

Realistic modelling of hydrogen bonding of 2-cyclohexenone with H₂O and H₃BO₃ in the outer coordination sphere of a chiral diene/Rh(I) complex by *ab initio* molecular dynamics.

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SUPPORTING INFORMATION

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1. Molecular dynamics methods

The three full DFT AIMD simulations **S1**, **S2** and **S3** (described in the main text) were carried out using the free open source software CP2K.¹ The simulations were performed in NVT ensemble at 300 K, and the equations of motion were integrated with a time step of 1.0 fs over total simulation length of 20 ps. Temperature was controlled via Nose thermostat.² All DFT computations were performed by CP2K's QUICKSTEP module³ using Perdew – Burke – Ernzerhof (PBE) exchange-correlation functional⁴ augmented with Grimme's DFT-D3 dispersion correction.⁵ For all atoms, atom kind-specific Goedecker – Teter – Hutter (GTH) pseudopotentials⁶ incorporating scalar-relativistic core corrections (where applicable) for the inner electrons and mixed Gaussian – plane waves (GPW)⁷ contracted double- ζ with polarisation (DZVP) MOLOPT basis set⁸ for the valence electrons were employed. Periodic boundary conditions were applied in all three dimensions in a cubic cell with edge length of 20.1 Å. The orbital transformation method⁹ was employed for an efficient wavefunction optimization. QUICKSTEP requires the use of a real-space (RS) integration grid to represent the electron density and the product Gaussian functions. RS grid(s) employs a multi-grid system for mapping the product Gaussians, so that wide and smooth Gaussian functions are mapped onto a coarser grid than narrow and sharp Gaussians. The electron density is always mapped onto the finest grid. Choosing a sufficiently fine integration grid for a calculation is crucial in obtaining meaningful and accurate results. The relative cutoff parameter was set to 50 Ry and the grid cutoff was 300 Ry for the BOMD simulations.¹⁰ With this setup for the grid cutoff, 60% of the Gaussian functions are spawned on the finest grid and less than 4% on the two coarsest.

The thermodynamic stability of the formed H-bonded complexes was investigated by well-tempered metadynamics (WTMetaD) simulations¹¹ **M1**, **M2** and **M3** (described in the text) with time step of 0.5 fs. The initial step **M1-3** was taken from step 20000 (or at 20th ps) of simulations **S1-3**, respectively. This method focuses the computational effort only on the physically relevant regions of the collective variable space by depositing adaptive Gaussian-shaped potentials at specified intervals. The WW parameter, which defines the Gaussian height, was 0.02 hartree, the ΔT parameter was 750 K, and the maximum interval between hills deposition was 100 steps. **M1-3** simulations were performed in the phase space of one or two collective variables (CV) as implemented in CP2K code. For system **M1** and **M2**, a single CV was defined as the coordination number of the ketone O atom (O_k) with respect to the O atom from the closest H₂O molecule or closest O atom from H₃BO₃, respectively. The cutoff distance (where CV = 0) was set to 3.7 Å for both. For **M3**, CV1 was defined as coordination number of the carbonyl O atom with respect to the B atom from H₃BO₃, and CV2 as the coordination number of the carbonyl O atom with the O atom from closest water molecule. The cutoff distances were set to 5.0 Å and 4.2 Å for CV1 and CV2, respectively.

2. Molecular dynamics restart files

The restart files at step 5000, after the initial thermal equilibration has occurred, are given below in their entirety for simulations **S1**, **S2** and **S3**. To reproduce the production part of the trajectory, run those files in a dedicated directory after entering the relevant basis set paths (marked in red).

Simulation S1

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  PRINT_LEVEL MEDIUM
  PROJECT_NAME MD
  RUN_TYPE MD
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&MOTION
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  ENSEMBLE NVT
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  STEP_START_VAL 5000
  TIME_START_VAL 4.9999999999995689E+03
  ECONS_START_VAL -3.3889856929344137E+03
  TEMPERATURE 3.0000000000000000E+02
&THERMOSTAT
  TYPE NOSE
  REGION GLOBAL
&NOSE
  LENGTH 4
  YOSHIDA 3
  MTS 2
&COORD
  1.8295652469857195E+01 9.7800992561186373E+00 4.5270578546405043E+00
&END COORD
&VELOCITY
  8.6775824218393374E-05 2.4952612515800068E-05 3.0135837709043843E-06
&END VELOCITY
&MASS
  1.6237299232570694E+06 1.6237299232570694E+06 1.6237299232570694E+06
&END MASS
&FORCE
  5.7601845135679237E-10 9.2369772848815942E-12 -3.2865883712449332E-10 3.7532732862611510E-11 -
&END FORCE
&END NOSE
&CSVR
  TIMECON 9.9999999999999986E+01
&END CSVR
&END THERMOSTAT
&AVERAGES T
&RESTART_AVERAGES
  ITIMES_START 1
  AVECPU 1.5875835823063701E+02
  AVEHUGONIOT 0.0000000000000000E+00
  AVETEMP_BARO 0.0000000000000000E+00
  AVEPOT -3.3897892214495191E+03
  AVEKIN 1.0178987102972687E+00
  AVETEMP 2.7507625746254149E+02
  AVEKIN_QM 0.0000000000000000E+00
  AVETEMP_QM 0.0000000000000000E+00
  AVEVOL 5.4800532563775429E+04
  AVECELL_A 3.7983495271001452E+01
  AVECELL_B 3.7983495271001452E+01
  AVECELL_C 3.7983495271001452E+01
  AVEALPHA 9.0000000000000000E+01
  AVEBETA 9.0000000000000000E+01
  AVEGAMMA 9.0000000000000000E+01
  AVE_ECONS 5.3505765414851236E+00
  AVE_PRESS 0.0000000000000000E+00
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&END AVERAGES
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  &TRAJECTORY SILENT
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  LOG_PRINT_KEY T
  FORMAT DCD_ALIGNED_CELL
  &EACH
    MD 1
  &END EACH
&END TRAJECTORY
&VELOCITIES OFF
  ADD_LAST NUMERIC
  LOG_PRINT_KEY T
  FORMAT XMOL
  &EACH
    MD 1
  &END EACH
&END VELOCITIES
&RESTART SILENT
  ADD_LAST NUMERIC
  LOG_PRINT_KEY T
  BACKUP_COPIES 0
  &EACH
    MD 10
  &END EACH
&END RESTART
&END PRINT
&END MOTION
&FORCE_EVAL
METHOD QS
&DFT
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  POTENTIAL_FILE_NAME insert basis set path here
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  CHARGE 0
  &SCF
    MAX_SCF 60
    EPS_SCF 9.9999999999999995E-07
    SCF_GUESS ATOMIC
    &OT T
      MINIMIZER DIIS
      PRECONDITIONER FULL_SINGLE_INVERSE
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    &RESTART SILENT
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&END SCF
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  REL_CUTOFF 5.0000000000000000E+01
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&END VDW_POTENTIAL
&END XC
&POISSON
&END POISSON
&LOCALIZE T
&END LOCALIZE
&END DFT
&SUBSYS
&CELL
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  C 0.000000000000000E+00 0.000000000000000E+00 2.0100000000000001E+01
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&COORD
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C 3.5922123059602664E+00 1.0264093753450179E+01 7.4226479927161302E+00
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H	1.5335170218949820E+01	1.1290650431073626E+01	8.2030077613795527E+00
H	-5.4224382956090516E+00	1.2242579023239205E+01	5.3320239546230273E+00
H	-5.8545919181672570E+00	1.3213563037008665E+01	6.8120728680876663E+00
O	1.3261787638162200E+01	9.1016608051992893E+00	1.8019354894400198E+01
O	1.0601982728779745E+01	8.6369258106493074E+00	-7.9994594891379522E-01
C	1.1185440737891600E+01	7.8051520616481085E+00	-1.8324059716550376E+00
C	1.1129802179449662E+01	9.9542883549194929E+00	-1.0326773979418808E+00
C	1.2731859902642661E+01	9.9482485540569972E+00	1.9031158202370474E+01
C	1.2677868077768144E+01	7.8585351674943089E+00	1.8301954822185571E+01
H	1.3123753403371749E+01	1.0948463188925389E+01	1.8797333997121267E+01
H	1.2972098551306306E+01	9.5618130511594579E+00	2.0005936188804633E+01
H	1.0728654980899826E+01	1.0549997358759553E+01	-1.7964087337497783E-01
H	1.0728342551174013E+01	1.0402471946046669E+01	-1.9375885153112951E+00
H	1.3175623757069982E+01	7.1465950183440672E+00	1.7659196491883652E+01
H	1.3091906287242344E+01	7.5766879633391158E+00	1.9359977475795311E+01
H	1.0783737862043298E+01	8.1017607101992937E+00	-2.8135057411505713E+00
H	1.0871403354433090E+01	6.7706874574057867E+00	-1.5640879028680827E+00
O	7.8098187877255825E+00	1.1099140015969808E+00	1.1265514285399666E+01
O	5.6932833414949506E+00	2.0889762692326701E+00	9.5866816006051341E+00
C	5.6007433063434409E+00	2.1963799627875082E+00	1.1023200394850360E+01
C	6.4080597291944335E+00	9.4326103699487973E-01	9.1766054745646244E+00
C	7.7998980116194021E+00	9.5013478086259684E-01	8.8592240604859089E+00
C	6.9556097013380436E+00	2.2256814172632127E+00	1.1714237227339037E+01
H	8.3175480415876137E+00	-1.0724878365284084E-02	9.6200081964121225E+00
H	8.4458056947673139E+00	1.7483811025534584E+00	9.3972675231957812E+00
H	6.6016136116252602E+00	1.1112366397268270E+00	8.1519391126073444E+00
H	5.8203471210629028E+00	6.8948754083657707E-02	4.0622219555395483E+00
H	6.8495537312133150E+00	2.0183099186584683E+00	1.2774031472311753E+01
H	7.4105836306961699E+00	3.1996099802795714E+00	1.1543592452536934E+01
H	5.0250258296254611E+00	1.3468265143081428E+00	1.1397536837975425E+01
H	5.0740796198425366E+00	3.1136232975806957E+00	1.1136958693652701E+01
O	1.6431761625110422E+01	1.2140733346528119E+01	1.0975586183762660E+01
O	-1.2712194309171256E+00	1.2198779381799115E+01	9.5291920355032946E+00
C	1.8615630418827866E+01	1.1127146369254408E+01	1.0399744273562543E+01
C	1.8380201407198594E+01	1.3345064879986621E+01	1.0184254872441198E+01
C	1.6841751487621192E+01	1.3190510396857427E+01	1.0129499794030522E+01
C	1.7039544806263237E+01	1.0907252773788953E+01	1.0690280800949015E+01
H	1.6391534324504008E+01	1.4050789274512113E+01	1.0599368999091549E+01
H	-3.5896690864361647E+00	1.2991153746858716E+01	9.1194911356822832E+00
H	-1.2653675046358295E+00	1.4165260079012739E+01	9.6449557836782063E+00
H	1.8729053981243883E+01	1.3462352569374490E+01	1.1187994272600795E+01
H	1.6999874944992559E+01	1.0251195551178656E+01	1.1571700770739659E+01
H	-3.6009486294773883E+00	1.0374476186923911E+01	9.8372081625937522E+00
H	1.9266103151304545E+01	1.1297620355105650E+01	1.1300388182553879E+01
H	1.8987071779704713E+01	1.0193742464813644E+01	9.8845263608136644E+00
O	1.4025240587827764E+01	7.3251363646092189E+00	2.3321097671869335E+00
O	1.1648712924876493E+01	5.7935590222676572E+00	3.1515570392006702E+00
C	1.2358111784129010E+01	5.4630606449477286E+00	1.9641339069526378E+00
C	1.1643658551026649E+01	7.2203817139781554E+00	3.2039128447909744E+00
C	1.3066979220316407E+01	7.8101409253128420E+00	3.3464815152806526E+00
C	1.3814698031348719E+01	5.9098633355051780E+00	2.0592716176758628E+00
H	1.3054529142551653E+01	8.8921601571016158E+00	3.1868956937950879E+00
H	1.3496980712496208E+01	7.5438629078026747E+00	4.2635143567782192E+00
H	1.1050053045149330E+01	7.5925935002783795E+00	4.0302685807678662E+00
H	1.1072102874457975E+01	7.6722665371342895E+00	2.3906405201240033E+00
H	1.4206241580283315E+01	5.6798830469552328E+00	1.0854408862512819E+00
H	1.4191893815956886E+01	5.2048036149387729E+00	2.8674804866243058E+00
H	1.1758284470609876E+01	5.9128703095497439E+00	1.1776621804490153E+00
H	1.2308656323515336E+01	4.3561360883756368E+00	1.7467467128627083E+00
O	1.5442794249313321E+01	2.5677784946546995E+00	5.4660579993738070E+00
O	1.3956029970873464E+01	3.9572018982014949E+00	7.7138199624699064E+00
C	1.4089420546567197E+01	4.3704584519985366E+00	6.3777878905543890E+00
C	1.5213379960970213E+01	3.2462386146743962E+00	7.8894260494420472E+00
C	1.5445849201847203E+01	2.1466706827962727E+00	6.8614584912122689E+00
C	1.4224111332625087E+01	3.2507963452223949E+00	5.3602678941246849E+00
H	1.6441872280226356E+01	1.7385634583054590E+00	6.9641795844128191E+00

