.32095300	8.73749500
H	1.62065700	-4.19706500	7.71749400

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C	-2.08349600	-3.26891300	-0.32279700
C	-2.07584500	-2.20927400	0.58395800
C	-1.25457900	-1.10103800	0.36806900
C	-0.44824100	-1.06841800	-0.77818900
C	-0.46198500	-2.12122000	-1.68433000
C	-1.27833400	-3.22817700	-1.45574300
H	-2.72658000	-4.12484400	-0.14013800
H	-2.71899900	-2.24868600	1.45744800
H	0.20476100	-0.21582000	-0.95923600
H	0.18115100	-2.08747500	-2.55820000
H	-1.27847300	-4.05767700	-2.15655800
P	-1.13011500	0.31129700	1.54350500
C	-2.49519100	-0.02646800	2.72262300
C	-3.71798200	0.64646400	2.69451900
C	-2.26675700	-0.98347600	3.72077800
C	-4.69567500	0.36587600	3.64789100
H	-3.90525200	1.39837500	1.93398900
C	-3.24945500	-1.27683500	4.65893600
H	-1.30241500	-1.48856900	3.76652700
C	-4.46643700	-0.59627900	4.62648700
H	-5.63860100	0.90336800	3.62342600
H	-3.06149000	-2.02205300	5.42573700
H	-5.22956200	-0.81087200	5.36820400
C	-1.75755500	1.70616900	0.53080100
C	-1.33432800	2.99864300	0.86199300
C	-2.65109400	1.51957800	-0.53063600
C	-1.80845700	4.09082100	0.13710000
H	-0.64581800	3.14977400	1.69142300
C	-3.11800500	2.61427400	-1.25142700
H	-2.97755400	0.51651100	-0.79271900
C	-2.69623700	3.90070000	-0.91808300
H	-1.47889800	5.09099300	0.40059300
H	-3.81095600	2.46340700	-2.07359800
H	-3.06008300	4.75385200	-1.48299800
P	2.81471300	-0.34934600	0.95154100
C	2.49740600	-2.02632000	0.27031600
C	1.65271800	-2.85442600	1.02109500
C	2.99842400	-2.49562900	-0.94630100

C	1.32726600	-4.12997400	0.57451500
H	1.22835600	-2.48068800	1.95200200
C	2.66469400	-3.77077200	-1.39884500
H	3.63779100	-1.86111500	-1.55282500
C	.83209800	-4.58904300	-0.64051700
H	0.66116500	-4.75490500	1.16128200
H	3.05497400	-4.12367400	-2.34889200
H	1.56741700	-5.57904100	-0.99987600
C	4.36531300	-0.55688500	1.90784600
C	4.72269800	-1.78095900	2.47785900
C	5.09980600	0.59036000	2.23628100
C	5.78936400	-1.85750200	3.37036800
H	4.15499100	-2.67698400	2.24175100
C	6.17399600	0.50812800	3.11530100
H	4.81713500	1.55323300	1.81783000
C	6.51549300	-0.71428500	3.69043800
H	6.04138000	-2.81001300	3.82689400
H	6.73227200	1.40495100	3.36612700
H	7.33948300	-0.77362000	4.39507900
C	3.34370900	0.65559000	-0.48735900
C	4.59765700	0.51708700	-1.09594600
C	2.45488000	1.62188900	-0.96988900
C	4.94027400	1.30872200	-2.18724900
H	5.30998700	-0.20181500	-0.69850600
C	2.79787600	2.41306900	-2.06499400
H	1.49838200	1.76845000	-0.47000100
C	4.03788100	2.25332500	-2.67610200
H	5.91454800	1.19469200	-2.65264400
H	2.10013300	3.16039900	-2.42959200
H	4.30909600	2.87275300	-3.52548800
Pd	1.03347500	0.72755600	2.45813900
C	-0.23843100	1.27455400	5.25094900
H	-0.11155100	1.87667500	6.15672300
H	0.13659500	0.26558600	5.42918400
H	-1.30334900	1.23605000	5.00233500
C	0.48344600	1.96913000	4.11590300
O	0.21329200	3.09229900	3.74139000
S	2.54062800	1.64768300	4.21129200
C	2.95460700	0.14590600	5.07223300
C	3.94984700	0.21217600	6.05544300
C	2.39706300	-1.10806400	4.79626800
C	4.38567400	-0.92644700	6.71799700
H	4.39772800	1.17338500	6.29099500
C	2.81686200	-2.24849100	5.47025300
H	1.62544300	-1.19601700	4.03354500
C	3.82846700	-2.17832900	6.43266600
H	5.17428700	-0.84840100	7.46257200
H	2.37484400	-3.21204800	5.22644900
N	4.31898800	-3.33809600	7.04567500
H	4.73626900	-3.17529200	7.95374100
H	3.64588200	-4.09283800	7.09236900

20-TS

C	-2.47423100	-3.25784000	-1.24914300
C	-2.49119800	-2.30475700	-0.22945400
C	-1.62260100	-1.21256000	-0.27362000
C	-0.74556600	-1.08884700	-1.35986200
C	-0.73555500	-2.03230800	-2.37809000

C	-1.60036200	-3.12445300	-2.32244300
H	-3.15471400	-4.10304100	-1.20264600
H	-3.19315600	-2.41269400	0.59211100
H	-0.05573900	-0.24737900	-1.40437300
H	-0.03725900	-1.92773100	-3.20261400
H	-1.58482000	-3.87126400	-3.11077100
P	-1.51387900	0.09187200	1.02199800
C	-2.94350900	-0.25999700	2.11501600
C	-4.05287900	0.58302100	2.20512100
C	-2.85652900	-1.36423200	2.97457200
C	-5.05961600	0.32295400	3.13406500
H	-4.12651200	1.45267700	1.55959900
C	-3.87060900	-1.63388400	3.88614200
H	-1.97580100	-2.00415400	2.93837200
C	-4.97393200	-0.78441000	3.97125100
H	-5.91170700	0.99222300	3.20188400
H	-3.79307300	-2.49431800	4.54370400
H	-5.75833400	-0.98242700	4.69505200
C	-2.03845000	1.56646700	0.06121900
C	-1.47830500	2.80884200	0.37485200
C	-2.98337200	1.47373800	-0.96865400
C	-1.86211000	3.94461100	-0.33845700
H	-0.76181500	2.89047400	1.18878700
C	-3.36312600	2.60970300	-1.67503600
H	-3.41632100	0.50817700	-1.21858500
C	-2.79992400	3.84650200	-1.36154400
H	-1.42479700	4.90636500	-0.08869400
H	-4.09538400	2.52959400	-2.47270300
H	-3.09385500	4.73201100	-1.91713500
P	2.45483700	-0.73278300	0.64967500
C	2.12416200	-2.27973500	-0.28363600
C	1.18648700	-3.16236600	0.26821400
C	2.73015400	-2.60525200	-1.49838600
C	0.87626500	-4.35732200	-0.37196400
H	0.67829400	-2.89124200	1.19288200
C	2.40999100	-3.79683000	-2.14641200
H	3.44532500	-1.92319700	-1.94849100
C	1.48788400	-4.67462100	-1.58332200
H	0.13790700	-5.02651300	0.05887800
H	2.88392800	-4.03822200	-3.09325900
H	1.23720800	-5.60025500	-2.09283000
C	3.88643100	-1.18143300	1.70437500
C	4.17875500	-2.50329400	2.05269100
C	4.57503200	-0.13904200	2.33934600
C	5.12279400	-2.77566700	3.04087300
H	3.65839500	-3.32241200	1.56376700
C	5.51947500	-0.41600200	3.32151900
H	4.34958900	0.89288400	2.08007100
C	5.78687200	-1.73476200	3.68457200
H	5.33207600	-3.80419700	3.31996700
H	6.03419600	0.40139600	3.81751700
H	6.50219000	-1.95157800	4.47141000
C	3.17881700	0.41273400	-0.58425800
C	4.48786300	0.29313900	-1.06710000
C	2.37472600	1.46078000	-1.04413500
C	4.96990900	1.18919300	-2.01631300
H	5.13073700	-0.49746800	-0.68719000
C	2.85733400	2.35576900	-1.99681200

H	1.37279000	1.58610100	-0.63613400
C	4.15309400	2.21733700	-2.48557200
H	5.98550100	1.08952700	-2.38700700
H	2.22404500	3.16603900	-2.34434300
H	.53353600	2.91756300	-3.22289700
Pd	.61795400	0.37223600	2.06484200
C	-0.79873400	0.75778600	4.78795600
H	-0.70682100	1.23624100	5.76933400
H	-0.41180100	-0.26076900	4.84793700
H	-1.85357600	0.73828900	4.50117700
C	-0.06478400	1.60590500	3.77029600
O	-0.45307400	2.69500400	3.39948500
S	1.92693800	1.48308900	3.91786100
C	2.39455100	0.09515400	4.92618200
C	3.10708400	0.35834500	6.10152700
C	2.16142900	-1.23588500	4.56004800
C	3.58820500	-0.68615800	6.88233600
H	3.29097400	1.38803500	6.39265400
C	2.63511500	-2.27399500	5.35117800
H	1.62217700	-1.45263200	3.64031300
C	3.35420600	-2.01221300	6.51850000
H	4.14978600	-0.46737400	7.78717100
H	2.46559700	-3.30380900	5.04506100
C	3.87534400	-3.13808300	7.35560500
H	4.07046100	-2.82443000	8.38138300
H	3.19458100	-3.98982100	7.36236700
Cl	5.45163400	-3.78515100	6.72822200

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C	-2.26808400	-3.31777000	-0.85201800
C	-2.30545800	-2.28086600	0.08053200
C	-1.44905900	-1.18549200	-0.04814200
C	-0.56541000	-1.14179000	-1.13536500
C	-0.53679500	-2.16928300	-2.06951000
C	-1.38513400	-3.26604500	-1.92499900
H	-2.93841900	-4.16456400	-0.73748300
H	-3.01057500	-2.32963900	0.90460200
H	0.11702400	-0.30045300	-1.24499700
H	0.16313200	-2.12385600	-2.89801100
H	-1.35141700	-4.07822300	-2.64506600
P	-1.36329900	0.19564700	1.16687600
C	-2.78648200	-0.14162400	2.27542700
C	-3.96085200	0.61351500	2.26724700
C	-2.64076700	-1.16205300	3.22539700
C	-4.97063400	0.35181200	3.19282100
H	-4.08583600	1.41415500	1.54467600
C	-3.65566900	-1.43579100	4.13420100
H	-1.71433400	-1.73432500	3.25740200
C	-4.82319800	-0.67215400	4.12276800
H	-5.87443800	0.95310900	3.18446100
H	-3.52998300	-2.22984100	4.86369100
H	-5.61025500	-0.87137400	4.84331000
C	-1.91984000	1.62318700	0.15881800
C	-1.47280700	2.89881800	0.52184400
C	-2.78410400	1.47597300	-0.93240200
C	-1.89377000	4.01410100	-0.20124500
H	-0.80686100	3.01850900	1.37454500
C	-3.19852700	2.59290500	-1.65103700

H	-3.12829800	0.48579000	-1.21976000
C	-2.75283100	3.86266200	-1.28589800
H	-1.54544400	5.00106600	0.08672900
H	-3.86849000	2.47286400	-2.49704200
H	-3.07494800	4.73294300	-1.84989000
P	2.62838700	-0.54068500	0.77761900
C	2.31288100	-2.19662800	0.04718500
C	1.38791600	-3.00727400	0.71746000
C	2.89992100	-2.66965800	-1.12871500
C	1.07037400	-4.27245900	0.23688100
H	0.89285800	-2.62537300	1.60921300
C	2.57247000	-3.93291800	-1.61795600
H	3.60283600	-2.04796100	-1.67573700
C	1.66284600	-4.73622600	-0.93584100
H	0.34259200	-4.88364200	0.76156500
H	3.02962700	-4.28906400	-2.53645700
H	1.40668700	-5.71792600	-1.32305700
C	4.10325800	-0.81450200	1.83319400
C	4.38302700	-2.06047600	2.40056700
C	4.84900900	0.30076700	2.23770200
C	5.38582700	-2.18961500	3.35894400
H	3.80639800	-2.93347700	2.10686200
C	5.85992200	0.16622500	3.18363800
H	4.62867500	1.28023500	1.81965000
C	6.12629400	-1.07830900	3.75160900
H	5.58215000	-3.16135900	3.80256800
H	6.43057900	1.03888600	3.48657800
H	6.90327300	-1.18068300	4.50304700
C	3.27128600	0.47932400	-0.60231900
C	4.55753100	0.33439700	-1.13773800
C	2.42648200	1.46897400	-1.11605000
C	4.97553200	1.14562400	-2.18810900
H	5.23551800	-0.40433800	-0.71691800
C	2.84467100	2.27847700	-2.17025700
H	1.44369400	1.61841500	-0.67084600
C	4.11751200	2.11417400	-2.70845300
H	5.97391300	1.02736100	-2.59798600
H	2.17972500	3.04336700	-2.55880500
H	4.44797100	2.74828900	-3.52542000
Pd	0.77371300	0.53808900	2.15731700
C	-0.67591300	1.08083000	4.89087300
H	-0.61568500	1.62905400	5.83715600
H	-0.38610000	0.04204000	5.05480500
H	-1.70571700	1.12237500	4.52505200
C	0.20559500	1.78234800	3.88195700
O	0.00850100	2.91450600	3.48736500
S	2.16170600	1.38472800	4.09118900
C	2.44909200	-0.16594500	4.91472300
C	3.38692800	-0.17617900	5.95454200
C	1.85251100	-1.37685000	4.54158100
C	3.73803700	-1.36135900	6.59006200
H	3.85717000	0.75452900	6.25721600
C	2.18125400	-2.56513500	5.18502900
H	1.13391700	-1.39283200	3.72450200
C	3.13169300	-2.54925700	6.19776200
H	4.47645600	-1.36639500	7.38475000
H	1.72186500	-3.50134600	4.88541600
Cl	3.58303700	-4.04492600	6.97879400

22-TS

C	-2.49043200	-3.22358500	-1.35198100
C	-2.50924600	-2.29307800	-0.31149100
C	-1.62412700	-1.21353000	-0.31882100
C	-0.72914800	-1.07860100	-1.38885700
C	-0.71720500	-1.99921300	-2.42754600
C	-1.59853000	-3.07935600	-2.40894600
H	-3.18369000	-4.05941700	-1.33454100
H	-3.22570800	-2.40787400	0.49644000
H	-0.02817600	-0.24530900	-1.40589100
H	-0.00818400	-1.88412000	-3.24127200
H	-1.58277800	-3.80800900	-3.21403900
P	-1.51886500	0.06907800	0.99755100
C	-2.96149200	-0.27500700	2.07307100
C	-4.03377800	0.60992600	2.19880500
C	-2.91653300	-1.41269100	2.89132900
C	-5.04784900	0.35710500	3.12177400
H	-4.07068100	1.50635100	1.58782600
C	-3.93848400	-1.67380300	3.79648700
H	-2.06336400	-2.08669400	2.82848300
C	-5.00570600	-0.78350300	3.91686100
H	-5.87018400	1.05901200	3.21948100
H	-3.89432500	-2.56000700	4.42197500
H	-5.79550700	-0.97568900	4.63633100
C	-2.00751400	1.56193100	0.04661700
C	-1.42066600	2.79007900	0.36689900
C	-2.95000500	1.49393800	-0.98746100
C	-1.77387900	3.93622500	-0.34577300
H	-0.71422500	2.85348100	1.19095400
C	-3.29976000	2.64028800	-1.69235900
H	-3.40381500	0.53949800	-1.24307300
C	-2.70855900	3.86267600	-1.37358700
H	-1.31653000	4.88697700	-0.08995300
H	-4.02996400	2.57941400	-2.49364000
H	-2.97961800	4.75607300	-1.92815500
P	2.42079500	-0.78942500	0.71603100
C	2.07676300	-2.30881800	-0.25778000
C	1.12601600	-3.19325200	0.26752200
C	2.69263600	-2.61578300	-1.47251300
C	0.80899400	-4.37088300	-0.40116100
H	0.61527100	-2.93845500	1.19528100
C	2.36764800	-3.79075000	-2.14770900
H	3.41909400	-1.93177500	-1.90107300
C	1.42974600	-4.66947100	-1.61255500
H	0.06048300	-5.04166000	0.00906800
H	2.84897900	-4.01797200	-3.09434200
H	1.17417900	-5.58143500	-2.14379900
C	3.86857700	-1.27836000	1.73182500
C	4.19968100	-2.61373400	1.97699300
C	4.55557400	-0.26609800	2.41600800
C	5.19082300	-2.93189800	2.90350500
H	3.67965400	-3.40962900	1.45150200
C	5.54223200	-0.58841400	3.34054100
H	4.29912300	0.77585200	2.23910200
C	5.85661600	-1.92284600	3.59287200
H	5.43614000	-3.97298500	3.09118300
H	6.05475200	0.20472300	3.87614300

H	6.61644000	-2.17387800	4.32674800
C	3.14135800	0.38496700	-0.49332600
C	4.44934300	0.27492500	-0.98091000
C	2.33721500	1.44314900	-0.92958600
C	4.92996400	1.18949000	-1.91297400
H	5.09246500	-0.52350600	-0.61821200
C	2.81840400	2.35686500	-1.86503600
H	1.33633200	1.56174700	-0.51714100
C	4.11282600	2.22726100	-2.35985200
H	5.94472400	1.09656400	-2.28771600
H	2.18476200	3.17458100	-2.19406700
H	4.49207000	2.94157500	-3.08417600
Pd	0.57319500	0.33946800	2.13347000
C	-0.87019700	0.67261300	4.80718400
H	-0.78760200	1.18659300	5.77084900
H	-0.42061500	-0.31845100	4.88983000
H	-1.92833800	0.58191200	4.54505400
C	-0.20598700	1.52908000	3.74779800
O	-0.62594300	2.61323200	3.40274600
S	1.86629800	1.47343400	3.94128100
C	2.35470900	0.12413600	4.99180100
C	2.99505300	0.42766800	6.19329400
C	2.20098400	-1.22711700	4.64609500
C	3.49272500	-0.57445500	7.02590700
H	3.11993700	1.46785000	6.47955000
C	2.67803500	-2.23093300	5.47118400
H	1.71077400	-1.48824000	3.71053500
C	3.33637400	-1.91168500	6.66344300
H	3.99284300	-0.29619300	7.94621200
H	2.57405400	-3.27703300	5.20222000
O	3.78555500	-2.96797100	7.39466800
C	4.46900500	-2.67997100	8.59189200
H	4.75416200	-3.64143900	9.01952900
H	5.37072200	-2.08346600	8.40370100
H	3.82663900	-2.14274700	9.30093800

23-TS

C	-2.48738500	-3.27150800	-1.23522400
C	-2.50051800	-2.31514200	-0.21849200
C	-1.62792500	-1.22634900	-0.26584700
C	-0.75155100	-1.10879300	-1.35349100
C	-0.74577200	-2.05500500	-2.36914100
C	-1.61377100	-3.14450100	-2.30943900
H	-3.17096500	-4.11402000	-1.18565100
H	-3.20270700	-2.41825300	0.60342900
H	-0.05842100	-0.27015700	-1.40071300
H	-0.04752300	-1.95517100	-3.19437200
H	-1.60146900	-3.89371800	-3.09554400
P	-1.50890600	0.07784800	1.02951800
C	-2.93915400	-0.26159600	2.12553200
C	-4.02889700	0.60443500	2.23533400
C	-2.86757500	-1.37565200	2.97396900
C	-5.03151800	0.35726000	3.17233200
H	-4.09000200	1.48186600	1.59914500
C	-3.87784900	-1.63213100	3.89353700
H	-2.00209900	-2.03498200	2.92196500
C	-4.96141900	-0.75969700	3.99823700
H	-5.86780300	1.04447800	3.25563500