H	1.4828703129281845E+01	1.1892871923674384E+00	6.9944436180314060E+00
H	1.5257452971300420E+01	2.7532201549475648E+00	8.8710819383832398E+00
H	1.6051725098038489E+01	4.0399139099209735E+00	7.8378157143361440E+00
H	1.4194361015725180E+01	3.4993214412696938E+00	4.2982431443332025E+00
H	1.3448617376414671E+01	2.5042356508231269E+00	5.5221607760151210E+00
H	1.494782509356008E+01	5.0804926013635230E+00	6.1921603283601740E+00
H	1.3213041104847161E+01	5.0223717740838199E+00	6.1603249849371240E+00
O	9.5782203669808776E+00	7.3981232321321162E+00	1.3282633222536907E+01
O	1.2422751320168086E+01	7.4299717407121397E+00	1.3002626028761540E+01
C	1.1541051903791613E+01	7.0263093315654688E+00	1.1885621974744739E+01
C	1.1860927506782360E+01	7.1314966192745226E+00	1.4243161311690766E+01
C	1.0487339989917881E+01	7.7080566188157098E+00	1.4398799954750407E+01
C	1.0228187613537008E+01	7.6916091878863995E+00	1.2018469115356027E+01
H	9.9018452927019744E+00	7.4580936442730019E+00	1.5300994953634424E+01
H	1.0501613796361937E+01	8.7879034053335658E+00	1.4477194850393410E+01
H	1.2549732277588310E+01	7.5961534662500965E+00	1.4988004436546399E+01
H	1.1858179721539566E+01	6.0520276869324281E+00	1.4423987485640742E+01
H	9.5672758395931439E+00	7.3192419170311114E+00	1.1235731404935803E+01
H	1.0329579699954797E+01	8.7862613034567971E+00	1.1979561675345563E+01
H	1.1513176444683006E+01	5.9192589861168825E+00	1.1959862048753816E+01
H	1.2036788581325007E+01	7.4131501781448419E+00	1.0976833782394952E+01
O	1.2928704951732783E+01	1.5414149482005326E+01	7.5630287323472434E+00
O	1.3173791838848675E+01	1.6667802050191732E+01	1.0009515281032874E+01
C	1.4140718760623999E+01	1.5717887107519742E+01	9.5825480894556563E+00
C	1.1865714825492608E+01	1.6462501754182284E+01	9.4979982387439161E+00
C	1.1902826114932628E+01	1.6328590182967208E+01	7.9647344928827115E+00
C	1.4247353194649479E+01	1.5697297465181265E+01	8.1130344023612526E+00
H	1.0965133039184240E+01	1.5861653079674831E+01	7.5668143679632687E+00
H	1.2153262959518832E+01	1.7320965765219064E+01	7.5992805420441014E+00
H	1.1265271050176926E+01	1.7342016262866014E+01	9.7076632579606255E+00
H	1.1496725056039532E+01	1.5432179057391460E+01	9.8434565926256319E+00
H	1.5018370411719697E+01	1.4912905732594549E+01	7.8259039780121888E+00
H	1.4648902330055705E+01	1.6638087332147769E+01	7.7519241521121298E+00
H	1.3959804538183615E+01	1.4670180924788150E+01	9.9929764365892098E+00
H	1.5052354000085966E+01	1.6042847243289636E+01	1.0037576306785668E+01
O	2.5132015223375461E+00	4.0133679180749233E+00	5.0237097922938485E+00
O	3.9839159618608577E+00	1.4873879964482775E+00	4.7329412319128004E+00
C	4.5010691150127018E+00	2.6170233143545221E+00	5.4482622657681841E+00
C	3.1412010854171282E+00	1.9484397930093149E+00	3.6866367677236767E+00
C	2.0770793834460650E+00	2.9436269325230460E+00	4.1476215382725581E+00
C	3.3985639892360036E+00	3.4798964302009003E+00	6.0991780328526541E+00
H	2.1699047111837466E+01	3.4831891935393831E+00	3.3246816361902529E+00
H	1.2381482712478165E+00	2.4510362686605882E+00	4.6408174118762737E+00
H	2.2814737877358088E+01	1.0038113888543925E+00	3.2755449150647733E+00
H	3.8261014974769623E+00	2.3860406810181241E+00	2.9159286812356666E+00
H	3.8014512202356281E+00	4.3548776077761833E+00	6.5909426036324898E+00
H	2.8520562487856753E+00	2.7696335719350236E+00	6.7901048688326764E+00
H	4.9922054431701257E+00	3.2286018183472542E+00	4.6796019093222059E+00
H	5.2616326773437434E+00	2.2779659301036772E+00	6.2112997491297319E+00
O	9.8816500444880706E+00	1.6674894581998590E+01	1.8855242982245201E+01
O	8.1764394923352359E+00	1.7641978629636462E+01	7.5682326574842662E-01
C	7.8839741225840259E+00	1.7829310616577590E+01	-6.5492695855957495E-01
C	9.5831341555270484E+00	1.7466461661654915E+01	1.0396281214279599E+00
C	1.0239754661828190E+01	1.6343513561495701E+01	2.0226412715188747E+01
C	8.4384715603185363E+00	1.6781445279949398E+01	-1.5564166550677896E+00
H	1.1322522724070877E+01	1.6391270203448624E+01	2.0275524098274285E+01
H	9.8312487068314933E+00	1.5373879984028502E+01	2.0544131854937788E+01
H	9.6238285959416814E+00	1.6971690566533994E+01	2.0413551635924829E+00
H	1.0224127377100547E+01	1.8373734580251927E+01	1.0213473298790441E+00
H	8.3801223426890825E+00	1.7129944986705908E+01	-2.6071870018283070E+00
H	8.0373809277918031E+00	1.5763717943321046E+01	1.8656747116866097E+01
H	8.2539642958559263E+00	1.8792160277833027E+01	-9.7076563618280576E-01
H	6.7956775873998163E+00	1.7885360950612558E+01	-7.0975682615079649E-01
O	1.9361570724233076E+01	1.8614001878514124E+01	1.4238016332788028E+01
O	6.3327188320556893E-01	1.9231680085473894E+01	1.6703990158454822E+01
C	1.2911376279182716E+00	1.9187473872464480E+01	1.5440504117576348E+01
C	-4.1653384624595646E-01	1.8239207093821090E+01	1.6720123729370520E+01
C	1.8679021436648103E+01	1.8454155148557394E+01	1.5559211568575547E+01
C	2.0456456876393990E+01	1.9654241062680125E+01	1.4422163836043520E+01
H	1.7965766612048373E+01	1.7564852265937564E+01	1.5466325715264412E+01
H	1.7998132331598505E+01	1.9261949869055364E+01	1.5822722491487996E+01
H	-1.0019555927709882E+00	1.8449995109900851E+01	1.7616888921984152E+01
H	5.3011211254541529E-02	1.7220440318387936E+01	1.6847591657460271E+01
H	2.0856766263888030E+01	1.9654865196420964E+01	1.3388264999631438E+01

H	1.9943112863308336E+01	2.0569125370800695E+01	1.4678523544545484E+01
H	1.6465261615453737E+00	1.8163231521764168E+01	1.5289311549093405E+01
H	2.2632819556627628E+00	1.9690283442887814E+01	1.5565158002837466E+01
O	1.9310925559547567E+01	3.4780207443606006E+00	1.3803621067775689E+01
O	1.7002407088902537E+01	4.6666764212530740E+00	1.2657259607811014E+01
C	1.7725625235731044E+01	3.5908157788210904E+00	1.1977623501878236E+01
C	1.7920792071588707E+01	5.4676952895784501E+00	1.3389371830758837E+01
C	1.8577090218573527E+01	4.6166348182289223E+00	1.4423472936367849E+01
C	1.8376753424119734E+01	2.6995278953752693E+00	1.3007767255387030E+01
H	1.9267485167026393E+01	5.2318915017619396E+00	1.5061184890930413E+01
H	1.7783850976708830E+01	4.2221162035032611E+00	1.5101747024958005E+01
H	1.7352221537982370E+01	6.3373651477080069E+00	1.3850330403659376E+01
H	1.8614061576244161E+01	5.9811720697274851E+00	1.2680743015452352E+01
H	1.8970123949760723E+01	1.9065024139146880E+00	1.2480523907007710E+01
H	1.7599917222028303E+01	2.3463382253080831E+00	1.3745264630859651E+01
H	1.8566664112551727E+01	4.0867529612002738E+00	1.1444441755320188E+01
H	1.6987902470957991E+01	3.0706767432084363E+00	1.1393737491562156E+01
O	1.8306211771034193E+00	1.8729126065254952E+01	1.1911817064395942E+01
O	3.3301209829827112E+00	1.6489801571056720E+01	1.0989558364095686E+01
C	3.8525940869507243E+00	1.7793072189252218E+01	1.0805151440406817E+01
C	1.8724138560110386E+00	1.6458204774613435E+01	1.1024334133977973E+01
C	1.3885547858503549E+00	1.7323043076083074E+01	1.2169820305605382E+01
C	3.3399920518455275E+00	1.8797457251629186E+01	1.1874912420934290E+01
H	3.3631328345455047E-01	1.7443814812935194E+01	1.2315976255731039E+01
H	1.8519204505267053E+00	1.6962546905749072E+01	1.3067724860842544E+01
H	1.5668380270968678E+00	1.5384474849995481E+01	1.1163669819152892E+01
H	1.4576825947885028E+00	1.6720449570408736E+01	1.0060517710436606E+01
H	3.6414543535187271E+00	1.9819018152241767E+01	1.1654376002635892E+01
H	3.7130913853654652E+00	1.8427012071011440E+01	1.2881369145660827E+01
H	3.5269478580183105E+00	1.8076959267932750E+01	9.7871444734438828E+00
H	4.9642276541585879E+00	1.7741222482478562E+01	1.0768983179201193E+01
O	1.3572622734175940E+01	-8.0285676623549274E-01	2.7829746905609669E+00
O	1.3128960345523364E+01	1.8000452391583563E+00	1.4195606465841335E+00
C	1.2093856390332704E+01	1.2075385589479462E+00	2.1012482490381270E+00
C	1.3927974152696226E+01	6.8237679196711765E-01	8.3805467570656300E-01
C	1.4518888147977588E+01	-1.4673954975014580E-01	1.9224651817162197E+00
C	1.2553187207465529E+01	1.2605361069041754E-01	3.1496250694722550E+00
H	1.5162725047360789E+01	1.9127687968390763E+01	1.4719426557530815E+00
H	1.5234298112833200E+01	2.0580806234600161E+01	2.5039850229812513E+00
H	1.4774142614715361E+01	2.1236222064568093E+01	2.8527512521699644E-01
H	1.3367392901924026E+01	6.0782004492768958E-02	1.4698167905687126E-01
H	1.1636699380829215E+01	-3.7586306719983142E-01	3.4176690074634215E+00
H	1.2909205068188962E+01	6.2811894788799982E-01	4.0193352732694319E+00
H	1.1323760214413682E+01	7.5785717388947471E-01	1.4892603399921844E+00
H	1.1626270063525144E+01	2.0317441218398264E+00	2.7203156484194086E+00
O	5.4133207162758019E+00	1.4007061829247662E+00	-9.6352828784099709E-01
O	6.4920438973455870E+00	2.0632495395151094E+00	1.6173394824893050E+00
C	7.1182947840400432E+00	2.6002208950385866E+00	3.141913661996706E-01
C	5.7984474520000937E+00	9.0645301349669816E-01	1.4784607221753576E+00
C	4.7471838288448280E+00	1.1272199896266486E+00	3.6425756134836723E-01
C	6.1250608998959981E+00	2.6901020660068045E+00	-7.6848301801181640E-01
H	4.1099034528326914E+00	2.9721349029973021E-01	2.165340564659378E-01
H	4.1684614615409146E+00	1.9692506485260839E+00	7.0833842772291999E-01
H	5.3950851407530420E+00	7.2738244082294223E-01	2.4647548267042034E+00
H	6.4083648194914913E+00	1.8397081643386635E-02	1.1461146868475887E+00
H	6.7972355460107261E+00	2.8115680436012123E+00	-1.5735213365756346E+00
H	5.5105885356062814E+00	3.6080183501054477E+00	-6.5061542652640703E-01
H	8.0061029978299789E+00	1.9583856624354499E+00	2.0123664650541931E-01
H	7.5069969260655443E+00	3.6009745974342131E+00	8.0095445539728638E-01
O	1.5986137641789666E+01	1.5524850994642657E+01	1.2077112557581722E+00
O	1.3284695414415165E+01	1.4551249790130692E+01	6.8929800393465268E-01
C	1.4368534470886781E+01	1.3741961370933382E+01	1.2582784173664496E+00
C	1.3937775030924115E+01	1.5517269489184597E+01	-1.7758450218577981E-01
C	1.4978070767672927E+01	1.6329758968786681E+01	5.7150753858537873E-01
C	1.5363591771069789E+01	1.4551001853636226E+01	2.0514335628834370E+00
H	1.5519661026536328E+01	1.7022159479533368E+01	-5.3706887255391016E-02
H	1.4386129550441115E+01	1.6936040877323695E+01	1.3215858805436020E+00
H	1.3182982745469396E+01	1.6207861645849661E+01	1.9535385939796150E+01
H	1.4378771115462895E+01	1.5088713713913645E+01	-1.0686323066600554E+00
H	1.6157963992970672E+01	1.3902087165089684E+01	2.4761382497371822E+00
H	1.4766960113654294E+01	1.5032463439026980E+01	2.8951414913040465E+00
H	1.4927201795620961E+01	1.3243920243120352E+01	4.5052172910764676E-01
H	1.3758655842675426E+01	1.3056727604288440E+01	1.8944094007775203E+00
O	1.4408263921783902E+01	1.4516376641518072E+01	1.4186060453887478E+01

O 1.7161958940108370E+01 1.5278693993117800E+01 1.4191817840811947E+01
C 1.6599069046395684E+01 1.4857406781799206E+01 1.2983315790292929E+01
C 1.6578983760053656E+01 1.4651482423695480E+01 1.5302961159737333E+01
C 1.5077067414287914E+01 1.4999318927543353E+01 1.5332501133731736E+01
C 1.5034541218520591E+01 1.5058098697272218E+01 1.2968559934243949E+01
H 1.4660806078346134E+01 1.4586423884733192E+01 1.6233020533605359E+01
H 1.4942293288286335E+01 1.6087498152763310E+01 1.5374796022288084E+01
H 1.7098452254177904E+01 1.4999188019558131E+01 1.6172234838376969E+01
H 1.6720801385485490E+01 1.3547179642709434E+01 1.5222025722733003E+01
H 1.4694719169596791E+01 1.4453109302721732E+01 1.2134933403738325E+01
H 1.4729348062369947E+01 1.6133194825854090E+01 1.2801410076142187E+01
H 1.6819879985178588E+01 1.3740952905244194E+01 1.2893093864436160E+01
H 1.7057829434054405E+01 1.5459904530995395E+01 1.2215287380743897E+01
O 1.7780355987590067E+01 5.1573248531578111E+00 3.2597212759388712E+00
O 1.7910880903447044E+01 2.7147981634660901E+01 5.3779745435129875E+00
C 1.8293433195334519E+01 7.3904289728758554E+00 4.0221926854428753E+00
C 1.8399851277836632E+01 5.7256782480031525E+00 5.6103058991262680E+00
C 1.7662830579994985E+01 4.8207679540285557E+00 4.6597436206372542E+00
C 1.7387705556693593E+01 6.5353300568314472E+00 3.1323603171377057E+00
H 1.8028803208190340E+01 3.7708484336000958E+00 4.7665591361604775E+00
H 1.657649374322926E+01 2.5120580936020350E+01 5.0415046603044642E+00
H 1.8105217110135051E+01 2.5582574973541895E+01 6.6626886563421293E+00
H 1.9536383533989913E+01 5.6210235690985044E+00 5.5772764668794306E+00
H 1.7525331123335278E+01 6.8132823314194351E+00 2.0728378220444061E+00
H 1.6332100859843976E+01 2.6824605538900308E+01 3.4618028709604167E+00
H 1.9332197612073973E+01 7.2185947655148892E+00 3.7247991754324907E+00
H 1.7936136025718373E+01 2.8542838975447637E+01 3.9168624036788406E+00
O -1.2779064291201675E-01 1.5767584474786053E+01 1.9105620579774108E+01
O 8.3759512033148598E-01 1.5025575691535940E+01 1.6033379576976727E+00
C 2.9342660065534443E-01 1.6343014265988316E+01 1.3708587280959248E+00
C 2.1563427714428204E+01 1.4504955880096425E+01 4.4231197096990943E-01
C 2.0638066288648020E+01 1.4449090526629460E+01 -7.1604217818581017E-01
C -7.7032258940575430E-01 1.6240267052943707E+01 2.0328832187761865E+01
H 2.1031689369706086E+01 1.4186919921598722E+01 1.8408986240517009E+01
H 1.9821832335628986E+01 1.3706122731796411E+01 1.9577630380114865E+01
H 2.1790788145483567E+01 1.3486503613532584E+01 6.9709644405694970E-01
H 2.2460377295745968E+01 1.5066727862322567E+01 9.9200258950088813E-02
H -1.1380635677122690E+00 1.7213002359892624E+01 2.0079825756061762E+01
H -1.5481124720412442E+00 1.5595672135253404E+01 7.024727602581613E+01
H 1.1000025487089149E+00 1.7018467319363740E+01 1.1103816082688855E+00
H -2.0825073770461294E-01 1.6594013029825547E+01 2.2812833402431845E+00
O 2.3459582042015356E+01 4.8925285034871226E+00 1.2166937442007589E+01
O 8.0392758168431799E-01 5.9960589733295722E+00 1.0927641143043608E+01
C 2.1115844265416627E+01 4.6361353695400691E+00 1.1417573843589953E+01
C 2.2145456116275685E+01 6.6896341641532659E+00 1.1055513309029884E+01
C 2.3052217590004805E+01 6.2459436834677158E+00 1.2237688482690585E+01
C 2.2549576233477893E+01 4.2570207554123494E+00 1.1272243544006715E+01
H 2.3884257707724252E+01 7.0464307220998705E+00 1.2279890782796024E+01
H 2.3094934648989751E+00 6.3647250681741738E+00 1.3214760197687058E+01
H 2.1906297453999343E+01 7.8147607670459234E+00 1.1222798203622524E+01
H 2.2635032570719886E+01 6.6674796166845001E+00 1.0060381484725138E+01
H 2.2951222983847622E+01 4.4667035111404125E+00 1.0244783732292239E+01
H 2.5902653237739557E+00 3.1717097439328561E+00 1.1412302916077470E+01
H 2.0469724791288193E+01 4.0329887768932648E+00 1.0735998858859160E+01
H 5.8124178636027757E-01 4.5873889155227801E+00 1.2413244757158427E+01
O 6.1089748042521448E+00 1.1942364414477559E+01 1.2060733208800082E+01
O 7.8470909575780103E+00 1.3848841264146623E+01 1.3394305282944229E+01
C 6.4117827050098946E+00 1.3818772399655375E+01 1.3468320756392108E+01
C 8.2819265620985103E+00 1.2991433805236467E+01 1.2273728128357572E+01
C 7.5193799534810832E+00 1.1647373439890417E+01 1.2160451937526879E+01
C 5.7219486577614234E+00 1.2504741779159200E+01 1.3308226252372695E+01
H 7.7424144507114070E+00 1.1092378566272384E+01 1.1245851477363191E+01
H 7.7196064472553836E+00 1.1000052664076321E+01 1.3034171152727241E+01
H 9.3329438818179931E+00 1.2782023283499901E+01 1.2487833075694299E+01
H 8.3101269696503959E+00 1.3622116064940100E+01 1.1366100281000110E+01
H 4.6248965286807717E+00 1.2677370441592705E+01 1.3173945744383589E+01
H 5.9281732804604887E+00 1.1890763918262333E+01 1.4149590990338439E+01
H 6.1425263459052912E+00 1.4483900937612537E+01 1.2616330999851357E+01
H 6.1581824418461117E+00 1.4272948654825280E+01 1.4429095565350259E+01
O 9.9959399914014497E+00 1.7719973334485378E+01 1.2638661824432779E+01
O 1.2827441859453549E+01 1.7260194102209582E+01 1.3513429640436708E+01
C 1.2336016077577685E+01 1.8514017034579467E+01 1.2942360464933985E+01
C 1.1792544309559544E+01 1.6193317830362204E+01 1.3365438163485322E+01
C 1.0405926143518418E+01 1.6693019931867752E+01 1.3577888553450641E+01