H	-3.81245600	-2.50058600	4.54174700
H	-5.74237200	-0.94755200	4.72839000
C	-2.02573100	1.55572300	0.06922400
C	-1.45682000	2.79436800	0.38188200
C	-2.97351000	1.47003900	-0.95848800
C	-1.83379400	3.93313200	-0.33019700
H	-0.73815300	2.87048900	1.19438200
C	-3.34644800	2.60878100	-1.66413700
H	-3.41400900	0.50766400	-1.20744000
C	-2.77403700	3.84159800	-1.35171400
H	-1.38949300	4.89182600	-0.08101100
H	-4.08077400	2.53390400	-2.46041800
H	-3.06286900	4.72913700	-1.90670300
P	2.47229200	-0.71422900	0.63647900
C	2.13736300	-2.26775300	-0.28332800
C	1.19982900	-3.14473700	0.27772100
C	2.74096800	-2.60368600	-1.49652700
C	0.88715600	-4.34457900	-0.35200200
H	0.69239600	-2.86473100	1.20020000
C	2.41829400	-3.80024900	-2.13403700
H	3.45617500	-1.92603500	-1.95342300
C	1.49630900	-4.67233800	-1.56180400
H	0.14870700	-5.00923300	0.08558700
H	2.89002900	-4.05008400	-3.07977500
H	1.24367100	-5.60183400	-2.06324300
C	3.91279000	-1.15544400	1.68336100
C	4.23318700	-2.47673800	2.00761700
C	4.58513800	-0.11067400	2.33283600
C	5.19252300	-2.74719800	2.98189100
H	3.72523100	-3.29771500	1.50909000
C	5.54539500	-0.38490200	3.30004500
H	4.33874500	0.92089500	2.09146700
C	5.84390700	-1.70463200	3.63573500
H	5.42636000	-3.77721500	3.23483900
H	6.05081000	0.43374000	3.80336900
H	6.57808100	-1.91859600	4.40611000
C	3.18805000	0.42287600	-0.60950200
C	4.49741100	0.30707400	-1.09221000
C	2.37523700	1.45893300	-1.08128200
C	4.97209000	1.19586100	-2.05194300
H	5.14620800	-0.47508100	-0.70495700
C	2.85044700	2.34609900	-2.04480400
H	1.37218900	1.58071000	-0.67488300
C	4.14718600	2.21222900	-2.53244500
H	5.98805500	1.09938000	-2.42244100
H	2.21041400	3.14673400	-2.40213600
H	4.52183000	2.90667300	-3.27813700
Pd	0.63407300	0.35229800	2.04807500
C	-0.78722200	0.71125300	4.79319900
H	-0.68601100	1.15299600	5.79099000
H	-0.40891100	-0.31214400	4.81551000
H	-1.84318100	0.71114900	4.51112200
C	-0.05091100	1.58842300	3.80317100
O	-0.45559800	2.66845800	3.42579000
S	1.91508100	1.48076300	3.93323200
C	2.37873700	0.09709400	4.94836700
C	3.01774600	0.36156100	6.16150600
C	2.21825100	-1.23564300	4.55009200

C	3.49308800	-0.67510400	6.95901300
H	3.15115400	1.39015700	6.48147700
C	2.69074700	-2.26933000	5.34327600
H	1.73584200	-1.45822100	3.60133600
C	3.32468600	-1.99917700	6.56029600
H	3.98967700	-0.43969200	7.89243800
H	2.57769100	-3.29446000	5.00446600
C	3.87396300	-3.16272300	7.36266700
Cl	5.34290700	-3.81158400	6.55164600
Cl	4.32216600	-2.71337400	9.02954000
Cl	2.67466500	-4.49177700	7.46655800

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C	-2.05202900	-2.96218100	-1.26077400
C	-2.16185400	-2.02784200	-0.23178600
C	-1.34350800	-0.89516000	-0.22247400
C	-0.43111600	-0.70656100	-1.26600600
C	-0.32004400	-1.63958400	-2.28977900
C	-1.12686000	-2.77593100	-2.28365800
H	-2.68622500	-3.84374700	-1.25508600
H	-2.88204600	-2.18643600	0.56545200
H	0.21599000	0.16795400	-1.26375600
H	0.41134000	-1.48959500	-3.07789300
H	-1.02725500	-3.51722700	-3.07057500
P	-1.35826800	0.36473400	1.11741200
C	-2.58660200	-0.33980600	2.29000400
C	-3.94901300	-0.02907200	2.25926000
C	-2.11441700	-1.22822600	3.26275900
C	-4.81821600	-0.59229500	3.19132200
H	-4.33052300	0.66637700	1.51731300
C	-2.98386600	-1.79749400	4.18788000
H	-1.05202800	-1.46174100	3.30471000
C	-4.33908400	-1.47532500	4.15558400
H	-5.87284000	-0.33566500	3.16560000
H	-2.60050300	-2.48063600	4.93952500
H	-5.01905700	-1.90693800	4.88345600
C	-2.25302100	1.75786300	0.32902300
C	-2.01764900	3.04918800	0.81377500
C	-3.16323600	1.56720700	-0.71809600
C	-2.70312700	4.13286000	0.26762100
H	-1.29272600	3.21020000	1.60839100
C	-3.84194800	2.65383500	-1.26053900
H	-3.33634600	0.56833400	-1.11068100
C	-3.61411700	3.93736000	-0.76620900
H	-2.51516200	5.13151700	0.64939900
H	-4.54728500	2.49943100	-2.07139400
H	-4.14236100	4.78427200	-1.19384400
P	2.63386100	-0.58771900	0.71270700
C	2.21128800	-2.24314300	0.02838000
C	1.19573000	-2.94634500	0.68744000
C	2.81229200	-2.81941200	-1.09350400
C	0.80167300	-4.20622700	0.24906800
H	0.69501200	-2.48891900	1.53987700
C	2.41189500	-4.07746400	-1.53854900
H	3.58521900	-2.28223000	-1.63417900
C	1.41073700	-4.77433900	-0.86724800
H	0.00503700	-4.73265600	0.76581000
H	2.88373800	-4.51301300	-2.41431600

H	1.09714800	-5.75243700	-1.21939100
C	4.03046800	-0.96153300	1.84575700
C	4.18467600	-2.20820800	2.45631700
C	4.87158400	0.09218100	2.22556500
C	5.15429500	-2.39502300	3.43938000
H	3.53727500	-3.03529600	2.17764900
C	5.84695100	-0.10047300	3.19764000
H	4.75413100	1.07120900	1.76844800
C	5.98467600	-1.34304100	3.81312400
H	5.25401800	-3.36496600	3.91688300
H	6.48739300	0.72746400	3.48568500
H	6.73427700	-1.48858000	4.58485600
C	3.48450000	0.28369200	-0.65973400
C	4.75967300	-0.08374800	-1.10909000
C	2.84294400	1.37417200	-1.25437300
C	5.36004800	0.60020900	-2.16023400
H	5.28562800	-0.89857400	-0.61760700
C	3.44476100	2.06028400	-2.30838100
H	1.87964800	1.70350400	-0.86932500
C	4.69907200	1.66881000	-2.76587500
H	6.34762400	0.30628700	-2.50223900
H	2.93854700	2.90717900	-2.76088300
H	5.17129100	2.20465300	-3.58355600
Pd	0.82484500	0.79421300	2.05684900
C	-0.54742200	1.57099300	4.73208700
H	-0.07587500	1.86999100	5.67558500
H	-0.54416100	0.47845700	4.70232300
C	0.31330100	2.12622100	3.60528600
O	0.24957900	3.26835200	3.21058400
S	2.37040000	1.51299500	3.87901700
C	2.47508000	0.01284100	4.82540500
C	3.31752200	0.00231100	5.94609700
C	1.79351500	-1.16690100	4.49817900
C	3.47476100	-1.15168900	6.70600100
H	3.85530100	0.90794800	6.21079800
C	1.93718100	-2.31432100	5.27171400
H	1.16045000	-1.18493800	3.61416600
C	2.78213900	-2.31551500	6.37769500
H	4.13822800	-1.13838100	7.56577700
H	1.39716500	-3.21586200	4.99449200
H	2.90111700	-3.21292500	6.97687700
C	-1.96040200	2.14071200	4.63822500
H	-2.60854900	1.68468700	5.39204100
H	-1.94193100	3.22258300	4.78931400
H	-2.40258400	1.94888900	3.65597100

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C	-2.71328100	-3.09821600	-1.34008800
C	-2.71786900	-2.17827400	-0.28992800
C	-1.78111300	-1.14378300	-0.25751500
C	-0.84818600	-1.04298400	-1.29907300
C	-0.85155300	-1.95121700	-2.34865600
C	-1.78392500	-2.98771100	-2.36839300
H	-3.44712300	-3.89891700	-1.35281300
H	-3.46189200	-2.26781100	0.49606700
H	-0.10468200	-0.24729800	-1.28462600
H	-0.11623600	-1.85961100	-3.14176500
H	-1.78047000	-3.70756100	-3.18149400