C	1.0789550174038082E+01	1.8828279775751128E+01	1.3015891558227622E+01
H	9.7533670733029556E+00	1.5823706059169925E+01	1.3375309931877576E+01
H	1.60036767597180731E+01	1.6901025417898364E+01	1.4587369259032657E+01
H	1.2106094721892491E+01	1.5434008118372319E+01	1.4064929271892630E+01
H	1.1971738826649821E+01	1.5934646558264561E+01	1.2298028145187267E+01
H	1.0641381028502298E+01	1.9662879162740126E+01	1.2288710229700461E+01
H	1.0587390677171060E+01	1.9008827816817156E+01	1.4096075232429117E+01
H	1.2556225958877969E+01	1.8515836038703263E+01	1.1861586370698719E+01
H	1.2922297364614767E+01	1.9263940246733640E+01	1.3437894870345341E+01
O	1.6152896849829236E+01	1.1152834380193081E+01	1.5611964565595388E+01
O	1.5531299012191290E+01	8.5486912804993782E+00	1.4458771313996417E+01
C	1.6567939955948841E+01	8.7369269019524989E+00	1.5432702234290309E+01
C	1.5452523137086015E+01	9.7542865285625293E+00	1.3653418599248678E+01
C	1.5161127079412813E+01	1.0980207804316235E+01	1.4562931855765058E+01
C	1.6204828063778404E+01	9.8755971407634568E+00	1.6393707914945590E+01
H	1.5276416431689157E+01	1.1896529671902030E+01	1.3987093342282957E+01
H	1.4178156546611568E+01	1.0795555952402895E+01	1.5041158131246522E+01
H	1.4619938225862967E+01	9.5806677185388764E+00	1.2954784106638453E+01
H	1.6360429185965042E+01	9.8756298088572780E+00	1.3072239392456765E+01
H	1.6877678593640614E+01	1.0125169033987239E+01	1.7161418133799796E+01
H	1.5267934557184109E+01	9.7009811849995540E+00	1.6888855237740316E+01
H	1.7502857723821762E+01	8.9229089080762751E+00	1.4889554778330981E+01
H	1.6676674476836126E+01	7.7986105104089667E+00	1.5911740521338748E+01
O	7.6512716587768512E+00	2.1455272992652478E+01	6.1550116493926721E+00
O	9.5139772954119728E+00	-3.1526438293062059E-01	4.7371629714126904E+00
C	9.9592145130889183E+00	4.8326799968805284E-01	5.8093666570757554E+00
C	8.3798849770273538E+00	2.0419222451719998E-01	4.0814198628213623E+00
C	7.1665273110840326E+00	5.5090051364093262E-01	4.9728318537663636E+00
C	8.7763866654651892E+00	7.1279717849619406E-01	6.8161303447390784E+00
H	6.3931745776133297E+00	2.1287274350348486E+01	4.4987886927817780E+00
H	6.6635349517803100E+00	1.9725808343731032E+01	5.3981363421314823E+00
H	7.9880518965595106E+00	-5.6807060233629658E-01	3.3938053261907273E+00
H	8.6774646772176407E+00	1.0997809634850415E+00	3.4721487919830092E+00
H	9.1212341787932090E+00	2.1462996263944373E+01	7.6665838643021580E+00
H	8.4706856928293526E+00	1.9833889595595593E+01	7.2310555011987301E+00
H	1.0271536618370835E+01	1.5391185036000774E+00	5.5001592589455717E+00
H	1.0839053862233595E+01	5.9231163274465953E-02	6.2959953357618703E+00
O	1.8715759070419203E+01	9.7513444614605298E+00	1.9995900741134948E-01
O	1.7589698124461826E+01	1.2364579153189093E+01	1.2852280079535550E-01
C	1.8054191136833609E+01	1.1730498342698640E+01	-1.0841142197701457E+00
C	1.8372365809484414E+01	1.1905701427873213E+01	1.2639200222051437E+00
C	1.8261304913142293E+01	1.0380366412014581E+01	1.4737353003356328E+00
C	1.7910305224790950E+01	1.0264479562428624E+01	-8.9012117356995824E-01
H	1.8919960674727125E+01	9.9407466281103662E+00	2.2615101747157267E+00
H	1.7256750340485624E+01	9.9660481250739501E+00	1.6473802326272802E+00
H	1.8071191344482308E+01	1.2507775093138358E+01	2.1216189774953356E+00
H	1.9394977285670407E+01	1.2171281256804740E+01	9.9685292067141151E-01
H	1.8289122091128828E+01	9.7442279574110415E+00	1.8332650819192452E+01
H	1.6857292848889163E+01	9.9341745097854748E+00	1.9412741419428883E+01
H	1.9126097903460497E+01	1.1974511328457442E+01	-1.3138426763025868E+00
H	1.7418171691444130E+01	1.2032147467448761E+01	1.8170658590220302E+01
O	8.1673862048711179E+00	5.1898610812675869E+00	1.6072031064497803E+01
O	5.840898016300840E+00	5.9405315936921905E+00	1.4769342448633278E+01
C	6.0872965359321434E+00	6.3417586124328915E+00	1.6168206565840375E+01
C	6.2876325782989326E+00	4.6171725272460025E+00	1.4628674365459007E+01
C	7.8017618573842773E+00	4.5689639927882872E+00	1.4857937820919220E+01
C	7.5577861841907090E+00	6.5470319079825341E+00	1.6285363058478683E+01
H	8.2988782071874549E+00	3.5647931913283388E+00	1.4896675676684753E+01
H	8.1829970542816284E+00	5.0985813607285717E+00	1.3973773194760275E+01
H	6.1162281427202299E+00	4.4010361665769686E+00	1.3540862118692479E+01
H	5.6411422620136484E+00	3.9052975325641679E+00	1.5147215141043167E+01
H	7.7935026698788201E+00	6.8503642937592248E+00	1.7338583769364259E+01
H	8.0083076087560450E+00	7.2473735502028998E+00	1.5566803165035365E+01
H	5.5799106615141687E+00	5.6339678758346459E+00	1.6807578600244465E+01
H	5.5024215970816517E+00	7.2720339489244656E+00	1.6273593981750484E+01
O	1.1053947390181502E+01	1.0814822416845137E+01	1.0721503122925792E+01
O	1.2788934619912677E+01	1.3006084028722947E+01	1.0835546110782563E+01
C	1.2243583428100795E+01	1.2603880325933813E+01	9.6243197830151903E+00
C	1.2984820552625951E+01	1.1956583576904633E+01	1.1783825924860013E+01
C	1.1670239059566857E+01	1.1128737107778136E+01	1.1940672546108509E+01
C	1.0879376786032328E+01	1.1947821710227261E+01	9.7334424652584008E+00
H	1.1874201357196743E+01	1.0124896651049644E+01	1.2402689507257302E+01
H	1.0992357808392939E+01	1.1692094523742421E+01	1.2663176105554951E+01
H	1.3294737637037816E+01	1.2436021274620417E+01	1.270198899799779E+01

H 1.3775341482900320E+01 1.1273177898389696E+01 1.1427004689780007E+01
H 1.0476076132782639E+01 1.1374259023566010E+01 8.8618396384589815E+00
H 1.0113587565480769E+01 1.2703638554767087E+01 1.0032385977511328E+01
H 1.2952093259411996E+01 1.1888102642775085E+01 9.2156237194508552E+00
H 1.2146261473652791E+01 1.3497546969063350E+01 8.9798296216850098E+00
O 1.0496282709711936E+01 1.2604485172948042E+01 1.5164391206576015E+01
O 1.1493149290923462E+01 1.3257030627135052E+01 1.7736893412416688E+01
C 1.0100948349736125E+01 1.3370284044527549E+01 1.7390958381257466E+01
C 1.2303406546817991E+01 1.3453770981833648E+01 1.6584743714074062E+01
C 1.1957147388763310E+01 1.2458697380057366E+01 1.5496048905907124E+01
C 9.6787771225512582E+00 1.2348385691631275E+01 1.6331220501718231E+01
H 1.2440710211699333E+01 1.2723981607099740E+01 1.4553493331107051E+01
H 1.2078812894801088E+01 1.1359067039195644E+01 1.5804072115306491E+01
H 1.3345720689117394E+01 1.3259329301206078E+01 1.6915462377455604E+01
H 1.2225143726130435E+01 1.4462223191205656E+01 1.6184809204201308E+01
H 8.6451562022288719E+00 1.2486302275036376E+01 1.6007748166258381E+01
H 9.7137845355480881E+00 1.1276748734427194E+01 1.6658060475659820E+01
H 9.9231453728693744E+00 1.4464969063345146E+01 1.7012109796630106E+01
H 9.5495182619519685E+00 1.3201978861650485E+01 1.8355303463301386E+01
O -2.2917672094791053E-01 1.4362414888093907E+01 6.6887287246400771E+00
O 2.3201544095907227E+00 1.4666910729786061E+01 7.9444606704141725E+00
C 1.3379731015668832E+00 1.3670672524894071E+01 8.3629903357593012E+00
C 1.6358199133218077E+00 1.5768672524714473E+01 7.2967715279781835E+00
C 8.1455922123722324E-01 1.5219483774413664E+01 6.2269128943107930E+00
C 4.4809830837897546E-01 1.3188014227361268E+01 7.2595396819869036E+00
H 3.5421795909631593E-01 1.5943529702929208E+01 5.5267200959741922E+00
H 1.4786446961974222E+00 1.4472598405411111E+01 5.7072884499162617E+00
H 2.3129587699514826E+00 1.6567881061968905E+01 6.9264322513610956E+00
H 9.0765684751481712E-01 1.6244703206879972E+01 7.9805459056750943E+00
H -3.9600063106186639E-01 1.2552677815405969E+01 7.7218198300382674E+00
H 9.6841337625177548E-01 1.2640415840160639E+01 6.4391471742407500E+00
H 7.6742361795900549E-01 1.4074332954174228E+01 9.2352133210453324E+00
H 1.9454442492124302E+00 1.2831231721337788E+01 8.8110494006256879E+00
O 2.8635792984562563E+00 1.7346492662215102E+01 3.1319118400144217E+00
O 5.5511654303082514E+00 1.6974721141408956E+01 4.0320908273006193E+00
C 5.2541326503672705E+00 1.7773364136514292E+01 2.8511046460260983E+00
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C 3.2349167770152487E+00 1.6546010866469143E+01 4.3496385025806115E+00
C 3.7998185374898861E+00 1.8366519764929166E+01 3.0418765005017763E+00
H 2.4465987709318071E+00 1.5783994874492777E+01 2.4603625613170426E+01
H 3.3579693115536986E+00 1.7141635728883458E+01 5.2757726040776820E+00
H 4.7496092360903690E+00 1.5373824571250230E+01 2.5210379640416889E+01
H 4.5652628715725427E+00 1.5161970315822188E+01 2.3466602297437479E+01
H 3.5258336853649137E+00 1.9064717846236086E+01 2.2470495851903465E+00
H 3.7822785194403572E+00 1.9014842575809848E+01 3.9662512963125662E+00
H 5.1565144024740643E+00 1.71463440999810278E+01 1.9600031184374862E+00
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H 2.2104635287420702E+01 3.1071550035223722E-01 -1.4395391295615316E+00
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C 4.3494193773183527E+00 1.7331897870972565E+01 1.7366308184640335E+01
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H 3.2955793086666811E+00 1.4012447477385841E+01 1.6026752525331133E+01
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H 1.1694648088002307E+01 4.3872555625454170E+00 1.3454873400210952E+01
H 1.2047869788090976E+01 2.1574175881518784E+01 1.4215210516057315E+01
H 1.1140498488354154E+01 2.2170844900233870E+01 1.2692933632349101E+01
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C 1.1906290692058241E+00 1.2226990039552591E+01 1.4346212625463284E+01
C -7.1571997210906138E-02 1.4051800496456295E+01 1.5134927292635869E+01
C 2.1362995528818049E-01 1.4788115488360583E+01 1.3826033731993936E+01
C 1.4596109361998775E+00 1.2990318346990447E+01 1.3055431159184405E+01
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H -7.0481553743597769E-02 1.4703162456266961E+01 1.6006342474059974E+01
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H 1.6793123203285452E+00 1.2267118636107368E+01 1.2265405021162763E+01
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H 3.4700365907203412E-01 1.1544135326303190E+01 1.4196155618635133E+01
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C 1.6908597059217676E+01 7.4895006878863386E+00 8.5126435774574549E+00
C 1.4905678311305994E+01 6.5275784559265615E+00 9.4642300000562685E+00
C 1.5331252788417448E+01 6.9978909872872688E+00 1.0820006090354557E+01
C 1.7342722063734847E+01 7.9467543028062222E+00 9.9190576881486106E+00
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O 9.8449096477118285E+00 1.4935333528189757E+01 3.4636692614344278E+00
O 1.0323639084434408E+01 1.4309865094304556E+01 6.2821058752889485E+00
C 1.1154584271384103E+01 1.3739241125105508E+01 5.2756573164421532E+00

C	9.0583416499060156E+00	1.4601520372274120E+01	5.7657316138832986E+00
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C	1.1186901148506779E+01	1.4654855932861302E+01	3.9620241602540789E+00
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H	1.1617889620506384E+01	1.4221219384045641E+01	3.0858992521293516E+00
H	1.1785241508676330E+01	1.5556849157489326E+01	4.0879061379088695E+00
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H	1.2129740816885471E+01	1.3724415741166258E+01	5.7613114694948129E+00
O	7.3714985305351233E+00	1.1008416120287052E+01	1.3638684988414453E+00
O	9.3550456701049463E+00	9.9656818445152009E+00	3.3025995554650431E+00
C	9.5584554311458554E+00	1.1219796261770906E+01	2.5108564976575307E+00
C	8.3377653734009876E+00	9.0854257227785151E+00	2.5856727980394583E+00
C	7.1320497885596117E+00	9.7937761369394760E+00	2.1830068098079716E+00
C	8.2184881826101535E+00	1.1908717789249405E+01	2.0914880300572189E+00
H	6.5536584628618186E+00	9.0613199872193579E+00	1.6237070842189412E+00
H	6.4834057174805810E+00	1.0127274594370283E+01	3.0350774937519018E+00
H	8.1916399912457845E+00	8.2683934779961152E+00	3.3018719304683812E+00
H	8.8657604075903809E+00	8.6042572773129926E+00	1.7202195376036808E+00
H	8.4634903515685238E+00	1.2638367183632660E+01	1.3200612406273862E+00
H	7.7975426323725836E+00	1.2396624304727229E+01	3.0068365087925231E+00
H	1.0039519157595235E+01	1.0901995733831587E+01	1.5252975494612846E+00
H	1.0189230579015041E+01	1.1792721959789441E+01	3.1949937726335826E+00
O	2.9593689635436840E+00	6.2038848095917061E+00	9.0421213134153178E-01
O	2.1566899940644660E+01	7.8916971306248618E+00	2.7442334785767510E+00
C	2.2157089010714945E+01	6.6319448953385596E+00	3.1490892263424151E+00
C	2.1308295433282936E+01	7.8191177802616618E+00	1.2783208619652224E+00
C	2.245212664377156E+01	7.4199285057003896E+00	4.4574037399259114E-01
C	2.3383743507301858E+01	6.2554076944912742E+00	2.2802524862227100E+00
H	1.9583290316283106E+00	7.2579597260864963E+00	-5.5184419265157181E-01
H	2.3254387826939833E+01	8.1584062316542081E+00	4.2287931451858968E-01
H	2.0907868539020566E+01	8.8107663096031441E+00	1.0633117049508960E+00
H	3.7920647226256599E-01	7.0483748403534765E+00	1.0702000144087001E+00
H	3.5980288909313494E+00	5.2400710039533465E+00	2.5178270044441518E+00
H	2.4239801327105553E+01	6.9319688928497403E+00	2.4457683028839901E+00
H	1.4138694014360162E+00	5.7663210518901016E+00	3.0316842910309147E+00
H	2.2371013340442818E+01	6.6469891983780078E+00	4.2354055760470697E+00
O	3.5890694023938354E+00	4.1947423170493261E+00	1.6564858503746620E+01
O	9.2901273652765659E-01	2.3765971848885005E+01	-2.7487707054839827E+00
C	2.0517929345179029E+00	2.3831758182608208E+01	-1.8324662857609515E+00
C	1.4042297490242748E+00	3.1561149700758167E+00	-4.0331025452200722E+00
C	2.5465304683459364E+00	4.0099081098223666E+00	-4.5338078625478273E+00
C	3.0253360064162105E+00	4.7289345402420917E+00	-2.3725445062488522E+00
H	2.3191799152531093E+01	3.4963166366804188E+00	1.4781854644901831E+01
H	2.3196492451129784E+00	5.0403589778754574E+00	-4.9283277504429464E+00
H	2.0655739048847362E+01	3.0632396102498105E+00	-4.7338717035447759E+00
H	2.1829338071578153E+01	2.2181222665637890E+01	1.6258666141372903E+01
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H	2.6235452960271863E+00	2.2860873178921359E+01	1.8343574999745346E+01
H	1.6998059936156464E+00	2.4098719661310930E+01	-8.4900618608275880E-01
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O	-3.4232174558676611E+00	1.7321332077451512E+01	6.1747737662156181E+00
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C	1.8426173450442903E+01	1.8362145657464740E+01	4.8735741801531711E+00
C	-2.3617917504978840E+00	1.6162291099895903E+01	4.2199953278270357E+00
H	1.8899340397542378E+01	1.9237899905276823E+01	4.4382225233713468E+00
H	1.9063267326191912E+01	1.8051992267170732E+01	5.6900563811215266E+00
H	1.7156456809781737E+01	1.9367415957287434E+01	6.2928729668731753E+00
H	1.6380528548730688E+01	1.8870234049836075E+01	4.7472506371653100E+00
H	-2.6649536879373095E+00	1.5682793503599651E+01	3.2696042482088643E+00
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H	-3.9227878663877340E+00	1.5415830499643466E+01	5.6149480491495289E+00
O	2.2923028489829087E+00	1.1298609939906507E+01	2.2238151556462487E+01
O	4.3593388064061127E+00	1.2474831879489216E+01	3.6294719998296667E+00
C	2.9305222163392157E+00	1.2741249209750199E+01	3.9971783784490658E+00
C	4.4649094871281747E+00	1.2318850780363375E+01	2.1790380340704369E+00
C	3.7073182598805574E+00	1.1110076945542694E+01	1.8409240250463501E+00
C	2.0012124240425608E+00	1.1664393170016568E+01	3.4752436770511550E+00
H	3.6826638227395447E+00	1.0849322455878784E+01	7.4449962365781919E-01

H	4.1112655027139544E+00	1.0176257363666508E+01	2.2427074424941917E+01
H	5.489035768837052E+00	1.2064348233497078E+01	2.0502066849830411E+00
H	4.2860815249173101E+00	1.3277921536538681E+01	1.5761597180585691E+00
H	2.1041108163184745E+01	1.1982579512137262E+01	2.3624544129442761E+01
H	2.0165102595991939E+00	1.0763715684917802E+01	2.4233730740522127E+01
H	2.2787167462089720E+01	1.3753919839859174E+01	3.6976727784523371E+00
H	2.3061882358249534E+01	1.2681838495141452E+01	5.1065895875262637E+00
O	7.3162416118911668E+00	1.7590562725612287E+01	7.7876911129224338E+00
O	6.2033307868278618E+00	1.5659416007333439E+01	9.4994670729117452E+00
C	7.6466944687844070E+00	1.5961827664532910E+01	9.5561559547807811E+00
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C	5.8622000323475127E+00	1.7399558447082427E+01	7.8967756662353743E+00
C	7.9484571456556967E+00	1.7375766228986627E+01	9.1086920439573138E+00
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C	1.0840595117801442E+01	6.2811385155999633E-01	-2.5050351388027861E+00
C	1.1577290642418093E+01	2.8607409565965427E+00	-2.4587391965503143E+00
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-1.70874556928602569E-04	2.9525289632904573E-04	-1.0896318688904776E-03
-3.5600797515570942E-04	-2.2235809584637701E-04	3.1607386305189356E-04
8.4528316776867366E-05	-2.0852162268959276E-05	2.0251260082538202E-05
1.4121353811058984E-04	-1.7968814076627142E-04	-1.2426291001770191E-04
-4.7875529056387947E-04	4.1622865936531697E-05	1.4861591850324295E-04
3.9929050040786663E-05	-6.0420447527577612E-05	-2.2086891015100219E-04
1.6729622444852559E-04	6.1760144103704994E-05	-1.9308841577173698E-04
1.0987712496722116E-03	8.1804314516384315E-04	4.9111442037979213E-04
-2.9008424238934847E-04	-9.6127872912690922E-04	-5.1795987277793360E-04
-2.4280891624978677E-04	-6.5340365711430946E-04	-6.0043747645409102E-04
4.9175007711405657E-04	7.6611802227194697E-04	6.8674335400097011E-04
6.2694941837123747E-06	8.0044023378926022E-04	-1.3031131920646997E-04
-1.3470355034467629E-04	-3.883305339994061E-04	-2.8652219144073157E-05
7.4431627238667427E-04	-4.5911615836201212E-04	-6.0555560112251583E-04
1.0787798954419070E-03	5.0182671370894300E-04	1.6573348436771089E-04
3.7713345064074539E-05	2.7424973105781504E-04	1.5585300526385504E-04
-1.0266368717586416E-04	-3.4311619054667097E-05	2.3302756299245625E-04
5.0938993649040841E-05	2.3277157891629793E-04	-1.6975947584410239E-04
2.3646129939385190E-04	-5.6912467838380351E-04	-9.2841858805103964E-05

&END VELOCITY

&KIND C

BASIS_SET DZVP-MOLOPT-SR-GTH

POTENTIAL GTH-PBE-q4

&POTENTIAL

2 2

0.338471240000000E+00 2 -0.8803673979999999E+01 0.133921085000000E+01

2

0.302575750000000E+00 1 0.962248665000001E+01

0.291506940000000E+00 0

&END POTENTIAL

&END KIND

&KIND O

BASIS_SET DZVP-MOLOPT-SR-GTH

POTENTIAL GTH-PBE-q6

&POTENTIAL

2 4

0.244554300000000E+00 2 -0.166672148000000E+02 0.248731132000000E+01

2

0.220955920000000E+00 1 0.183374581100000E+02

0.211332470000000E+00 0

&END POTENTIAL

&END KIND

&KIND H

BASIS_SET DZVP-MOLOPT-SR-GTH

POTENTIAL GTH-PBE-q1

&POTENTIAL

1

0.200000000000000E+00 2 -0.417890044000000E+01 0.724463310000000E+00

0

&END POTENTIAL

&END KIND

&KIND Rh

BASIS_SET DZVP-MOLOPT-SR-GTH

POTENTIAL GTH-PBE-q17

&POTENTIAL

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0.420000000000000E+00 2 0.262067934000000E+02 -0.493738335000000E+01