P	-1.63550400	0.10175600	1.09074100
C	-3.12414200	-0.19352800	2.11885900
C	-4.18445300	0.71089000	2.20824700
C	-3.14295900	-1.34453700	2.91916200
C	-5.24672000	0.46318600	3.07708900
H	-4.17647500	1.61578200	1.60852200
C	-4.20899500	-1.59724600	3.77487400
H	-2.31082500	-2.04578900	2.86968600
C	-5.26363200	-0.68877600	3.85765300
H	-6.06071300	1.17826200	3.14550600
H	-4.21096900	-2.49388000	4.38699900
H	-6.08996600	-0.87549100	4.53639700
C	-2.01315200	1.64756400	0.17394900
C	-1.39458900	2.83501700	0.57925400
C	-2.89015600	1.66444000	-0.91784200
C	-1.64897100	4.02265900	-0.10536300
H	-0.73952600	2.83188300	1.44665800
C	-3.14079400	2.85222700	-1.59690500
H	-3.36841000	0.74327500	-1.24147700
C	-2.51723600	4.03214900	-1.19287800
H	-1.16681300	4.94028000	0.21716600
H	-3.81803500	2.85642800	-2.44550500
H	-2.71071800	4.95772800	-1.72684100
P	2.30532900	-0.88755000	0.90838600
C	1.89272600	-2.38178900	-0.07929500
C	0.88454700	-3.21562800	0.41948600
C	2.51959200	-2.71801500	-1.28120600
C	0.52021300	-4.37233500	-0.26260500
H	0.36683600	-2.93575600	1.33597800
C	2.14883700	-3.87126800	-1.96921400
H	3.29163900	-2.07291000	-1.69002400
C	1.15233700	-4.69989700	-1.46014900
H	-0.27209500	-5.00389800	0.12720500
H	2.63957900	-4.12107400	-2.90525700
H	0.86076400	-5.59509500	-2.00140400
C	3.78108000	-1.42845600	1.85878900
C	4.12119200	-2.77131200	2.03282200
C	4.50637400	-0.44463300	2.54631400
C	5.16755900	-3.12568900	2.88517000
H	3.57009600	-3.54561000	1.50652200
C	5.54982400	-0.80067900	3.39088200
H	4.23337500	0.60312200	2.43414800
C	5.88155700	-2.14436000	3.56456700
H	5.42352700	-4.17355300	3.01311700
H	6.09251900	-0.02945700	3.92853900
H	6.69344100	-2.42222800	4.23051000
C	3.02558200	0.27966400	-0.31141700
C	4.32174400	0.14806000	-0.82444500
C	2.23235400	1.35276800	-0.73160700
C	4.79971300	1.05392500	-1.76649800
H	4.95883800	-0.66054200	-0.47388200
C	2.71045800	2.25754800	-1.67712800
H	1.24233000	1.48987400	-0.29912500
C	3.99219600	2.10534200	-2.19821300
H	5.80510200	0.94298200	-2.16111600
H	2.08424400	3.08608200	-1.99319800
H	4.36916000	2.81250300	-2.93070700
Pd	0.45751600	0.27486400	2.26885300

C	-0.90296400	0.33454000	4.96360400
H	-0.13828200	0.17449600	5.73073900
H	-1.02853400	-0.62459700	4.44556000
C	-0.38837900	1.36628300	3.95767700
O	-0.97277000	2.39057100	3.68275600
S	1.65956000	1.60257100	4.01472800
C	2.44535900	0.33225300	4.98103600
C	3.38580200	0.73517100	5.93337500
C	2.24285900	-1.03929000	4.78064400
C	4.13507300	-0.20900200	6.63026300
H	3.54658100	1.79496400	6.10866100
C	2.98606800	-1.97199400	5.49076500
H	1.52518200	-1.37474500	4.03432700
C	3.95514400	-1.57519900	6.41615800
H	4.87788000	0.12705500	7.34992800
H	2.83505100	-3.03134900	5.29592700
C	4.77998000	-2.60414200	7.14421200
H	4.17429100	-3.16540100	7.86435900
H	5.20424400	-3.32836800	6.43995000
H	5.60412900	-2.13856600	7.69157600
C	-2.22402700	0.78995100	5.57453600
H	-2.09063700	1.72721800	6.12065100
H	-2.97285100	0.95953000	4.79670700
H	-2.60338300	0.03051000	6.26437000

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C	-2.19800400	-3.00412000	-1.12789500
C	-2.25109400	-2.07273700	-0.09099500
C	-1.44910100	-0.92937900	-0.13365300
C	-0.60975100	-0.72887000	-1.23572400
C	-0.55749000	-1.65717000	-2.26796200
C	-1.34816600	-2.80359300	-2.21117500
H	-2.82030900	-3.89304900	-1.08280200
H	-2.91661100	-2.24182800	0.75065400
H	0.02343000	0.15518200	-1.27768400
H	0.11669300	-1.49573600	-3.10348800
H	-1.29436700	-3.54068700	-3.00658900
P	-1.37820300	0.32947800	1.20665000
C	-2.60740500	-0.31335200	2.41272400
C	-3.94056500	0.10327900	2.45621200
C	-2.16117300	-1.25789200	3.34430500
C	-4.80572200	-0.411176500	3.41957900
H	-4.30192900	0.84220700	1.74709900
C	-3.02777300	-1.78174200	4.29837700
H	-1.12107800	-1.57921100	3.32245200
C	-4.35321200	-1.35322600	4.34015000
H	-5.83683100	-0.07329900	3.45059900
H	-2.66594300	-2.51310900	5.01442500
H	-5.03008000	-1.74971700	5.09039700
C	-2.22398000	1.75805900	0.42695500
C	-1.88310000	3.04370600	0.86122400
C	-3.19018500	1.59992500	-0.57477800
C	-2.51600000	4.15583600	0.30799800
H	-1.12026900	3.17711400	1.62515300
C	-3.81693200	2.71382600	-1.12388400
H	-3.44624400	0.60369500	-0.92667900
C	-3.48069700	3.99289100	-0.68186200
H	-2.24486500	5.15016100	0.64875800

H	-4.56487300	2.58428300	-1.90007000
H	-3.96727600	4.86127300	-1.11567900
P	2.59507900	-0.63048600	0.56923600
C	2.16524900	-2.25092700	-0.18200200
C	1.19961400	-3.00658800	0.49347300
C	2.71742400	-2.75662100	-1.36158700
C	0.81330300	-4.25543000	0.01894200
H	0.73150800	-2.59726300	1.38771600
C	2.32008500	-4.00130800	-1.84520100
H	3.44832600	-2.17480200	-1.91485100
C	1.37532000	-4.75495600	-1.15367900
H	0.05766700	-4.82536000	0.55072400
H	2.75172500	-4.38350900	-2.76541200
H	1.06717600	-5.72416800	-1.53402200
C	4.05608100	-1.02923700	1.60786900
C	4.21685500	-2.28409100	2.20240900
C	4.92845800	0.00783700	1.96276000
C	5.22512000	-2.49556200	3.14061500
H	3.54802800	-3.09992700	1.94087900
C	5.94135900	-0.20891100	2.89147500
H	4.80715500	0.99269800	1.51898600
C	6.08744900	-1.45955800	3.48879500
H	5.33474400	-3.47374200	3.59959900
H	6.60877400	0.60537100	3.15690600
H	6.86810100	-1.62508200	4.22493500
C	3.31309500	0.37495100	-0.78464600
C	4.55117100	0.10549300	-1.38287400
C	2.58745300	1.49637800	-1.19979400
C	5.03078100	0.92232800	-2.40186000
H	5.14713400	-0.73451900	-1.03360500
C	3.06787000	2.31397700	-2.22070300
H	1.65235400	1.74217100	-0.69844300
C	4.28607500	2.02291200	-2.82602600
H	5.99115500	0.70719200	-2.86034100
H	2.49625100	3.18329400	-2.52990400
H	4.66582900	2.66162900	-3.61754600
Pd	0.86288100	0.68629400	1.98418100
C	-0.33214600	1.52750600	4.74995400
H	0.14586000	1.77959300	5.70494700
H	-0.37964100	0.43688400	4.69156300
C	0.55398100	2.07558200	3.63944400
O	0.46995100	3.20272600	3.19945200
S	2.49318700	1.47716100	3.75902800
C	2.65664300	-0.01766200	4.69650600
C	3.61603800	-0.03684500	5.72113300
C	1.92305300	-1.18508500	4.43488200
C	3.84525500	-1.18830900	6.45944500
H	4.18820500	0.86136200	5.92990600
C	2.12720000	-2.33686400	5.18006700
H	1.20090700	-1.18825700	3.62237100
C	3.09201700	-2.32161000	6.17819400
H	4.58831800	-1.22198800	7.24706800
H	1.57212600	-3.24678300	4.98556900
N	3.32945400	-3.54277400	6.95122800
O	2.64606200	-4.51779900	6.69090500
O	4.19710200	-3.51131000	7.80564100
C	-1.71844000	2.15826100	4.66541200
H	-2.39025000	1.70460300	5.39944300

H	-1.65746300	3.23316900	4.84994200
H	-2.15789600	2.01535100	3.67387800

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C	-2.33471500	-2.88107100	-1.47591200
C	-2.35178900	-2.04047700	-0.36358900
C	-1.50330400	-0.93140400	-0.30803600
C	-0.64663600	-0.67691500	-1.38484900
C	-0.62942300	-1.51655100	-2.49243000
C	-1.47409400	-2.62360800	-2.53873200
H	-2.99750700	-3.74083800	-1.50779800
H	-3.03189100	-2.24795100	0.45713300
H	0.02122300	0.18224600	-1.35429700
H	0.05409700	-1.31453000	-3.31122800
H	-1.45459900	-3.28634700	-3.39844100
P	-1.47169000	0.26405000	1.09458000
C	-2.71371400	-0.44645500	2.23888600
C	-4.00510300	0.06244500	2.38583600
C	-2.32492400	-1.55550300	2.99945300
C	-4.89434300	-0.53142300	3.27905300
H	-4.31369000	0.93276500	1.81464100
C	-3.21913100	-2.15868400	3.87668400
H	-1.30794900	-1.93594500	2.91253900
C	-4.50642200	-1.64332000	4.02034900
H	-5.89171300	-0.11936100	3.39665400
H	-2.90726900	-3.01862200	4.46127100
H	-5.20131200	-2.10206100	4.71685600
C	-2.30165400	1.69790400	0.30589100
C	-1.85535900	2.99148600	0.58781800
C	-3.36262700	1.51215100	-0.59151900
C	-2.47815300	4.08760200	-0.00976200
H	-1.02947200	3.14908300	1.27592000
C	-3.98207000	2.60854100	-1.17968400
H	-3.69834700	0.50643900	-0.83322900
C	-3.53984800	3.89902300	-0.88765500
H	-2.12586800	5.08907600	0.21649700
H	-4.80403400	2.45686800	-1.87256100
H	-4.02168200	4.75430300	-1.35183900
P	2.39069100	-0.92174800	0.62265900
C	1.97883400	-2.37677500	-0.42221100
C	0.99605700	-3.24621700	0.06493700
C	2.59474300	-2.66327600	-1.64249000
C	0.65930100	-4.39907400	-0.63784200
H	0.48040600	-3.00715000	0.99364800
C	2.24696200	-3.80983400	-2.35292500
H	3.33921000	-1.98602500	-2.04875700
C	1.28700500	-4.68312000	-1.84852400
H	-0.10770300	-5.06276200	-0.25067300
H	2.73057600	-4.02118300	-3.30192700
H	1.01921000	-5.57703400	-2.40359900
C	3.80611300	-1.54917700	1.61469200
C	3.92828000	-2.90320600	1.94128400
C	4.68473500	-0.62534600	2.19595200
C	4.90142700	-3.32318400	2.84477700
H	3.26209000	-3.63474300	1.49261300
C	5.65420600	-1.04981500	3.09898200
H	4.60113700	0.43008000	1.95156400
C	5.76003400	-2.39800000	3.43197300