3

```

0.345446220000000E+00 2 -0.452482320000000E+00 0.389280438000000E+01
-0.502558885000000E+01
0.378380140000000E+00 2 -0.941112419999999E+00 -0.569931000000000E-02
0.674351000000000E-02
0.433747250000000E+00 2 0.157423622000000E+01 -0.301217170000000E+01
0.341548166000000E+01
&END POTENTIAL
&END KIND
&KIND B
BASIS_SET DZVP-MOLOPT-SR-GTH
POTENTIAL GTH-PBE-q3
&END KIND
&TOPOLOGY
NUMBER_OF_ATOMS 780
MULTIPLE_UNIT_CELL 1 1 1
&END TOPOLOGY
&END SUBSYS
&END FORCE_EVAL

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Simulation S2

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&GLOBAL
PRINT_LEVEL MEDIUM
PROJECT_NAME MD
RUN_TYPE MD
&END GLOBAL
&MOTION
&MD
ENSEMBLE NVT
STEPS 750
TIMESTEP 9.999999999999978E-01
STEP_START_VAL 5000
TIME_START_VAL 4.999999999995689E+03
ECONS_START_VAL -3.3824714789750383E+03
TEMPERATURE 3.000000000000000E+02
&THERMOSTAT
TYPE NOSE
REGION GLOBAL
&NOSE
LENGTH 4
YOSHIDA 3
MTS 2
&COORD
-2.2631887530026021E-01 1.3771861412010548E+01 6.0300772339181332E+00
3.0636929763953081E+01
&END COORD
&VELOCITY
-7.1656370278467617E-07 5.3308840457186362E-05 1.3335818563807413E-05
1.7363656282596911E-04
&END VELOCITY
&MASS
3.7021042250261183E+09 1.6237299232570694E+06 1.6237299232570694E+06
1.6237299232570694E+06
&END MASS
&FORCE
-2.5125118706431411E-11 5.8559673303749689E-10 2.2567323323886988E-09 -
4.0725608173426026E-10
&END FORCE
&END NOSE
&CSVR
TIMECON 9.999999999999986E+01
&END CSVR
&END THERMOSTAT
&AVERAGES T
&RESTART_AVERAGES
ITIMES_START 1
AVECPU 1.4783757815133711E+02
AVEHUGONIOT 0.000000000000000E+00
AVETEMP_BARO 0.000000000000000E+00
AVEPOT -3.3831612795156052E+03
AVEKIN 9.3099527417576555E-01
AVETEMP 2.5743856665699087E+02
AVEKIN_QM 0.000000000000000E+00

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AVETEMP_QM      0.000000000000000E+00
AVEVOL          5.4800532563775429E+04
AVECELL_A      3.7983495271001452E+01
AVECELL_B      3.7983495271001452E+01
AVECELL_C      3.7983495271001452E+01
AVEALPHA       9.000000000000000E+01
AVEBETA        9.000000000000000E+01
AVEGAMMA       9.000000000000000E+01
AVE_ECONS      5.6058531947087200E+00
AVE_PRESS      0.000000000000000E+00
AVE_PXX        0.000000000000000E+00
&END RESTART_AVERAGES
&END AVERAGES
&END MD
&PRINT
&TRAJECTORY SILENT
  ADD_LAST NUMERIC
  LOG_PRINT_KEY T
  FORMAT DCD_ALIGNED_CELL
  &EACH
    MD 1
  &END EACH
&END TRAJECTORY
&VELOCITIES OFF
  ADD_LAST NUMERIC
  LOG_PRINT_KEY T
  FORMAT XMOL
  &EACH
    MD 1
  &END EACH
&END VELOCITIES
&RESTART SILENT
  ADD_LAST NUMERIC
  LOG_PRINT_KEY T
  BACKUP_COPIES 0
  &EACH
    MD 10
  &END EACH
&END RESTART
&END PRINT
&END MOTION
&FORCE_EVAL
METHOD QS
&DFT
  BASIS_SET_FILE_NAME insert basis set path here
  POTENTIAL_FILE_NAME insert basis set path here
  MULTIPLICITY 1
  CHARGE 0
  &SCF
    MAX_SCF 60
    EPS_SCF 9.999999999999995E-07
    SCF_GUESS ATOMIC
    &OT T
      MINIMIZER DIIS
      PRECONDITIONER FULL_SINGLE_INVERSE
    &END OT
    &OUTER_SCF T
      EPS_SCF 9.999999999999995E-07
      MAX_SCF 5
    &END OUTER_SCF
  &PRINT
    &RESTART SILENT
      ADD_LAST NUMERIC
      COMMON_ITERATION_LEVELS 1
      FILENAME =./WFN_restart.wfn
      LOG_PRINT_KEY T
    &EACH
      QS_SCF 0
    &END EACH
  &END RESTART
&END PRINT
&END SCF
&QS
  EPS_DEFAULT 9.999999999999998E-13

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&END QS
&MGRID
  NGRIDS 5
  CUTOFF 3.000000000000000E+02
  REL_CUTOFF 5.000000000000000E+01
&END MGRID
&XC
  DENSITY_CUTOFF 1.000000000000000E-10
  GRADIENT_CUTOFF 1.000000000000000E-10
  TAU_CUTOFF 1.000000000000000E-10
  &XC_FUNCTIONAL NO_SHORTCUT
  &PBE T
  &END PBE
&END XC_FUNCTIONAL
&VDW_POTENTIAL
  POTENTIAL_TYPE PAIR_POTENTIAL
  &PAIR_POTENTIAL
  TYPE DFTD3(BJ)
  PARAMETER_FILE_NAME dftd3.dat
  REFERENCE_FUNCTIONAL PBE
  &END PAIR_POTENTIAL
&END VDW_POTENTIAL
&END XC
&POISSON
&END POISSON
&LOCALIZE T
&END LOCALIZE
&END DFT
&SUBSYS
&CELL
  A 2.0100000000000001E+01 0.000000000000000E+00 0.000000000000000E+00
  B 0.000000000000000E+00 2.0100000000000001E+01 0.000000000000000E+00
  C 0.000000000000000E+00 0.000000000000000E+00 2.0100000000000001E+01
  PERIODIC XYZ
  MULTIPLE_UNIT_CELL 1 1 1
&END CELL
&COORD
Rh 1.0396636922105996E+01 1.1029521772537862E+01 1.0990855317859909E+01
C 8.7010401779321747E+00 1.2720905006854606E+01 1.0949634592224202E+01
C 1.0742367257682579E+01 1.3725535780623117E+01 1.1870067427313105E+01
C 1.3685638688516727E+01 1.3033540553539035E+01 1.1963817619684045E+01
C 7.2283488170754344E+00 1.2262950567345840E+01 1.1020101631000374E+01
C 6.7418085993768031E+00 1.1641880851652283E+01 1.2229988191742963E+01
C 9.4573196763673266E+00 1.2862947494532818E+01 1.2111186297737779E+01
C 9.3275123498772299E+00 1.3367093731297558E+01 9.6816725702913526E+00
C 4.9550044998265239E+00 1.2036417400794068E+01 1.0165564703502790E+01
C 1.5794632405748780E+01 1.2977178873419849E+01 1.0865673267447365E+01
C 1.0368179395255162E+01 1.5065847174839091E+01 1.1197730875314878E+01
C 1.0645861298463021E+01 1.2599867379558544E+01 9.6537342511675419E+00
C 5.4598499721603915E+00 1.1124521325311575E+01 1.2358907008893970E+01
C 1.1474053279625613E+01 1.2914750652655002E+01 1.0780298991722129E+01
C 1.3700576270414761E+01 1.3064812056422427E+01 9.6142804110819533E+00
C 6.2233560862172395E+00 1.2526325151547592E+01 9.9896716548016986E+00
C 9.5030485533784930E+00 1.4844576445579431E+01 9.9244249770285293E+00
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C 1.2913397466756127E+01 1.3045313399125479E+01 1.0765530389276817E+01
C 1.5120569322257152E+01 1.3127546305669464E+01 9.6157258683068889E+00
C 1.5080335064622275E+01 1.2952124709739849E+01 1.2058614461927087E+01
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H 1.6891459620707138E+01 1.2960664220589692E+01 1.0954821734845309E+01
H 1.3233009168248808E+01 1.3194076226155689E+01 8.6496667379244574E+00
H 1.5591234852663627E+01 1.3174223783378604E+01 8.6714470262052803E+00
H 1.5490749521217680E+01 1.2748100351450507E+01 1.3028090346316365E+01
H 7.4386518308367746E+00 1.1455567946557023E+01 1.3062327173127867E+01
H 4.2240108512073347E+00 1.2430838121223767E+01 9.4110057069306166E+00
H 5.0899599138975908E+00 1.0588440824907389E+01 1.3197522134586064E+01
H 6.5473320600790537E+00 1.3081091779019134E+01 9.0771247579846310E+00
H 3.4887502027934461E+00 1.1137588473532205E+01 1.1390276920320959E+01
H 1.1430178346911280E+01 1.3822249845210644E+01 1.2749203953101599E+01
H 8.7208739549023324E+00 1.3046961333347499E+01 8.8011565007673394E+00
H 9.8774410224546099E+00 1.5751612744308352E+01 1.1951512456923151E+01
H 1.1261699093844037E+01 1.5598530503014992E+01 1.0984518598903596E+01
H 1.0029239669087209E+01 1.5321855817750093E+01 9.1177057112107267E+00
H 8.5118627677138630E+00 1.5206773023928653E+01 1.0115664206458606E+01

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H	1.1155640449501837E+01	1.2387889451213383E+01	8.6366757160294387E+00
H	9.2192564502526064E+00	1.2757790757984759E+01	1.3192379826918817E+01
C	1.1586917365660527E+01	9.7759080280306634E+00	9.7789624644434081E+00
C	1.2949182281427335E+01	9.9511171633586475E+00	9.5412789521294137E+00
C	1.1037861030223016E+01	8.6850507444805825E+00	9.0883476303761039E+00
C	1.3729918681173379E+01	9.2332663982632326E+00	8.6478961054123999E+00
H	1.3422759527619043E+01	1.0717435420934409E+01	1.0180813767600567E+01
C	1.1722092843124903E+01	7.9656594254046400E+00	8.1061484896797360E+00
H	9.9967711785951092E+00	8.3727434019744376E+00	9.2606955099657782E+00
C	1.3087552498632919E+01	8.2094615170884904E+00	7.9023945923110865E+00
H	1.4809871226782283E+01	9.3362087052789740E+00	8.7201703001337378E+00
H	1.1144823780333111E+01	7.2877856479158263E+00	7.4493367061668794E+00
H	1.3577726036736422E+01	7.6783802145322309E+00	7.1288420091525140E+00
C	1.0851657105264612E+01	9.1128340745631800E+00	1.2221005772107798E+01
C	9.5888416628368152E+00	9.6994180986975937E+00	1.2620098866084934E+01
H	1.0857900625515159E+01	8.2982253341570207E+00	1.1488121488950599E+01
H	8.6277112622473826E+00	9.4066159186710543E+00	1.2203823412193627E+01
C	9.4544586238219441E+00	1.0032365715195384E+01	1.4001366747095627E+01
O	8.3807186396310804E+00	1.0096293628670768E+01	1.4642287293120688E+01
C	1.0753151719077575E+01	1.0333153952302379E+01	1.4763021650975322E+01
H	1.0465497530106893E+01	1.1214964894538088E+01	1.5324957488859928E+01
C	1.2107521453153916E+01	9.3182021794808776E+00	1.2964418750281556E+01
C	1.1964817553391274E+01	1.0468803993406773E+01	1.3916071986149165E+01
H	1.0884929495786746E+01	9.5411224807099284E+00	1.5471335409611301E+01
H	1.1882222661907869E+01	1.1395460308464218E+01	1.3318703153971908E+01
H	1.28657441111139053E+01	1.0517997934038553E+01	1.4576098784930313E+01
H	1.2296511746959634E+01	8.3914478215700949E+00	1.3511657758610824E+01
H	1.2981325233197476E+01	9.3781479984417651E+00	1.2281078402760544E+01
H	1.4808870815414526E+01	6.7074892686022860E+00	1.4214509773141126E+01
O	1.8722859484541850E+01	1.9330476555537210E+01	7.3704719361107536E+00
H	1.7949861093444941E+01	1.8747294404679597E+01	7.2049142270772411E+00
H	1.9438759995674129E+01	1.8659732416891078E+01	7.4797921732808277E+00
O	1.5347203593802236E+01	7.3252740332083288E+00	1.3693584490321523E+01
H	1.6159988368782869E+01	6.8402727033426771E+00	1.3609794845551233E+01
O	1.3862749015667200E+01	1.7186345167374711E+01	1.1287988422937367E+01
B	5.6067766278856439E+00	9.5674679100115334E+00	1.7569825967187796E+01
O	6.4995168547471991E+00	1.2857282686116234E+01	6.2175239559804467E+00
O	6.2965751799565108E+00	9.1955804963626271E+00	1.6402633246360431E+01
H	1.3784218217615837E+01	1.7379067189338976E+01	1.0330407749966991E+01
H	1.4155880672799773E+01	1.6283914649332939E+01	1.1246916202349691E+01
O	4.7747251151983807E+00	3.7073972164647109E+00	1.1916887528866118E+01
O	6.1522298160073445E+00	1.0274681927365545E+01	1.8631882931641762E+01
O	4.3313577969765156E+00	9.0570170271459780E+00	1.7683890124091526E+01
H	5.0824543141036322E+00	2.8283807091168423E+00	1.1801509781517531E+01
H	5.5275832896969437E+00	1.0151430185594750E+01	1.9400068529133112E+01
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H	6.5008524604807539E+00	1.1933161913941586E+01	3.9987128847706352E+00
H	7.0703033620442266E+00	9.7055102805918398E+00	1.6216366426575220E+01
H	7.3609389799819525E+00	1.3243086834104110E+01	6.0077634129542625E+00
H	6.8313910701905805E+00	9.8632483178286705E+00	9.6863387580551823E+00
H	8.6838295574669750E+00	8.1791418569024437E+00	8.0014777570604600E+00
H	7.9106285216513967E+00	7.7749357403517658E+00	9.4833595417586167E+00
O	2.7303709936875831E+00	1.7218661302681102E+01	1.1470881668314448E+00
O	1.6076881019871023E+00	1.5255804306009836E+01	2.8459018381010863E+00
C	8.1766473794653582E-01	1.6286343291829699E+01	2.2571687948088082E+00
C	3.0439795996234684E+00	1.5452789945507243E+01	2.8491294913562806E+00
C	3.4242918926402579E+00	1.5995076546775650E+01	1.4532767539132603E+00
C	1.3701021171298846E+00	1.6836350331832051E+01	9.9005595512554645E-01
H	4.4645567574615219E+00	1.6282869661710134E+01	1.2551179595133590E+00
H	3.2683442607467237E+00	1.5278000019533632E+01	5.9948902320084474E-01
H	3.5362373492336561E+00	1.4482502442925162E+01	3.0822147732044547E+00
H	3.3051555714461500E+00	1.6275448148797892E+01	3.5157381750301600E+00
H	7.5773406945944277E-01	1.7673404491531407E+01	7.5240182997610028E-01
H	1.3372497425354595E+00	1.6059081271620826E+01	2.5457672469392484E-01
H	6.8353597893015861E-01	1.7153612608217923E+01	2.8868804408130795E+00
H	-7.40641405540114030E-02	1.5682904663203745E+01	1.9886665743542504E+00
O	1.0984616680656803E+01	9.4878007305223999E+00	2.0618391995795658E+01
O	8.7558531187217774E+00	1.1153425976831883E+01	2.0444907034025974E+01
C	8.8737319552001441E+00	1.0013009625344973E+01	1.9580304535472919E+01
C	1.0019389538512648E+01	1.1636313240560586E+01	2.0830829813550135E+01
C	1.0827338884285936E+01	1.0613720787318352E+01	2.1489150599394815E+01
C	9.6462785876818167E+00	8.9400815183541251E+00	2.0273778618411399E+01
H	1.1839823011995135E+01	1.0937495765939005E+01	2.1733896481605104E+01

H	1.0320181863410449E+01	1.0308493493044093E+01	2.2392859424348622E+01
H	9.7903224521543564E+00	1.2471384671005559E+01	2.1501197046451871E+01
H	1.56807487533597E+01	1.2069401054554060E+01	1.9966963332243900E+01
H	9.8182252068725546E+00	8.0336040676823810E+00	1.9670668423086390E+01
H	9.1602116391075512E+00	8.6660710186218566E+00	2.1181598838082429E+01
H	9.4340244135537024E+00	1.0249261454547847E+01	1.8632664298331772E+01
H	7.8094723370656123E+00	9.7496262777627951E+00	1.9222941172408607E+01
O	1.6850602669139050E+01	1.6911992699927570E+01	6.9196283236152940E+00