H	4.98646800	-4.37785600	3.08935200
H	6.32082700	-0.32163600	3.55046200
H	6.51106000	-2.72671700	4.14365000
C	3.19472800	0.28034200	-0.50672300
C	4.46776500	0.07419000	-1.05508800
C	2.51229300	1.46541400	-0.80190800
C	5.02535400	1.01700600	-1.91247800
H	5.02857000	-0.81970100	-0.79295000
C	3.07219700	2.41008800	-1.65987900
H	1.54683400	1.66326700	-0.33807400
C	4.32469200	2.18269100	-2.22097200
H	6.01135500	0.84756300	-2.33414300
H	2.53318800	3.32686200	-1.87600800
H	4.76367300	2.91908400	-2.88704000
Pd	0.73856700	0.52406200	2.07280900
C	-0.48132600	2.01021300	4.55957900
C	0.47992100	2.15207300	3.32127100
O	0.50699200	3.22215700	2.74572900
S	2.39219700	1.46312400	3.66438800
C	2.59644800	0.19018700	4.89182100
C	3.07988600	0.56893100	6.14471000
C	2.37595400	-1.16589600	4.62975800
C	3.35084100	-0.39544500	7.11223800
H	3.24061400	1.62128800	6.35921200
C	2.64871500	-2.11771100	5.60157300
H	1.98402400	-1.47022400	3.66294900
C	3.14512900	-1.75053400	6.85739100
H	3.72449700	-0.08436100	8.08451200
H	2.47940300	-3.16906800	5.37965600
C	3.46165400	-2.79919200	7.89227500
H	4.36132500	-3.36163000	7.61797400
H	3.63571700	-2.34901300	8.87302200
H	2.64419800	-3.52035100	7.99005700
Cl	-2.10099500	2.53130900	4.01581700
Cl	0.08058900	3.10223800	5.85038700
Cl	-0.59102800	0.35619100	5.18035400

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C	-2.31643000	-2.78185100	-1.46068400
C	-2.27919600	-1.94926800	-0.34339700
C	-1.45526400	-0.82012100	-0.33687500
C	-0.66782300	-0.54472800	-1.46003400
C	-0.70350900	-1.37738300	-2.57275600
C	-1.53029900	-2.49881700	-2.57427900
H	-2.95864600	-3.65773600	-1.45682900
H	-2.89489300	-2.17782400	0.52224700
H	-0.01133900	0.32415800	-1.45656100
H	-0.07596600	-1.15907100	-3.43121700
H	-1.55040600	-3.15686700	-3.43759600
P	-1.36528300	0.36971400	1.06259600
C	-2.32066300	-0.47544400	2.38339100
C	-3.70386100	-0.35517300	2.53810300
C	-1.60005300	-1.26151400	3.28929400
C	-4.35118700	-1.01121900	3.58229700
H	-4.27456500	0.27138500	1.85888800
C	-2.24780700	-1.91872800	4.33115500
H	-0.51764000	-1.33597300	3.19327700
C	-3.62664500	-1.79206700	4.47969200

H	-5.42474100	-0.90123000	3.70181600
H	-1.67057200	-2.51330600	5.03288900
H	-4.13447100	-2.29206600	5.29857100
C	-2.46408900	1.70344000	0.44183100
C	-2.18674800	3.02794700	0.79363300
C	-3.56035500	1.42556600	-0.38613300
C	-3.01347100	4.05561000	0.34228200
H	-1.32817300	3.26132100	1.41599900
C	-4.38400900	2.45467900	-0.82919700
H	-3.76492600	0.40233000	-0.69113900
C	-4.11215200	3.77202000	-0.46246100
H	-2.79008900	5.08046700	0.62153000
H	-5.23356600	2.22866800	-1.46642200
H	-4.75329700	4.57563300	-0.81225900
P	2.50378400	-0.82127300	0.41315400
C	2.03157600	-2.27349900	-0.60933400
C	1.04473400	-3.12255500	-0.09227500
C	2.59893300	-2.57027100	-1.85026900
C	0.66810700	-4.27101500	-0.78085100
H	0.56011500	-2.87402000	0.85120600
C	2.20605000	-3.71013600	-2.54881000
H	3.34488500	-1.90887300	-2.27946000
C	1.25082100	-4.56770400	-2.01139300
H	-0.09747000	-4.92076800	-0.36780700
H	2.65390000	-3.92891200	-3.51362800
H	0.95067400	-5.45827100	-2.55533700
C	3.77968000	-1.53195900	1.53414300
C	3.78054700	-2.87793500	1.91228400
C	4.67293800	-0.65003500	2.15624900
C	4.64525400	-3.32781200	2.90817300
H	3.10591500	-3.58122700	1.43270200
C	5.53498800	-1.10377600	3.14907000
H	4.68316400	0.39878400	1.87377500
C	5.51692600	-2.44219400	3.53472100
H	4.63544100	-4.37587900	3.19263200
H	6.21277900	-0.40478900	3.62925800
H	6.18259000	-2.79335700	4.31700000
C	3.50867900	0.22545100	-0.70561100
C	4.79104200	-0.14445600	-1.13145300
C	2.97241500	1.44346100	-1.13324500
C	5.50999900	0.67786500	-1.99163000
H	5.22629800	-1.07511200	-0.77540900
C	3.69393000	2.26748100	-1.99577600
H	1.99523100	1.75778400	-0.77000800
C	4.95941300	1.88273100	-2.42793000
H	6.50300500	0.38316700	-2.31672300
H	3.27085800	3.21360800	-2.31823100
H	5.52492800	2.52634100	-3.09479400
Pd	0.90745300	0.76431300	1.81445200
C	-0.25773600	1.91039200	4.41381400
H	0.13654600	2.47089500	5.26452300
H	-0.20943700	0.84049100	4.61647300
C	0.53012000	2.29255900	3.15819600
O	0.47769600	3.38771100	2.64644900
S	2.53421400	1.60692000	3.51049500
C	2.45979300	0.32623800	4.74519400
C	2.78483900	0.65291900	6.06740300
C	2.12377900	-0.99881800	4.45012000

C	2.77489200	-0.32101100	7.05883900
H	3.04481500	1.67910200	6.31140100
C	2.11320400	-1.96597900	5.45052300
H	1.88675300	-1.27487400	3.42665400
C	2.44018400	-1.64676500	6.76960000
H	3.02802800	-0.04594200	8.08014600
H	1.85761700	-2.99205300	5.19493200
C	2.46265500	-2.70046200	7.84683400
H	3.48477900	-3.04954700	8.03319200
H	2.07353100	-2.31072100	8.79207700
H	1.86335400	-3.57031900	7.56467700
Cl	-1.97709200	2.36093200	4.22180200

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C	-1.21291100	-3.19824900	0.31891600
C	-1.05163700	-1.99783800	1.00741400
C	-0.35054500	-0.94031500	0.42165300
C	0.19077400	-1.10641900	-0.85784900
C	0.02975000	-2.30511600	-1.54425000
C	-0.67452000	-3.35341600	-0.95595500
H	-1.75756000	-4.01503500	0.78341800
H	-1.47793300	-1.88228600	1.99981300
H	0.75413200	-0.29348000	-1.31394200
H	0.46886700	-2.42645500	-2.52956500
H	-0.79061700	-4.29438800	-1.48515700
P	-0.14714600	0.69995200	1.22300000
C	-0.70970000	0.39312800	2.94235600
C	-2.05284100	0.45964900	3.32059900
C	0.25761200	0.08684500	3.90447300
C	-2.42012300	0.21532700	4.64169900
H	-2.81076800	0.71324600	2.58402000
C	-0.11048900	-0.15927300	5.22365100
H	1.30928700	0.06726900	3.62320800
C	-1.45170800	-0.09450800	5.59360600
H	-3.46541600	0.27485700	4.92908700
H	0.65309400	-0.38377100	5.96237500
H	-1.74090600	-0.27637700	6.62417300
C	-1.53383300	1.64398200	0.46640700
C	-1.56512700	3.03653200	0.60989800
C	-2.57030600	1.00385100	-0.22567000
C	-2.62145400	3.76912300	0.07531700
H	-0.77160800	3.55186300	1.13659900
C	-3.62260700	1.74372600	-0.75776300
H	-2.55992200	-0.07455500	-0.35079800
C	-3.65033900	3.12774500	-0.60852300
H	-2.63235600	4.84827800	0.19156500
H	-4.42033400	1.23527600	-1.29064300
H	-4.46991700	3.70389000	-1.02754900
P	3.66420100	-0.48071100	0.21114400
C	3.17828500	-2.23467200	-0.03748200
C	2.41529400	-2.82553200	0.97777000
C	3.51446000	-2.99214200	-1.16173600
C	2.02660200	-4.15748800	0.88761700
H	2.11024600	-2.23041100	1.83743500
C	3.10972400	-4.32216500	-1.25916800
H	4.08422900	-2.54380000	-1.96969700
C	2.37428200	-4.90884900	-0.23360500
H	1.43272300	-4.60116000	1.68085000