O	1.7590769853689409E+01	1.4047183663553335E+01	6.9752232077628396E+00
C	1.8028013188710343E+01	1.5038517094638925E+01	7.9858129132141791E+00
C	1.7550425901928087E+01	1.4697368418769608E+01	5.7323489404957781E+00
C	1.663593122008697E+01	1.5983491070354495E+01	5.8918628791594720E+00
C	1.7019580939334123E+01	1.6142781948222407E+01	8.1493499613653135E+00
H	1.6799034358437940E+01	1.6575434630767106E+01	4.9405949378722438E+00
H	1.5544737852950888E+01	1.5753958386515842E+01	5.8277023627622775E+00
H	1.7042738587490433E+01	1.3927652284405223E+01	5.1289535344477031E+00
H	1.8540918992093239E+01	1.5008745207084282E+01	5.3686238415679544E+00
H	1.7493476102130028E+01	1.6759026366864816E+01	8.9373335363648216E+00
H	1.6001183121433158E+01	1.5804259937698323E+01	8.4600371775918735E+00
H	1.8964778120632271E+01	1.5575826886076555E+01	7.7198039290430938E+00
H	1.8167739574653911E+01	1.4431450890982626E+01	8.8591071330252999E+00
O	6.5025463305984275E+00	1.9266505291991642E+01	1.6683891113300060E+01
O	4.7715499285908871E+00	2.1248685348927758E+01	1.7694704553589069E+01
C	4.2670045949831747E+00	2.0386798985292689E+01	1.6699062753096850E+01
C	6.2020611416490556E+00	2.1499288205864318E+01	1.7527248818523404E+01
C	6.9182108685715642E+00	2.0178501830392218E+01	1.7781936586775558E+01
C	5.0445316970695080E+00	1.9062426633175932E+01	1.6713000318373258E+01
H	7.9928329187936269E+00	2.0331991413016066E+01	1.7578928164656300E+01
H	6.6838077856237339E+00	1.9782201569514950E+01	1.8821295085880198E+01
H	6.5460083057750840E+00	2.2229899945583245E+01	1.8320927456043655E+01
H	6.4985427827838924E+00	2.1833712905449648E+01	1.6512028587462030E+01
H	4.7008839192426226E+00	1.8348678383917385E+01	1.5943409094421574E+01
H	4.8383716421339926E+00	1.8544817585151236E+01	1.7713783827438125E+01
H	4.4446574782927808E+00	2.0873027593572079E+01	1.5688627730808435E+01
H	3.2214380487507799E+00	2.0182366708261696E+01	1.6928003250609045E+01
O	1.6574623827568885E+01	2.0784580901764603E+01	1.1719391524135736E+01
O	1.7653917579091033E+01	1.8235195177693914E+01	1.2608432902270289E+01
C	1.7591479727086899E+01	1.8569116187484575E+01	1.1245674674369187E+01
C	1.6502849230076354E+01	1.8864028093920961E+01	1.3193800643264764E+01
C	1.6407147984259030E+01	2.0436990035633830E+01	1.3065975500101711E+01
C	1.7667834798771427E+01	2.0058151603742811E+01	1.1064598675258509E+01
H	1.5372512101475278E+01	2.0762413703674131E+01	1.3387349559213384E+01
H	1.7175816141758055E+01	2.0884242459966455E+01	1.3763133467640905E+01
H	1.6567245451645025E+01	1.8706480890131473E+01	1.4290550946734339E+01
H	1.5583586256740887E+01	1.8333364574523831E+01	1.2812242010963953E+01
H	1.7516159846185513E+01	2.0302948847808619E+01	1.0029492794151347E+01
H	1.8667672557737248E+01	2.0420095735619824E+01	1.1441295922828051E+01
H	1.6760034975402020E+01	1.8012953648891994E+01	1.0710122654636942E+01
H	1.8524082298535717E+01	1.8293128938144985E+01	1.0716480302476405E+01
O	1.9193124590751260E+01	3.2037507639116800E+00	1.8483546348603888E+01
O	2.0477188647703361E+01	7.0662674829000260E-01	1.7700923011934137E+01
C	2.1179534241511444E+01	1.7040187652922356E+00	1.8400680939394551E+01
C	1.9520740601236049E+01	1.3292811916872382E+00	1.6870443927826155E+01
C	1.8530888586650210E+01	2.1499118869477618E+00	1.7734266475942729E+01
C	2.0283867598122473E+01	2.6722053608680305E+00	1.9236346282813905E+01
H	1.7800521202599878E+01	2.6272626304891165E+00	1.7074231398351728E+01
H	1.7951379440753072E+01	1.4179894675633056E+00	1.8471095322206377E+01
H	1.8848950097952219E+01	5.5997831420380373E-01	1.6436685497311213E+01
H	1.9997419360570849E+01	1.9034822418223805E+00	1.6084137880829100E+01
H	2.0793743899928923E+01	3.4895019861212813E+00	1.9648525520293113E+01
H	1.9957188835779192E+01	2.0581354176024562E+00	2.0133929176335577E+01
H	2.1664686916150536E+01	2.3262521442078539E+00	1.7640287822869567E+01
H	2.1887666047394529E+01	1.1797280384585018E+00	1.9095699172780648E+01
O	1.3862717750727402E+01	4.8887616995538323E+00	1.5090632552516603E+01
O	1.3038841459516897E+01	2.1863909101348469E+00	1.5055240863329908E+01
C	1.4033380047021499E+01	2.6669015767400155E+00	1.5941825321245039E+01
C	1.3002320868591319E+01	2.9744731932550752E+00	1.3783885801718629E+01
C	1.2868105729145274E+01	4.4506477116151668E+00	1.4084219451031696E+01
C	1.3752059854202251E+01	4.1398736760524395E+00	1.6294591948360221E+01
H	1.3133355056407433E+01	4.9601053829240493E+00	1.3141998926161039E+01
H	1.1857422852406989E+01	4.7281191368468738E+00	1.4368107782765387E+01
H	1.2110391721001298E+01	2.5827885582111030E+00	1.3343591331813778E+01
H	1.3964759453229659E+01	2.8783065209167100E+00	1.3257051984101958E+01
H	1.4495874601057588E+01	4.6154154317810399E+00	1.6922040276366221E+01

H	1.2800649661750462E+01	4.3120513795807778E+00	1.6724935341002201E+01
H	1.4994416204518677E+01	2.6916510516909971E+00	1.5376326465457637E+01
H	1.4026953830893181E+01	1.9902032156947471E+00	1.6891229575388127E+01
O	1.4719464093490616E+01	4.6837527432389496E+00	1.0727923977127061E+01
O	1.2339582820102395E+01	3.7030028272599917E+00	9.3505009396879686E+00
C	1.2482409603490236E+01	5.0798253275797443E+00	9.8841154192955702E+00
C	1.3275778658187416E+01	2.8128694238449476E+00	1.0021358095053156E+01
C	1.4735898836662900E+01	3.3162576460169091E+00	1.0101966645210720E+01
C	1.3933800559176271E+01	5.5193957991320604E+00	9.9179866603626170E+00
H	1.5363072540676592E+01	2.5813848473234917E+00	1.0608062766286563E+01
H	1.5204524549885528E+01	3.3946711444097590E+00	9.0761243634700630E+00
H	1.3261084217453222E+01	1.8915786052345087E+00	9.3413297789973342E+00
H	1.2811599739037135E+01	2.5418429054594385E+00	1.1039040638295251E+01
H	1.3993225442840210E+01	6.5115754815673448E+00	1.0321645199341296E+01
H	1.4285850588116011E+01	5.5546520429725303E+00	8.8701023702818969E+00
H	1.2130533572181351E+01	5.1167590141542538E+00	1.0945723657324214E+01
H	1.1843699252004718E+01	5.7234692014052415E+00	9.2413048512208515E+00
O	1.2085761658283335E+01	1.4749012060097519E+01	1.9625389601848308E+01
O	1.4433548628754272E+01	1.5890020401487705E+01	2.0960962827414150E+01
C	1.3693253622073591E+01	1.4771837304757483E+01	2.1580340413758005E+01
C	1.3628371701888586E+01	1.6578256526690438E+01	2.0039530168269430E+01
C	1.2914953564971162E+01	1.5725653170525680E+01	1.9010123330885289E+01
C	1.2945975680836291E+01	1.3929333874754148E+01	2.0435407615327087E+01
H	1.2240986466065129E+01	1.6467385856242853E+01	1.8435829994093787E+01
H	1.3564712317773504E+01	1.5346860611180364E+01	1.8182915301577026E+01
H	1.4204144519251189E+01	1.7324712636945598E+01	1.9523140248752483E+01
H	1.2791780950297358E+01	1.7203177340818574E+01	2.0526383398806409E+01
H	1.2260598819624748E+01	1.3096489473627560E+01	2.0941241218370980E+01
H	1.3711432205824075E+01	1.3379589795432715E+01	1.9884517300568564E+01
H	1.2939127768153110E+01	1.5231427960928047E+01	2.2267478257062329E+01
H	1.4304878157080880E+01	1.4123516315644297E+01	2.2198567737719451E+01
O	5.340853839533398E+00	6.7386571930000576E+00	1.9686483854987962E+00
O	7.8197328506710431E+00	6.1136822362322745E+00	7.1745222557017352E-01
C	6.7031078819243755E+00	6.6936135755007289E+00	2.5555070680615154E-02
C	7.5305285869023866E+00	5.5661066487477058E+00	2.0138560890299093E+00
C	6.4845786000892867E+00	6.4655858389149747E+00	2.7375357850421231E+00
C	5.7575729134426830E+00	7.5727289430491753E+00	8.4461521615410262E-01
H	6.0571021867412824E+00	5.9988824792888487E+00	3.6723086840357628E+00
H	6.9502199535383093E+00	7.4019027918186131E+00	3.0669292712120502E+00
H	8.5029349775671399E+00	5.6649142715867464E+00	2.5303119951370925E+00
H	7.2327568723392783E+00	4.5093993759218272E+00	1.8758529479967168E+00
H	4.8840213104672516E+00	7.9231370151531966E+00	3.3404867849008413E-01
H	6.3602652804537394E+00	8.4614756756511795E+00	1.1940694917439527E+00
H	6.0672957779382086E+00	5.8802461823810841E+00	-4.2655621488368783E-01
H	7.1970745530457298E+00	7.2215251978289885E+00	-8.2407564741172068E-01
O	7.7975626108949633E-02	1.0586032774647808E+01	6.5222845844438799E+00
O	2.7524117553703009E+00	1.0042933904407793E+01	5.4496455726898363E+00
C	2.4141504027359177E+00	1.1357824450341361E+01	5.9083501295813932E+00
C	1.5911767249741455E+00	9.3461844347756795E+00	4.8843091967589860E+00
C	5.9601152154761661E-01	9.3588007002433855E+00	5.9781256944869252E+00
C	1.2861511962751486E+00	1.1234746911769378E+01	6.9288612725168530E+00
H	-3.6258988722736613E-01	8.8522372801189206E+00	5.7749042111737223E+00
H	1.1303204615009363E+00	8.7881691864425111E+00	6.7812438714174599E+00
H	1.8459623438888859E+00	8.3394827756252941E+00	4.5771580692914231E+00
H	1.2808844502076311E+00	9.9338861269981713E+00	3.9970368277461312E+00
H	9.2454391496045663E-01	1.2251901560270337E+01	7.0813826140635960E+00
H	1.6883751400512454E+00	1.0820547748592276E+01	7.8297590849671979E+00
H	2.2385417826126113E+00	1.2048239175809558E+01	5.0574644474514603E+00
H	3.3214954910219618E+00	1.1707873998027136E+01	6.4346401383612433E+00
O	1.7350677849322352E+01	8.1103809505016855E+00	8.0846264044593816E+00
O	1.7799874595583645E+01	9.6385736835197182E+00	1.0439185317263982E+01
C	1.6861159395828640E+01	8.5854566922059004E+00	1.0488444182639197E+01
C	1.7850071327399249E+01	1.0245562092130353E+01	9.1452804797402241E+00
C	1.8253352184138862E+01	9.2277585057492217E+00	8.0858798727492527E+00
C	1.7220508328137495E+01	7.5162051691977396E+00	9.4222550327986259E+00
H	1.8290391220458346E+01	9.5946607607038423E+00	7.0569292240338264E+00
H	1.9279816484731587E+01	8.9161772229015295E+00	8.3048000209434267E+00
H	1.8587271601960079E+01	1.1039762423080735E+01	9.3524709388571310E+00
H	1.6894291621824305E+01	1.0722092548202065E+01	8.9047527083206557E+00
H	1.6434617369124346E+01	6.8115101344297120E+00	9.3025588414112974E+00
H	1.8223367638927296E+01	7.0474868076968731E+00	9.7588618551598909E+00
H	1.5813267094374044E+01	8.9992183171269087E+00	1.0324841461959275E+01
H	1.6895186638388619E+01	8.1361595280581138E+00	1.1460232788627994E+01
O	1.0924877705492126E+01	5.3662751528238442E+00	2.5575987620808491E+00

O	1.2285112410071784E+01	6.9178853957134505E+00	4.4981334687297059E+00
C	1.1775689632671442E+01	5.6081711644679348E+00	4.8160259003992678E+00
C	1.1641254333348773E+01	7.5052676941559904E+00	3.2999154450542068E+00
C	1.1555940360520980E+01	6.5710977066190672E+00	2.1133724623757342E+00
C	1.1816400551652695E+01	4.8019217771075366E+00	3.5826890118853854E+00
H	1.0937032903142592E+01	7.0406263154574162E+00	1.3634744985493170E+00
H	1.2589497175732555E+01	6.3923755745629061E+00	1.7712115316718806E+00
H	1.2168093515428497E+01	8.4190822399004634E+00	3.0329313983615549E+00
H	1.0622654706975865E+01	7.7211587570519882E+00	3.6008085057113965E+00
H	1.1404838562315305E+01	3.8253137802762045E+00	3.7420601894736762E+00
H	1.2805328842633829E+01	4.7337986199920916E+00	3.2127699783342960E+00
H	1.0744336891943382E+01	5.5954701260134412E+00	5.2669337182846201E+00
H	1.2458893947233198E+01	5.2566607505078986E+00	5.6013270639836001E+00
O	1.9173796948357637E+01	1.9126910965577089E+01	2.2436716846632788E+01
O	1.6623738507904932E+01	1.8638683198967268E+01	2.1141597104209193E+01
C	1.6944755770636579E+01	1.8032351512668328E+01	2.2354354350828146E+01
C	1.7857634418112116E+01	1.8920931059857100E+01	2.0462788614001671E+01
C	1.8832586303160301E+01	1.9825572466479283E+01	2.1231884913061442E+01
C	1.7970559769020571E+01	1.8873201305929360E+01	2.3072586650197724E+01
H	1.9777305363465455E+01	1.9961900133086804E+01	2.0683048071829948E+01
H	1.8378961378377447E+01	2.0756480193599991E+01	2.1534360420800198E+01
H	1.7555480400235233E+01	1.9329569443013110E+01	1.9508431557430569E+01
H	1.8383281905037094E+01	1.7980123304229281E+01	2.0288956538075944E+01
H	1.8257413874579957E+01	1.8300149670306112E+01	2.3953638964072297E+01
H	1.7442840688495188E+01	1.9844441150220337E+01	2.3375632021054759E+01
H	1.7328140489544669E+01	1.7018076752255425E+01	2.2190399494311883E+01
H	1.6089994644606545E+01	1.7981628956349475E+01	2.3045378077438869E+01
O	1.3216978851992129E+01	9.2349607023594498E+00	1.7479540033938409E+01
O	1.5736850409830112E+01	8.1844121161233776E+00	1.8303946203920340E+01
C	1.4986430536630273E+01	7.5653443621279575E+00	1.7173405011825377E+01
C	1.4841920431360441E+01	8.6561787349006281E+00	1.9295000008617311E+01
C	1.3973836195185026E+01	9.7520820595065043E+00	1.8640908574620912E+01
C	1.4018371788826840E+01	8.5272230465944077E+00	1.6534500467360026E+01
H	1.3130631931026397E+01	1.0185585935633796E+01	1.9208539679428554E+01
H	1.4622515754459855E+01	1.0577566263046759E+01	1.8248563913995181E+01
H	1.5548183061183687E+01	9.0602951073837481E+00	1.9985053017814618E+01