H	3.37446800	-4.90072100	-2.13910000
H	2.06177500	-5.94588600	-0.31130900
C	5.22537400	-0.63064800	1.17467800
C	5.48851600	-1.71622300	2.01509800
C	6.09640200	0.46620100	1.18312300
C	6.59289800	-1.69419800	2.86468600
H	4.83317900	-2.58246300	2.01103500
C	7.19516100	0.48505300	2.03554400
H	5.90242400	1.31725400	0.53703400
C	7.44141300	-0.59100500	2.88493500
H	6.78784500	-2.54327000	3.51317200
H	7.85089000	1.35007800	2.04324400
H	8.29373800	-0.57056300	3.55689900
C	4.27084200	0.08350300	-1.42288400
C	5.46454400	-0.38835200	-1.98386100
C	3.52471100	1.04356800	-2.11239600
C	5.88598000	0.07125000	-3.22664900
H	6.06844700	-1.10606000	-1.43366300
C	3.94920400	1.50561900	-3.35752900
H	2.62151600	1.45005300	-1.65974100
C	5.12561300	1.01576400	-3.91595600
H	6.81271200	-0.29932100	-3.65380700
H	3.36725900	2.25753100	-3.88091800
H	5.46066900	1.37976300	-4.88231400
Pd	2.16149000	1.43847900	1.20783100
C	1.29048000	3.40828300	3.34170600
H	1.52915000	4.40420100	3.72909500
C	1.75474200	3.31077000	1.88975600
O	1.43843300	4.11966800	1.05202300
S	3.96313900	2.97589000	2.01182800
C	4.37619100	2.26441100	3.58938700
C	4.12323100	0.92741200	3.92470200
C	5.02450900	3.06851200	4.53305100
C	4.51094700	0.41790500	5.15789000
H	3.64312100	0.27598100	3.19973900
C	5.41425600	2.54761700	5.76331600
H	5.22659600	4.10854300	4.29370400
C	5.16678700	1.21601700	6.09903500
H	4.31309500	-0.62771300	5.38591800
H	5.91919700	3.19289500	6.47830600
C	5.60334700	0.64358700	7.42326500
H	4.77350500	0.14517600	7.93475400
H	6.39604200	-0.10081400	7.28875100
H	5.98735000	1.42386100	8.08564300
H	1.73182100	2.62970400	3.96794400
F	-0.08418500	3.25306800	3.33447400

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C	-3.03263700	-3.05098800	-0.86134300
C	-2.90227400	-2.04395000	0.09560400
C	-1.82351300	-1.15877100	0.04888000
C	-0.89453900	-1.28702300	-0.99309700
C	-1.03011600	-2.28202800	-1.95267100
C	-2.09733900	-3.17673200	-1.88237400
H	-3.87648300	-3.73245500	-0.80793100
H	-3.65360900	-1.94755000	0.87221000
H	-0.05443900	-0.59823000	-1.05593400
H	-0.29095500	-2.36938600	-2.74289600

H	-2.20034300	-3.96270700	-2.62440700
P	-1.49671900	0.15957900	1.29746200
C	-3.01133100	0.17807700	2.32969300
C	-3.83642800	1.30061200	2.42289600
C	-3.29687300	-0.94274400	3.12201500
C	-4.94321700	1.29132800	3.27049500
H	-3.61632100	2.18620400	1.83498200
C	-4.41494700	-0.95900200	3.94728700
H	-2.63627400	-1.80670600	3.09568900
C	-5.24190100	0.16077600	4.02363400
H	-5.57605800	2.17142400	3.33316600
H	-4.62463500	-1.83652900	4.55141400
H	-6.10945300	0.15374400	4.67658400
C	-1.66856300	1.67702600	0.26694500
C	-1.02209500	2.84418700	0.69413200
C	-2.40347200	1.69599900	-0.92325000
C	-1.10455900	4.00758100	-0.06867100
H	-0.46724300	2.84050000	1.62996100
C	-2.47768700	2.85929300	-1.68475300
H	-2.91127000	0.79640900	-1.25957100
C	-1.82499500	4.01507800	-1.26088200
H	-0.60023500	4.90725000	0.27041300
H	-3.04664700	2.86202200	-2.60952500
H	-1.88108300	4.92104500	-1.85713400
P	2.46012100	-0.55183800	0.70295400
C	2.07900900	-2.20338900	-0.00826500
C	1.24244500	-3.02959100	0.75192300
C	2.52905200	-2.65084100	-1.25359300
C	0.86551200	-4.28266800	0.28085800
H	0.86025900	-2.66424500	1.70424100
C	2.14630700	-3.90395300	-1.72784600
H	3.16568100	-2.01480500	-1.86241000
C	1.31365300	-4.71891800	-0.96381100
H	0.20438900	-4.90707100	0.87355400
H	2.49450000	-4.24138700	-2.69961900
H	1.00676800	-5.68927100	-1.34227800
C	4.10260100	-0.80260100	1.48271100
C	4.68807400	-2.05905600	1.65747300
C	4.70536600	0.32014500	2.06917300
C	5.85075700	-2.19165400	2.41770500
H	4.23091600	-2.93795100	1.21159800
C	5.86956800	0.18615700	2.81494500
H	4.24125500	1.29814400	1.95956400
C	6.44032500	-1.07389500	2.99938900
H	6.29480200	-3.17352700	2.55266500
H	6.32242800	1.06178900	3.26944100
H	7.34057500	-1.18038000	3.59668000
C	2.87770300	0.48981700	-0.74932000
C	4.11651600	0.42676400	-1.39882500
C	1.91507500	1.39765400	-1.20444500
C	4.37512500	1.23901400	-2.49858300
H	4.88257200	-0.25191700	-1.03123200
C	2.17311800	2.20667800	-2.30893000
H	0.96515800	1.48682800	-0.68099000
C	3.40192000	2.12603000	-2.95769900
H	5.33930900	1.18419700	-2.99499600
H	1.41510300	2.90643700	-2.64758800
H	3.60894400	2.76122300	-3.81366100

Pd	0.70728300	0.24857800	2.30757000
C	-0.08340700	1.31006100	4.18516100
O	-0.55169100	2.39021000	3.85520500
S	1.82441600	1.30343300	4.35827500
C	-0.85073400	0.32290400	5.01821600
C	-0.56143900	-1.04306200	5.08340500
C	-1.92018400	0.83780900	5.75447400
C	-1.31603700	-1.87637800	5.90253700
H	0.25011200	-1.45306800	4.48818400
C	-2.66782600	0.00331000	6.57867700
H	-2.15015600	1.89417500	5.66071100
C	-2.36271900	-1.35328200	6.66040100
H	-1.08086900	-2.93525600	5.95283500
H	-3.49813600	0.41080900	7.14791100
H	-2.94579300	-2.00473200	7.30500600
C	2.30807400	-0.05367600	5.41221700
C	3.03643400	-1.12717300	4.89512900
C	2.00723000	-0.00989300	6.77580100
C	3.45324900	-2.15365400	5.73748300
H	3.27156800	-1.15883000	3.83610900
C	2.41488800	-1.04629200	7.61038400
H	1.44138700	0.82826600	7.17202300
C	3.13877500	-2.11886800	7.09428700
H	4.02450300	-2.98022400	5.32511900
H	2.16686000	-1.01380300	8.66678700
H	3.45924500	-2.92374300	7.74864000

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C	-3.01528500	-3.06999400	-0.84643400
C	-2.88908000	-2.05940200	0.10727100
C	-1.81477200	-1.16906400	0.05695900
C	-0.88581200	-1.29602400	-0.98524700
C	-1.01731200	-2.29467700	-1.94160400
C	-2.08016100	-3.19430200	-1.86777300
H	-3.85577200	-3.75538000	-0.79027100
H	-3.64038700	-1.96405400	0.88400900
H	-0.04932800	-0.60307000	-1.05130800
H	-0.27849300	-2.38075500	-2.73227500
H	-2.17996400	-3.98293000	-2.60743500
P	-1.49438400	0.15374700	1.30222100
C	-3.01218900	0.17326100	2.32968300
C	-3.84211700	1.29306800	2.41210200
C	-3.29664400	-0.94370800	3.12773700
C	-4.95224000	1.28485300	3.25532300
H	-3.62307000	2.17570500	1.81941100
C	-4.41798500	-0.95910000	3.94859300
H	-2.63268500	-1.80525900	3.10962100
C	-5.24946800	0.15798500	4.01449800
H	-5.58866800	2.16287500	3.30996100
H	-4.62668300	-1.83353200	4.55750500
H	-6.11945600	0.15181100	4.66420600
C	-1.66443400	1.66792900	0.26653000
C	-1.02477400	2.83840000	0.69511100
C	-2.39098600	1.68118800	-0.92885400
C	-1.10532200	3.99918300	-0.07186900
H	-0.47698000	2.83939200	1.63516400
C	-2.46330200	2.84202700	-1.69433300
H	-2.89372300	0.77922400	-1.26631900

C	-1.81710300	4.00100400	-1.26929600
H	-0.60633700	4.90141300	0.26830200
H	-3.02578000	2.84030600	-2.62307200
H	-1.87165100	4.90504100	-1.86862200
P	2.46087300	-0.54224800	0.71582800
C	2.08549100	-2.19662700	0.00857800
C	1.25173700	-3.02371700	0.77090600
C	2.53762600	-2.64581200	-1.23534700
C	0.87945200	-4.27939500	0.30306600
H	0.86806200	-2.65715100	1.72219300
C	2.15971500	-3.90164500	-1.70622200
H	3.17222500	-2.00907300	-1.84556500
C	1.32970200	-4.71746500	-0.94021200
H	0.22039200	-4.90460600	0.89720700
H	2.50954900	-4.24057000	-2.67689000
H	1.02655100	-5.69000800	-1.31607300
C	4.10325900	-0.78653700	1.49765800
C	4.69614500	-2.04005200	1.66842400
C	4.69851700	0.33776200	2.08860600
C	5.85879400	-2.16831100	2.42938600
H	4.24455900	-2.92017300	1.21935000
C	5.86253600	0.20807600	2.83540800
H	4.22912700	1.31344900	1.98154500
C	6.44072100	-1.04910300	3.01592200
H	6.30845400	-3.14800600	2.56151500
H	6.30939300	1.08482100	3.29367000
H	7.34076900	-1.15221100	3.61411600
C	2.87628900	0.49749000	-0.73841500
C	4.11608600	0.43778000	-1.38631800
C	1.91087900	1.40092300	-1.19633900
C	4.37292600	1.24895800	-2.48728500
H	4.88420600	-0.23733500	-1.01648600
C	2.16718500	2.20893800	-2.30195200
H	0.96006800	1.48771500	-0.67421400
C	3.39703400	2.13161600	-2.94912000
H	5.33788600	1.19682900	-2.98248400
H	1.40696000	2.90538500	-2.64244800
H	3.60281400	2.76609500	-3.80591600
Pd	0.70472500	0.25546700	2.32902200
C	-0.08964700	1.30752400	4.18397300
O	-0.55368900	2.39023700	3.85300200
S	1.82282300	1.30269600	4.37545600
C	-0.86046500	0.32983500	5.02575300
C	-0.57506100	-1.03625200	5.10324700
C	-1.93082300	0.85334700	5.75466900
C	-1.33462100	-1.86079400	5.92696300
H	0.23726700	-1.45332200	4.51416500
C	-2.68368600	0.02774800	6.58297800
H	-2.15737200	1.90952300	5.65106900
C	-2.38261700	-1.32903800	6.67678900
H	-1.10271700	-2.91998000	5.98647600
H	-3.51491400	0.44221400	7.14584900
H	-2.96990300	-1.97383700	7.32429100
C	2.30494100	-0.06157400	5.41833200
C	3.02436000	-1.13841000	4.89977400
C	2.01621700	-0.02543000	6.78541500
C	3.44087700	-2.16753300	5.73891600
H	3.25811700	-1.17251100	3.84046000