H	1.4203867779466661E+01	7.8325971448798590E+00	1.9714346408761120E+01
H	1.3272124317338138E+01	7.9760329558307603E+00	1.5883576883665219E+01
H	1.4532208146518135E+01	9.1766417596148102E+00	1.5796202546706827E+01
H	1.4459592264206368E+01	6.6404728599229710E+00	1.7500432527815182E+01
H	1.5780040449910775E+01	7.3935096385695571E+00	1.6430987797720825E+01
O	3.8937261279597841E+00	5.8168056819902452E+00	1.5093587034326514E+01
O	2.0571788184175488E+00	4.8649634846391603E+00	1.7059277456953041E+01
C	3.3193964157012603E+00	5.4390734296663554E+00	1.7503197844929389E+01
C	2.1612356094642560E+00	4.1382163174229154E+00	1.5733664282587357E+01
C	2.6870309001703245E+00	5.0907713500730800E+00	1.4667022884607904E+01
C	3.8714818234582586E+00	6.3676596120659807E+00	1.6391357954169035E+01
H	2.9311154108433435E+00	4.4532392084140504E+00	1.3756732222457533E+01
H	1.9329760244739635E+00	5.8185925570963040E+00	1.4302989740262420E+01
H	1.1361547216875763E+00	3.7902639629740142E+00	1.5563291387466956E+01
H	2.8558001912835560E+00	3.2850224956476373E+00	1.5894865335442764E+01
H	4.9231532645186933E+00	6.6248168465871853E+00	1.6745657527678059E+01
H	3.1740228158469566E+00	7.2285963490751870E+00	1.6392963602852209E+01
H	3.9798003899806043E+00	4.6000363948282432E+00	1.7702422174168696E+01
H	3.1401586475168566E+00	6.0290994465620784E+00	1.8442260224660973E+01
O	9.0456416694667521E+00	4.4197577174494453E+00	1.2399425452653492E+01
O	6.4470536755990624E+00	5.6927570460962631E+00	1.2479983873116183E+01
C	7.2481969353891067E+00	5.6808337384069887E+00	1.1323345861300343E+01
C	7.2494258965565361E+00	5.5064011851536705E+00	1.3711782388467862E+01
C	8.0939653930524553E+00	4.2533893463507875E+00	1.3563309314593498E+01
C	8.1359721054708096E+00	4.4809119842958740E+00	1.1164164374978647E+01
H	8.8174667925370631E+00	4.0641549111366491E+00	1.4406520975940207E+01
H	7.5268180385596768E+00	3.3807317261643122E+00	1.3316476489328615E+01
H	6.5807147772151451E+00	5.3643253472428745E+00	1.4570102767447008E+01
H	7.8507955213372735E+00	6.3906672768861528E+00	1.3937693031035664E+01
H	8.8623195903862939E+00	4.6392499574003185E+00	1.0392498479756165E+01
H	7.6904422495639775E+00	3.5078355624313677E+00	1.0973439564576017E+01
H	7.9353250363103607E+00	6.5613620208692165E+00	1.1249939272409900E+01
H	6.5185153326107468E+00	5.6559925204086863E+00	1.0451250873387563E+01
O	1.0987697016507671E+01	1.3851704346328583E+01	1.5353898976297717E+01
O	1.3400247527844069E+01	1.5431684831997211E+01	1.5523880010920248E+01
C	1.2364393978437040E+01	1.5777963507596109E+01	1.4577995480715037E+01
C	1.3466635857167404E+01	1.3983416107495438E+01	1.5685980970033411E+01
C	1.2118825042171586E+01	1.3478211156669255E+01	1.6216588595797692E+01

C	1.0997967547611996E+01	1.5255924043025791E+01	1.5037155873210855E+01
H	1.2105043724775241E+01	1.2389202447520136E+01	1.6175421603374293E+01
H	1.1866572530814866E+01	1.3753898475669599E+01	1.7271206708628011E+01
H	1.4261403252992585E+01	1.3733285199038704E+01	1.6370497305833627E+01
H	1.3619383447930813E+01	1.3556623848814148E+01	1.4678008644855911E+01
H	1.0250607405752216E+01	1.5343946368252691E+01	1.4251857985357240E+01
H	1.0723777219327539E+01	1.5973905728994421E+01	1.5821731744416692E+01
H	1.2556450925531893E+01	1.5471952190747871E+01	1.3556476865156737E+01
H	1.2364494671820568E+01	1.6898420388750782E+01	1.4588570190088202E+01
O	1.6387505437276517E+00	2.7782924965774134E+00	1.0128206401424547E+01
O	-4.4874963480067526E-01	4.8278213805074666E+00	1.0187697500147323E+01
C	8.1663097945316931E-01	5.0549863654453429E+00	1.0797767791442270E+01
C	-7.5170541029581184E-01	3.4163450195939995E+00	1.0223059151704827E+01
C	3.6166010575458746E-01	2.5252717311738340E+00	9.5191362606735161E+00
C	1.9275933206761724E+00	4.1607806851098967E+00	1.0097708497116065E+01
H	3.6653111941666691E-02	1.5226498807241662E+00	9.8018364770849402E+00
H	5.3782670037445879E-01	2.6175783570083433E+00	8.4457665692584136E+00
H	-1.7871535426829515E+00	3.2782739778481607E+00	9.8154955390467400E+00
H	-7.3349698017466636E-01	3.0026784676906537E+00	1.1199205917997505E+01
H	2.9530345661320245E+00	4.3014722492381621E+00	1.0595527791672012E+01
H	2.0369591861936396E+00	4.4637749049163356E+00	9.0782893543375653E+00
H	8.5645997568150167E-01	4.7388033490437174E+00	1.1854826473674525E+01
H	1.0439965304239907E+00	6.0826258135687175E+00	1.0700421610477100E+01
O	7.0687707998393021E+00	1.2270598586879748E+00	1.2518668032961559E+01
O	9.4248751067936496E+00	-3.2655049326290747E-01	1.3079178812001739E+01
C	8.7508616509150254E+00	4.2879553779322277E-01	1.4100192609347850E+01
C	9.3798775899350471E+00	4.7513421377300369E-01	1.1832796586674922E+01
C	7.8902145933195333E+00	6.1875038791158787E-01	1.1499233963834271E+01
C	7.2317896238679138E+00	5.1869396400859591E-01	1.3790108330265516E+01
H	7.6321483308999785E+00	1.0519445618129828E+00	1.0500093658666668E+01
H	7.4977444826154551E+00	-4.6000253103583011E-01	1.1452695425340236E+01
H	9.7618440850934807E+00	-2.2919006179199655E-01	1.0974594106870482E+01
H	9.8548625501258282E+00	1.3744220623617254E+00	1.2073499300865141E+01
H	6.8107301054141480E+00	1.1777218051409493E+00	1.4533753033716412E+01
H	6.7722323290093422E+00	-4.8363557008233998E-01	1.3711653370831801E+01
H	9.2617928766448472E+00	1.3779723426707651E+00	1.4254572158362114E+01
H	9.0279656758994022E+00	-2.0377692397907179E-01	1.5006366631622994E+01
O	1.7335560431083085E+01	3.6911775796593340E+00	1.4620076039922385E+01
O	1.7987891709637733E+01	6.4822502611236521E+00	1.3865993451711665E+01
C	1.7965624124302444E+01	5.3263427377927490E+00	1.2920516886710869E+01
C	1.8166890867938729E+01	5.8290705988835931E+00	1.5184582931141209E+01
C	1.7055148222252317E+01	4.7736273125307802E+00	1.5491167465708353E+01
C	1.6999300388065759E+01	4.1218111509622375E+00	1.3293459258593661E+01
H	1.7211418571333308E+01	4.5071311747664877E+00	1.6557957994691346E+01
H	1.6017522341082717E+01	5.1108998506495231E+00	1.5309273786512898E+01
H	1.8150035710047394E+01	6.6513400099517241E+00	1.5845780210550608E+01
H	1.917773063680988E+01	5.4005273036716428E+00	1.5234559154497708E+01
H	1.7355859696217028E+01	3.2847128862816648E+00	1.2695621875230616E+01
H	1.5925842642589359E+01	4.3732243190036089E+00	1.3187774732384197E+01
H	1.8949851401955993E+01	4.9273558829912414E+00	1.3012386782942901E+01
H	1.7660871810250018E+01	5.6564339617176218E+00	1.1931620372421067E+01
O	-1.4238416281284974E-01	8.6341476380766906E+00	1.9016960095900856E+01
O	5.8991827933747747E-01	6.2514113356091778E+00	2.0406482971153583E+01
C	-7.4901130520861570E-01	6.5134187180992775E+00	1.9877389216922751E+01
C	1.1882048365797226E+00	7.5399465916555908E+00	2.0686603897737438E+01
C	1.1965443768584920E+00	8.4231477878805361E+00	1.9502169651202713E+01
C	-6.1621642719658398E-01	7.3584092695393464E+00	1.8655231647436786E+01
H	1.5433373185748833E+00	9.4246863304117099E+00	1.9727220600834240E+01
H	1.8539492494239755E+00	8.0293180757005764E+00	1.8728320379624289E+01
H	2.2272392094074247E+00	7.3532973205188483E+00	2.1045793536087967E+01
H	7.3022825989078444E-01	8.1142749828112510E+00	2.1551409883312786E+01
H	-1.5503198000127976E+00	7.5641778573910710E+00	1.8090693279775042E+01
H	5.3330350993270978E-02	6.8754910261464248E+00	1.7901654976702105E+01
H	-1.2877883415590925E+00	7.0371472804656170E+00	2.0646804113462181E+01
H	-1.2063582226420064E+00	5.5385006556751515E+00	1.9661810317718864E+01
O	1.4463140096294323E+01	1.8952273094313181E+01	4.1364326150166519E+00
O	1.2178124235502661E+01	2.0173783836808962E+01	2.6897125925838830E+00
C	1.2973821351657080E+01	2.0903999375942821E+01	3.5942991279992076E+00
C	1.2212016063359735E+01	1.8808698817476248E+01	2.9797453207141653E+00
C	1.3641792118104423E+01	1.8265417168275558E+01	3.2517258188546201E+00
C	1.4357378740367233E+01	2.0350780155025181E+01	3.7598966048947906E+00
H	1.3429010962128190E+01	1.7232941052913922E+01	3.5492482060963026E+00
H	1.4065861451088429E+01	1.8119372626518718E+01	2.2360253643743988E+00
H	1.1812193023799372E+01	1.8293721580650548E+01	2.0927168826245883E+00

H	1.1525152085362839E+01	1.8523555881058400E+01	3.8439305321758410E+00
H	1.4838935885183371E+01	2.0899736914371694E+01	4.5892048217857511E+00
H	1.4903504736968905E+01	2.0556221697160371E+01	2.8352146859650778E+00
H	1.2390405940054398E+01	2.1027662967513045E+01	4.5134070225527960E+00
H	1.3190516065444845E+01	2.1948554199975032E+01	3.2143339227133443E+00
O	7.6571456406952567E+00	3.8202166610537684E+00	8.0990905058923328E+00
O	8.1535977226170218E+00	2.9501887829568179E+00	5.4300257391257167E+00
C	7.9445164541694053E+00	4.3606623633679815E+00	5.729245924222238E+00
C	7.3112034536323316E+00	2.1715226490325046E+00	6.3718198396129750E+00
C	7.7466723980903760E+00	2.4061047261712747E+00	7.7943117500030725E+00
C	8.3510402925452834E+00	4.6703221667141896E+00	7.1725934386057908E+00
H	7.1817428956713547E+00	1.8361613414119222E+00	8.6107219886334647E+00
H	8.8404206912524792E+00	2.1187076525105919E+00	7.9888964955035044E+00
H	7.5231090267636009E+00	1.1256808312741196E+00	6.1308552109482841E+00
H	6.1972329150058831E+00	2.4349408783820339E+00	6.2573107811328912E+00
H	8.1396195732945209E+00	5.7307623878869638E+00	7.4655438802195837E+00
H	9.4261220805904777E+00	4.4231983588452701E+00	7.3720904487407166E+00
H	6.8668448887615900E+00	4.6536635767721890E+00	5.6403236597915232E+00
H	8.5722994501581198E+00	4.9671080863763484E+00	5.0184014847923226E+00
O	1.7037673399246604E+01	3.9144001464880325E+00	7.0506473163817551E+00
O	1.7494325125989999E+01	2.4118445814197398E+00	4.62926745193909509E+00
C	1.6676680194863934E+01	3.6198275180721198E+00	4.7343753044003103E+00
C	1.7438908150783409E+01	1.7944512921584999E+00	5.9306563347848016E+00
C	1.7817394996666469E+01	2.7216315082111118E+00	7.0921991279999332E+00
C	1.17176491814382871E+01	4.6212689595528627E+00	5.7950976385012760E+00
H	1.7581670097977135E+01	2.2846938951250841E+00	8.0559979717793748E+00
H	1.8882459275444486E+01	2.9766863627178677E+00	7.1440322305872543E+00
H	1.8112673716345796E+01	9.4491347843770335E-01	6.0201286951652380E+00
H	1.6358792958314062E+01	1.4728948770091070E+00	6.0779606277985945E+00
H	1.6630811856126293E+01	5.5965498294776301E+00	5.9026973220889385E+00
H	1.8225768041570554E+01	4.8224201019760482E+00	5.5639083859180918E+00
H	1.5622874145622591E+01	3.2657261016102752E+00	5.0593845507089128E+00
H	1.6622468002496646E+01	3.9012800605085949E+00	3.7040309015770823E+00
O	-1.3642732352744973E+00	9.5533285708729760E+00	1.5826785474893697E+01
O	-2.8028635186876065E+00	1.2003058604220060E+01	1.5367796945973549E+01
C	-1.9927925663256572E+00	1.1825901872805439E+01	1.6592056462080759E+01
C	-3.2638268203846463E+00	1.0752276362018268E+01	1.4951170730181964E+01
C	-2.1089710473742969E+00	9.7355490626512537E+00	1.4650652858787888E+01
C	-8.064219232771287E-01	1.0830988400466939E+01	1.6213406522669572E+01
H	-2.5305311937185260E+00	8.7652906643789734E+00	1.4402636076701457E+01
H	-1.5264088556178441E+00	1.0142846486125496E+01	1.3833178233639719E+01
H	-3.8829533476943321E+00	1.1000697949189602E+01	1.4048411861942196E+01
H	-3.9231993748812544E+00	1.0283731067093825E+01	1.5695609247574234E+01
H	-1.1227953674611339E-01	1.0702552524288603E+01	1.7032323017818072E+01
H	-2.1153897863004956E-01	1.1215665668626487E+01	1.5340833208916642E+01
H	-2.5942157026398065E+00	1.1404636910460381E+01	1.7380081675628201E+01
H	-1.6795881720448962E+00	1.2820244263331350E+01	1.6859851960537391E+01
O	2.4927003827398386E+00	1.4806126407242136E+01	7.8069722447706358E+00
O	6.9562212215379204E-01	1.7000015813401077E+01	7.5883053243970027E+00
C	1.2367350865814890E+00	1.6354654942534264E+01	6.4324750826686570E+00
C	1.5454704519419942E+00	1.6898152265455401E+01	8.7278481935587013E+00
C	1.9804245729767780E+00	1.5439344821201757E+01	8.9484747342505280E+00
C	1.5852450625353030E+00	1.4888328557400552E+01	6.6809645194141059E+00
H	2.8008660426130740E+00	1.5526305932224659E+01	9.6615099865301186E+00
H	1.2030195714120662E+00	1.4805490191439581E+01	9.4545823830410765E+00
H	8.8433404972140361E-01	1.7269964132455971E+01	9.5117885320469693E+00
H	2.3730289461521075E+00	1.7657294683481762E+01	8.6563835588868336E+00
H	2.1431862045156911E+00	1.4505763081239722E+01	5.8241523941643223E+00
H	7.2373099337521918E-01	1.4333731861792248E+01	6.8983218374804034E+00
H	2.1104730324368579E+00	1.6883829124402432E+01	5.9727644588006621E+00
H	4.0054242748855506E-01	1.6328571005652485E+01	5.7206410369194174E+00
O	1.3241549275493593E+01	1.9019775830398505E+01	1.7632181435646913E+01
O	1.0546701579211923E+01	1.9736209278967198E+01	1.7566916678981809E+01