C	2.42676200	-1.06484500	7.61101300
H	1.45883000	0.81308500	7.19301400
C	3.14410800	-2.15211300	7.10277300
H	4.00844200	-2.99483200	5.31931300
H	2.18854200	-1.03125000	8.67143300
C	3.56894200	-3.27999300	8.00795400
H	2.71375100	-3.90963800	8.27779200
H	4.31326200	-3.91814900	7.52455300
H	3.99939300	-2.89932700	8.93921800

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C	-2.99553100	-2.78521100	-1.24103300
C	-2.86580500	-1.85806000	-0.20682800
C	-1.76759600	-0.99627200	-0.16186500
C	-0.81792000	-1.06364200	-1.19027100
C	-0.95120600	-1.98092000	-2.22499400
C	-2.03899000	-2.85329900	-2.24745100
H	-3.85432900	-3.44962700	-1.25806100
H	-3.63059700	-1.80730900	0.56099400
H	0.04221200	-0.39724700	-1.17609100
H	-0.19336400	-2.02887500	-3.00101400
H	-2.13889700	-3.58056100	-3.04760200
P	-1.46146400	0.22753000	1.18455500
C	-2.91928600	0.02751100	2.27615300
C	-3.79388300	1.07695100	2.56135800
C	-3.09653000	-1.20285600	2.92522000
C	-4.84953000	0.88681200	3.45311600
H	-3.64923800	2.04517800	2.09208500
C	-4.16095400	-1.39686600	3.79575500
H	-2.39538200	-2.01533800	2.74248500
C	-5.04269000	-0.34899000	4.06090500
H	-5.52420600	1.71022900	3.66723000
H	-4.28985000	-2.35791900	4.28419500
H	-5.86874900	-0.49519700	4.75045800
C	-1.78748900	1.80816400	0.30281500
C	-1.08703200	2.95469600	0.69327600
C	-2.71134800	1.89152500	-0.74535500
C	-1.30447700	4.16529300	0.03743400
H	-0.39052500	2.90049500	1.52616400
C	-2.92484000	3.10131900	-1.39836100
H	-3.25766800	1.00412800	-1.05432600
C	-2.21879400	4.23888300	-1.00959500
H	-0.75788100	5.05010300	0.34869800
H	-3.64055400	3.15636600	-2.21301400
H	-2.38432400	5.18207100	-1.52161300
P	2.48275900	-0.68101200	0.77872700
C	1.93787000	-2.27709700	0.04083700
C	0.92150000	-2.97021900	0.70834800
C	2.44482900	-2.79846100	-1.15291900
C	0.41636900	-4.16010600	0.19255600
H	0.50251400	-2.54870700	1.62119900
C	1.93712200	-3.98679800	-1.67168500
H	3.22381600	-2.26651600	-1.69096000
C	0.92104200	-4.66619900	-1.00219100
H	-0.38685000	-4.67595000	0.70933600
H	2.33092500	-4.37914500	-2.60452800
H	0.51788600	-5.58531400	-1.41646700
C	4.09078100	-1.11489300	1.55299200

C	4.35223800	-2.40611100	2.02039800
C	4.98819400	-0.08365000	1.86596000
C	5.48579600	-2.66009500	2.79172700
H	3.66541800	-3.21552900	1.78780100
C	6.12114100	-0.34104100	2.62994800
H	4.78926900	0.92799900	1.51891200
C	6.36954400	-1.62979400	3.10244700
H	5.67661600	-3.66724100	3.15077600
H	6.80605700	0.46745200	2.86624200
H	7.24824400	-1.82975600	3.70759300
C	3.00454200	0.33912500	-0.65665600
C	4.20476400	0.12802400	-1.34707300
C	2.16368000	1.38250600	-1.05896200
C	4.54065100	0.92598400	-2.43590900
H	4.88593300	-0.65276700	-1.01738500
C	2.49838900	2.17838700	-2.15310800
H	1.24829700	1.58057600	-0.50339900
C	3.68441400	1.94799400	-2.84390700
H	5.47409000	0.75425100	-2.96310900
H	1.83497900	2.98344800	-2.45371100
H	3.94970300	2.57058900	-3.69279600
Pd	0.71398100	0.30654600	2.24436200
C	-0.25423800	1.34349500	4.12148400
O	-0.87035000	2.34668700	3.81178200
S	1.64496400	1.58024500	4.27650200
C	-0.85949600	0.23342500	4.93138900
C	-0.37850900	-1.07965300	4.95229200
C	-1.96981700	0.57572000	5.70609300
C	-0.98708300	-2.03042500	5.76376800
H	0.47376600	-1.35595700	4.33575500
C	-2.56696600	-0.37466400	6.52795700
H	-2.35032900	1.59033500	5.64712200
C	-2.07242700	-1.67590700	6.56451700
H	-0.60535400	-3.04665100	5.78116900
H	-3.42723700	-0.10086300	7.13123200
H	-2.53495500	-2.41694100	7.20975300
C	2.25842900	0.36218500	5.42292100
C	3.20552900	-0.57728600	5.00452300
C	1.82703500	0.37701800	6.75454900
C	3.71140200	-1.50840500	5.90288300
H	3.54043600	-0.58639100	3.97287900
C	2.31440500	-0.55817000	7.65749000
H	1.09337200	1.11037300	7.07405400
C	3.24813200	-1.48554900	7.21172200
H	4.44418500	-2.24471000	5.59581000
H	1.98687500	-0.57944400	8.68946600
N	3.76483300	-2.48001800	8.16166600
O	3.34197600	-2.44336200	9.30265400
O	4.58353500	-3.28098000	7.74825200

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C	-3.00866100	-3.05596600	-0.87294300
C	-2.88052900	-2.05704100	0.09260800
C	-1.80601900	-1.16635700	0.05187800
C	-0.87930200	-1.28045200	-0.99373700
C	-1.01233800	-2.26790400	-1.96160600
C	-2.07500400	-3.16839700	-1.89692400

H	-3.84941500	-3.74154600	-0.82366400
H	-3.63080200	-1.97137100	0.87133800
H	-0.04328200	-0.58652900	-1.05347400
H	-0.27462200	-2.34472700	-2.75429300
H	-2.17589600	-3.94833000	-2.64560500
P	-1.48636300	0.14348300	1.31190800
C	-2.99929200	0.13436600	2.34692900
C	-3.84067200	1.24359700	2.45213300
C	-3.27085300	-1.00013200	3.12427600
C	-4.95015000	1.20703100	3.29575000
H	-3.63189100	2.13979200	1.87605800
C	-4.39254200	-1.04444800	3.94344000
H	-2.59798400	-1.85418100	3.08868700
C	-5.23629800	0.06186000	4.03152500
H	-5.59574400	2.07706400	3.36813300
H	-4.59521200	-1.93662100	4.52910100
H	-6.10676600	0.03354400	4.68012200
C	-1.67667700	1.66789200	0.29506300
C	-1.03302700	2.83575300	0.72427600
C	-2.42294700	1.69043600	-0.88820000
C	-1.12966500	4.00371700	-0.02995600
H	-0.46902900	2.82920000	1.65454800
C	-2.51147900	2.85835500	-1.64077400
H	-2.92824500	0.78995900	-1.22598900
C	-1.86150700	4.01510500	-1.21509000
H	-0.62736600	4.90400300	0.31049300
H	-3.08904600	2.86395200	-2.56017400
H	-1.92863800	4.92482400	-1.80449700
P	2.46840000	-0.54885900	0.70613600
C	2.08991900	-2.19545000	-0.01678100
C	1.25621100	-3.02805500	0.73952600
C	2.53942600	-2.63408200	-1.26543400
C	0.88142400	-4.27901900	0.26132700
H	0.87493800	-2.66952300	1.69484900
C	2.15887900	-3.88516700	-1.74672300
H	3.17397100	-1.99291700	-1.87115300
C	1.32902900	-4.70662300	-0.98653300
H	0.22261300	-4.90854200	0.85117500
H	2.50656200	-4.21607400	-2.72092900
H	1.02401200	-5.67542700	-1.37047600
C	4.11270300	-0.80198900	1.48073300
C	4.70206600	-2.05856700	1.64153100
C	4.71246500	0.31631200	2.07847700
C	5.86545600	-2.19587300	2.39968200
H	4.24684500	-2.93397200	1.18695300
C	5.87725600	0.17760000	2.82254900
H	4.24669200	1.29439400	1.97819800
C	6.45169300	-1.08262300	2.99331600
H	6.31236900	-3.17779700	2.52428300
H	6.32774400	1.04965200	3.28617000
H	7.35230400	-1.19293100	3.58938100
C	2.87705300	0.50828900	-0.73713100
C	4.11380000	0.45877300	-1.39173000
C	1.90864900	1.41689600	-1.17818900
C	4.36440400	1.28544400	-2.48264500
H	4.88474600	-0.21997800	-1.03457100
C	2.15846200	2.24005700	-2.27394300
H	0.96045900	1.49583300	-0.65005900

C	3.38535600	2.17308800	-2.92783300
H	5.32711900	1.24159700	-2.98299100
H	1.39576200	2.94011800	-2.60132900
H	3.58630200	2.81968000	-3.77669400
Pd	0.71707000	0.24006400	2.33456600
C	-0.06082100	1.28671300	4.18993800
O	-0.50667600	2.37885700	3.86562500
S	1.85807700	1.25933200	4.38167500
C	-0.84506200	0.31687900	5.02443800
C	-0.57422300	-1.04960500	5.11345400
C	-1.92522600	0.84498300	5.73746300
C	-1.35563500	-1.86475500	5.92666500
H	0.24441800	-1.47975400	4.54269700
C	-2.69517800	0.02513600	6.55084600
H	-2.14438400	1.90274500	5.63385900
C	-2.42006500	-1.34105000	6.66277100
H	-1.12968500	-2.92616300	5.99341900
H	-3.53487400	0.44724300	7.09876500
C	-3.27835200	-2.22400900	7.53198600
H	-3.41307200	-1.78924500	8.52726800
H	-4.27675300	-2.35062000	7.09678800
H	-2.83697000	-3.21693200	7.65117000
C	2.32814200	-0.11753700	5.41444900
C	3.04074900	-1.19460000	4.88230200
C	2.03073600	-0.08831500	6.77926700
C	3.44457200	-2.23795100	5.71007600
H	3.27414600	-1.21536900	3.82260500
C	2.42622100	-1.14075200	7.59962900
H	1.47674400	0.75202400	7.18737800
C	3.13363900	-2.21674500	7.06808100
H	4.00304900	-3.06706800	5.28543300
H	2.18100200	-1.11842300	8.65699200
H	3.44395000	-3.03477700	7.71090100

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C	-2.95075700	-3.11585100	-0.80292100
C	-2.83292500	-2.10609700	0.15251300
C	-1.78494900	-1.18610600	0.08492400
C	-0.87289300	-1.28388400	-0.97526400
C	-0.99636300	-2.28223700	-1.93310000
C	-2.03313900	-3.21027300	-1.84299900
H	-3.77062000	-3.82448600	-0.73260200
H	-3.57093100	-2.03514100	0.94436500
H	-0.05654500	-0.56871000	-1.05517100
H	-0.27082900	-2.34593100	-2.73812600
H	-2.12578400	-3.99842500	-2.58413100
P	-1.48042700	0.13530100	1.33622400
C	-3.00611200	0.12763800	2.35440100
C	-3.88656100	1.21077400	2.39410000
C	-3.25836500	-0.98311900	3.17098300
C	-5.01334600	1.17050000	3.21402000
H	-3.69551900	2.08863300	1.78464700
C	-4.39477900	-1.03193500	3.97039500
H	-2.55917600	-1.81624700	3.18098600
C	-5.27657800	0.04778800	3.99188400
H	-5.69005500	2.01936400	3.23511000
H	-4.57591300	-1.90164100	4.59611400
H	-6.16126100	0.01701700	4.62112600

C	-1.66792200	1.65250600	0.30831400
C	-1.03914500	2.82680200	0.74210400
C	-2.39894700	1.66493800	-0.88461200
C	-1.13396400	3.99090400	-0.01839900
H	-0.48639800	2.82796200	1.67936900
C	-2.48611800	2.82935500	-1.64283800
H	-2.89371100	0.75978800	-1.22531100
C	-1.85006300	3.99242200	-1.21319000
H	-0.64267300	4.89606300	0.32516500
H	-3.05185600	2.82736000	-2.56957500
H	-1.91592000	4.89933200	-1.80707900
P	2.46561100	-0.54691800	0.70521800
C	2.09454800	-2.18954700	-0.02834300
C	1.26855000	-3.03167700	0.72582900
C	2.54730200	-2.61975800	-1.27872600
C	0.90506600	-4.28455000	0.24410600
H	0.88478300	-2.67968600	1.68266200
C	2.17836900	-3.87301700	-1.76336500
H	3.17616600	-1.97108500	-1.88251200
C	1.35694100	-4.70451400	-1.00486600
H	0.25160300	-4.92146000	0.83194800
H	2.52886200	-4.19815700	-2.73851200
H	1.06166100	-5.67542900	-1.39117700
C	4.11483600	-0.79695400	1.46977000
C	4.71965000	-2.04948800	1.60249900
C	4.70447200	0.31654300	2.08598100
C	5.88905100	-2.18781200	2.35093400
H	4.27164100	-2.92119400	1.13395600
C	5.87487000	0.17675400	2.82116700
H	4.22728900	1.29094800	2.00691200
C	6.46522400	-1.07948800	2.96335100
H	6.34787200	-3.16666100	2.45435700
H	6.31753500	1.04478700	3.29962900
H	7.37039100	-1.19090700	3.55227300
C	2.85727500	0.52966000	-0.72820800
C	4.08893100	0.49957700	-1.39360600
C	1.87906500	1.43786500	-1.14730200
C	4.32378100	1.34544800	-2.47342500
H	4.86865500	-0.17774900	-1.05307300
C	2.11280200	2.28024300	-2.23171700
H	0.93544300	1.50218400	-0.60974800
C	3.33467500	2.23277000	-2.89651800
H	5.28268400	1.31748600	-2.98215800
H	1.34163400	2.97966100	-2.54024100
H	3.52405000	2.89473800	-3.73614500
Pd	0.72531100	0.24152700	2.37245100
C	-0.01020000	1.29508200	4.19489000
O	-0.41431900	2.40492200	3.87138900
S	1.92477300	1.21797100	4.39528500
C	-0.82164300	0.36867800	5.04807800
C	-0.58681500	-1.00469500	5.17828300
C	-1.90508000	0.93650500	5.72187700
C	-1.40436100	-1.79030600	5.97760500
H	0.23327300	-1.46808000	4.63716300
C	-2.72488700	0.15959400	6.52885200
H	-2.09703500	1.99617100	5.58985100
C	-2.47660100	-1.20694500	6.65467100
H	-1.23363200	-2.85618100	6.08555800

H	-3.57734400	0.60686500	7.03594000
C	2.36646100	-0.18274200	5.40689500
C	3.03056900	-1.28192900	4.85616400
C	2.08692700	-0.15661900	6.77560900
C	3.40147700	-2.34910400	5.66881400
H	3.25156100	-1.30067700	3.79360400
C	2.44990800	-1.23211000	7.58127600
H	1.57090700	0.70051500	7.19810300
C	3.10689900	-2.33012800	7.03068300
H	3.92099000	-3.19589600	5.22999700
H	2.21731800	-1.21139200	8.64150400
H	3.39055500	-3.16726100	7.66099600
O	-3.26651000	-2.02643500	7.40197300
H	-3.95703100	-1.49600000	7.82427100

4. The calculation details of the solvent effect

In order to examine the solvent effect, the C-S bond BDE and BDFE values of 34 thioesters were investigated in the solvent phase (solvent = THF, SMD model). All these calculations are based on the optimized structures in the gas phase. The LanL2DZ basis set combined with the polarization function ($\zeta(f) = 1.472$) were used for Pd atom, and the 6-311+G(2df,2p) basis set was used for the other atoms. The results are shown in Table S2. In solvent the BDE and BDFE data are decline compared with that of the gas phase. There still has a better linear relationship between BDE and BDFE values of the solvent phase, as shown Figure S3. The linear equation still is $BDE = BDFE + 12.98$.

Table S2. The calculated bond dissociation enthalpy (BDE, kcal•mol⁻¹) and bond dissociation free energy (BDFE, kcal•mol⁻¹) of the C-S bond cleavage process for selected thioesters **1-34** in the solvent phase.

Thioester	1	2	3	4	5	6	7	8	9	10
BDE	74.67	74.45	74.55	74.60	74.34	74.44	73.83	74.12	73.90	74.22
BDFE	61.97	60.83	61.39	63.28	61.74	61.85	60.48	61.17	61.06	61.43
	11	12	13	14	15	16	17	18	19	20
BDE	73.23	75.00	72.73	73.49	64.28	63.00	72.12	64.38	59.59	65.63
BDFE	60.70	61.54	59.32	60.15	51.10	50.38	58.85	51.43	46.28	52.64
	21	22	23	24	25	26	27	28	29	30
BDE	65.45	62.65	66.51	72.65	66.57	64.30	65.73	65.46	65.70	71.99
BDFE	52.20	49.72	53.56	59.78	54.27	51.99	51.95	53.08	51.84	58.84
	31	32	33	34						
BDE	63.63	71.23	71.82	71.65						
BDFE	50.66	58.06	58.53	58.43						

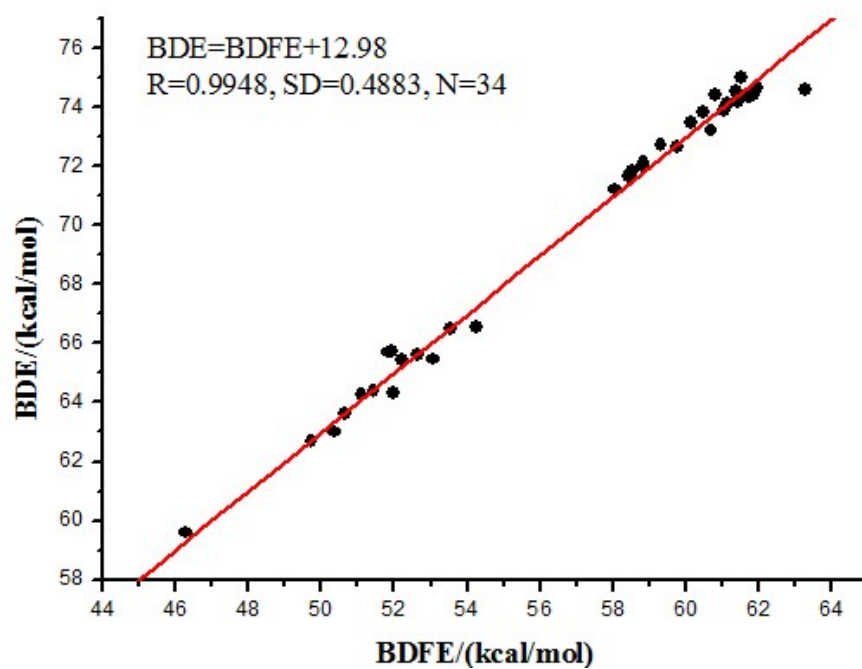


Figure S3. The linear correlation plots between BDE and BDFE values (in solvent).