C	1.1197416207295548E+01	1.9430820810528189E+01	1.8843995735708521E+01
C	1.1191479168390897E+01	1.8958492254318475E+01	1.6526513656998219E+01
C	1.2663224427951723E+01	1.9272734329440620E+01	1.6420042461875916E+01
C	1.2692240616909425E+01	1.9837092871742435E+01	1.8648904228664282E+01
H	1.3068326763807347E+01	1.8702197590059424E+01	1.5589063717791481E+01
H	1.2795024921687542E+01	2.0301195445569277E+01	1.6209561870579609E+01
H	1.0644740983391859E+01	1.9157274907204215E+01	1.5553109819741914E+01
H	1.1099631800249783E+01	1.7881053512635589E+01	1.7624136540827324E+01
H	1.3298901029106887E+01	1.9667007667212388E+01	1.9567116578168520E+01
H	1.2765228953664273E+01	2.0874358783272520E+01	1.8470357408655882E+01
H	1.1112308679769090E+01	1.8338103649771128E+01	1.9189813950528148E+01

H	1.0727922661243431E+01	2.0045070813081473E+01	1.9632822515407987E+01
O	1.0002252467785050E+01	1.5889618302137002E+01	3.1382434232394032E+00
O	8.6668397631146394E+00	1.4048328233038220E+01	4.7173247826251581E+00
C	7.9134735937122676E+00	1.4752077789073997E+01	3.6685316751163808E+00
C	9.7852533462051046E+00	1.4921660957865669E+01	5.1659379229061599E+00
C	1.0746543158002607E+01	1.5060280316564748E+01	4.0380251420735718E+00
C	8.8886110882052520E+00	1.5136046614004133E+01	2.5805466305800473E+00
H	1.1694899747340417E+01	1.5574662233790832E+01	4.2704790093489624E+00
H	1.0927219810121889E+01	1.4093487150562590E+01	3.5554057659892044E+00
H	1.0305252801701602E+01	1.4363194925370536E+01	5.9774055149836460E+00
H	9.3189917381245593E+00	1.5866306273559642E+01	5.4888852545930238E+00
H	8.3841000454553694E+00	1.5787416519745856E+01	1.8579398706684720E+00
H	9.2590762038468117E+00	1.4330513445181179E+01	1.9082342154404814E+00
H	7.5278877219449072E+00	1.5652846938390665E+01	4.1865055791558321E+00
H	7.0205531748879864E+00	1.4165064095851253E+01	3.3858585679776616E+00
O	3.0495390866677203E+00	8.5570023187201176E+00	9.8084263270550114E+00
O	2.2554904760332830E+00	7.4024759795960922E+00	1.2234669506138905E+01
C	1.4147111745569301E+00	8.4618851130530128E+00	1.1719129277990016E+01
C	3.6680204787035477E+00	7.4746223015746134E+00	1.1871689822602370E+01
C	3.7500319264057307E+00	7.3880111258638657E+00	1.0308839316882377E+01
C	1.6394658701245732E+00	8.6208405255091307E+00	1.0172533191407457E+01
H	4.7996356249711374E+00	7.4467989284274356E+00	9.9838963634304303E+00
H	3.3641350516977102E+00	6.5091223730844829E+00	9.8040219879993913E+00
H	4.1665623331142267E+00	6.7118914228795150E+00	1.2473256870182800E+01
H	4.0408675146348507E+00	8.4563595320728560E+00	1.2176277823604259E+01
H	1.2442852260414299E+00	9.6129396019733235E+00	9.8440637715788153E+00
H	1.1739630130033776E+00	7.8438299180672546E+00	9.5839256422675287E+00
H	1.6528422524908553E+00	9.4030113961143531E+00	1.2249122271231915E+01
H	3.7984023432716135E-01	8.1151352114489388E+00	1.2022966658241081E+01
O	5.6252493855035706E+00	2.1435909498119345E+00	2.0761089707220361E+01
O	2.9102142224924488E+00	1.3942037175737816E+00	2.1119127819471665E+01
C	3.8545223005341449E+00	3.8939706718118011E-01	2.0789830002868097E+01
C	3.3230050456279288E+00	2.7310317240723765E+00	2.0594035828696633E+01
C	4.6418220906625303E+00	3.1433305994492495E+00	2.117245169113069E+01
C	5.2649252047928536E+00	8.5682284990689717E-01	2.1317188457813351E+01
H	4.8484511151327014E+00	4.1045361219485672E+00	2.0685751629452287E+01
H	4.6500108296901423E+00	3.2431966815565736E+00	2.2238839302509163E+01
H	2.5261760567916771E+00	3.4453966766738144E+00	2.0798577773187461E+01
H	3.4487750075549783E+00	2.6067834346281713E+00	1.9489558461904558E+01
H	6.0324831119853846E+00	1.6205046714252949E-01	2.0895022403823106E+01
H	5.4132147996189985E+00	8.8896039689001705E-01	2.2421317174203942E+01
H	3.8793106509269890E+00	1.9823285522228695E-01	1.9707244753051715E+01
H	3.5552203490779410E+00	-5.0911461440673456E-01	2.1350775637880783E+01
O	1.3972242754457063E+00	2.1230000874423933E+01	6.2713103881562260E+00
O	3.2610381122224115E+00	1.9551522833855337E+01	5.2229019942253458E+00
C	3.4300191600382228E+00	2.0131593985681310E+01	6.5140407833496337E+00
C	2.5209275454963178E+00	2.0414107021169393E+01	4.3502751994889124E+00
C	1.2267700502530408E+00	2.0592935174720193E+01	5.0286395049961898E+00
C	2.1080053020870189E+00	2.0379528523253569E+01	7.1845507547700702E+00
H	5.4153946061309965E-01	2.1236381099178921E+01	4.4624432276276718E+00
H	7.6918620635079216E-01	1.9602459180174961E+01	5.0674520599981241E+00
H	2.5197849100500882E+00	1.9961650176820626E+01	3.3827680041770614E+00
H	3.0694502930533409E+00	2.1393610572780982E+01	4.3776700080343574E+00
H	2.2290385137075370E+00	2.1002339617201908E+01	8.1201471915874581E+00
H	1.5491728223475221E+00	1.9438869564497868E+01	7.2324261643429013E+00
H	3.8540746925531546E+00	2.1163316400863003E+01	6.3840855243581771E+00
H	4.1087259647464025E+00	1.9464782841348388E+01	7.1008107942027081E+00
O	2.2655585347000091E+00	4.4275375619594612E+00	6.5248986515935687E+00
O	2.4267864078933106E+00	6.0089931261123022E+00	4.2814143495367682E+00
C	1.7253735665981285E+00	4.7731961232747890E+00	4.0825505202909715E+00
C	3.5924519233300756E+00	5.8447131648544115E+00	5.0167100839245107E+00
C	3.2091087408843686E+00	5.4985933327353234E+00	6.4508994178857515E+00
C	1.2478901230595363E+00	4.4481733666287031E+00	5.4897419621465122E+00
H	3.9791579234659817E+00	5.2449985746680179E+00	7.1853515299432624E+00
H	2.7654533157032546E+00	6.4206884760155187E+00	6.8325239242382034E+00
H	4.1840221024020625E+00	6.7684942339580418E+00	4.7981095997317871E+00
H	4.2802243484506102E+00	5.1274478940393449E+00	4.4790893560190019E+00
H	6.5803942913646252E-01	3.4973472489435662E+00	5.6110252023195990E+00
H	5.7339885597642126E-01	5.2373881336927779E+00	5.8012720957085229E+00
H	2.2331056838245260E+00	3.9110481315624965E+00	3.6677421104547769E+00
H	7.8007022441643226E-01	5.0234933437859164E+00	3.5545741674277163E+00
O	3.9738659646828660E+00	1.0593711172822614E+01	1.0207957884171877E+00
O	4.8447729690320038E+00	1.2852328153583551E+01	2.4664702786998220E+00
C	4.9152263773392271E+00	1.2744258554645663E+01	9.7993607515581216E-01

C	4.8160397924859426E+00	1.1479778527074794E+01	3.0406104380001424E+00
C	3.6846238607716639E+00	1.0654857466195827E+01	2.3880878094803397E+00
C	3.7620924085542131E+00	1.1931718907968712E+01	4.5214327641315555E-01
H	3.7303538537085874E+00	9.6185404574046558E+00	2.7658462484606114E+00
H	2.6847777352815547E+00	1.1000194079363204E+01	2.6708120664417874E+00
H	4.5095347018950926E+00	1.1712812166644378E+01	4.0690156804893096E+00
H	5.7810786644386045E+00	1.0945272044218163E+01	2.9843747226654780E+00
H	3.7608189164769992E+00	1.1825262782151512E+01	-6.8494776404415714E-01
H	2.7247783347933154E+00	1.2161907889460775E+01	6.5339744506828656E-01
H	5.8176696257015790E+00	1.2229019741294513E+01	6.4727475980306770E-01
H	4.9439367613712770E+00	1.3760183961558562E+01	6.0177769369330381E-01
O	1.8474581685632881E+01	9.0378851875808532E+00	2.3869759855009942E+01
O	1.6448696321452452E+01	6.9022666889021194E+00	2.3742641863632656E+01
C	1.7762452451488212E+01	6.7501182981863472E+00	2.3196902720163866E+01
C	1.6123433286446982E+01	8.3361772197371344E+00	2.3814799383807152E+01
C	1.7185177326793042E+01	9.1523792714810561E+00	2.4533555871196651E+01
C	1.8775084169975571E+01	7.6417138631265047E+00	2.3917296856098002E+01
H	1.6947115717608039E+01	1.0218449755562915E+01	2.4561624659292029E+01
H	1.7257799479869202E+01	8.7579009317430696E+00	2.5531619253227710E+01
H	1.5151906100590942E+01	8.3694837123023493E+00	2.4304487401338104E+01
H	1.6077595718045046E+01	8.7520338074525093E+00	2.2762879656957644E+01
H	1.9745497805310865E+01	7.5971489001963155E+00	2.3454741036670345E+01
H	1.8957777601845638E+01	7.4468963194633240E+00	2.4961966779480033E+01
H	1.7683268817276126E+01	6.9099200707649766E+00	2.2119181880293720E+01
H	1.7997355515755366E+01	5.6345150396811485E+00	2.3327986811749874E+01
O	7.2904174576213006E+00	1.5698755540332414E+01	1.1927200504698760E+01
O	5.0546918621307215E+00	1.6302349617252787E+01	1.3504105429201475E+01
C	5.1413483210263227E+00	1.6833011321426628E+01	1.2128595513216204E+01
C	6.3556047492658880E+00	1.6060098330101514E+01	1.4111100250808896E+01
C	7.2330958167165340E+00	1.5166151546869465E+01	1.3282292276710525E+01
C	6.0221732632608989E+00	1.5860460469816131E+01	1.1365553682060609E+01
H	8.2750929733494978E+00	1.5177052596407256E+01	1.3665408802485512E+01
H	6.9039807535029274E+00	1.4107720010202520E+01	1.3210626297723850E+01
H	6.0915871157903840E+00	1.5569131933834708E+01	1.5018265223595757E+01
H	6.9357640021094786E+00	1.7046491910231040E+01	1.4292822310492038E+01
H	6.1779438427256137E+00	1.6269921472054062E+01	1.0348476640691549E+01
H	5.4975155471539230E+00	1.4945086826585317E+01	1.1116839581298491E+01
H	5.5421149257141247E+00	1.7855907865535929E+01	1.2079323340956108E+01
H	4.0329900777193428E+00	1.6881709538849329E+01	1.1756612693259694E+01
O	2.3122203355425199E+00	1.9010989993886493E+01	1.4176243790234738E+01
O	1.1184274532205287E+00	1.9324060061658852E+01	1.1712931733732781E+01
C	1.7115974646787941E+00	1.8054036882677952E+01	1.2096674475029038E+01
C	1.7630704064419864E+00	2.0453478638438483E+01	1.2416141488064170E+01
C	1.6439425130902676E+00	2.0202993057213792E+01	1.3877046460845216E+01
C	1.7902220613302340E+00	1.7858154776320639E+01	1.3577896251262713E+01
H	2.0815040580394788E+00	2.0999132527894837E+01	1.4560944115425231E+01
H	6.3583436928568315E-01	2.0151306567242258E+01	1.4212421676876991E+01
H	1.2201343696368394E+00	2.1291466284913675E+01	1.1933673365762367E+01
H	2.7953238467165575E+00	2.0593964305156980E+01	1.2144422060269973E+01
H	2.3891978393373114E+00	1.7008095607301165E+01	1.3950885907310246E+01
H	7.6004131155324917E-01	1.7681901086233967E+01	1.4014557109018519E+01
H	2.7496849466374917E+00	1.8037522191700894E+01	1.1706227042309104E+01
H	1.14912527113945794E+00	1.7304936807965515E+01	1.1518414573674793E+01
O	3.2819223150387349E+00	1.4917700644065102E+01	1.5863544756369876E+01
O	3.0729961261157221E+00	1.2399835053633970E+01	1.7271655164553835E+01
C	2.9148652993749038E+00	1.2450606758909322E+01	1.5836339797578280E+01
C	2.4427619829633000E+00	1.3678416340413870E+01	1.7766351434951492E+01
C	3.2058872210047138E+00	1.4880087688877655E+01	1.7283202542827532E+01
C	3.6265368292994471E+00	1.3659499876964727E+01	1.5276731028717659E+01
H	2.5967716951136657E+00	1.5767220984685935E+01	1.7571380642135921E+01
H	4.1829065831979948E+00	1.4783075070489573E+01	1.7786037601527131E+01
H	2.5233424139376246E+00	1.3692562917904011E+01	1.8867579494918179E+01
H	1.3920021139541923E+00	1.3573922496045855E+01	1.7512129623390994E+01
H	3.550885093381233E+00	1.3807913776706950E+01	1.4177686495320099E+01
H	4.7230637305959835E+00	1.3467060024124004E+01	1.5468199793909672E+01
H	1.8004589758285288E+00	1.2409242889857488E+01	1.5581456166122956E+01
H	3.4011566730703171E+00	1.1584929058124517E+01	1.5389395019336678E+01
O	9.0221151678317266E+00	2.0477285002344310E+01	4.0172590713251193E+00
O	7.9140548220466984E+00	1.9471525497994136E+01	1.5443171190490668E+00
C	8.4566087484611288E+00	1.8612385611788838E+01	2.5934676841338433E+00
C	8.5688356951982794E+00	2.0814201878380054E+01	1.6592490821671202E+00
C	8.5322754362559063E+00	2.1400311514923057E+01	3.0056874021691820E+00
C	8.3844780789488844E+00	1.9215291503086885E+01	4.0106885073939260E+00
H	9.1648814376937953E+00	2.2279341901822644E+01	3.0003404473057214E+00

H	7.5607997676482768E+00	2.1775154759851297E+01	3.2579973862991287E+00
H	7.9905513324683737E+00	2.1424973390275824E+01	9.5897001406695503E-01
H	9.6870281608104580E+00	2.0679358825711979E+01	1.4173768378713960E+00
H	8.9993280947362866E+00	1.8643937574622733E+01	4.7181311394876833E+00
H	7.3439516641721445E+00	1.9290633119499827E+01	4.4304472318636190E+00
H	9.5644802370924626E+00	1.8461004477506023E+01	2.4248696945569099E+00
H	7.9435984266948143E+00	1.7649680473489664E+01	2.5532952461215093E+00
O	1.1621229310567077E+01	1.9067899558081947E+01	7.1151282095356505E+00
O	1.3554498500201412E+01	1.7318662140826067E+01	8.2152321380410349E+00
C	1.3953694382496060E+01	1.8600653147797320E+01	7.7241220389643130E+00
C	1.2558199237385155E+01	1.6749222287408784E+01	7.3631481257287152E+00
C	1.1341405249467753E+01	1.7708946707201385E+01	7.3555293824121231E+00
C	1.2786008467659098E+01	1.9608089630915870E+01	7.7415555155155404E+00
H	1.0554855523724688E+01	1.7396780373803985E+01	6.6184818704389148E+00
H	1.0819375394494244E+01	1.7594365324392427E+01	8.2941925227028488E+00
H	1.2148257572631813E+01	1.5864594307557191E+01	7.8048508715820981E+00
H	1.2849612396252590E+01	1.6489031767490129E+01	6.3513249132288507E+00
H	1.2997092672568712E+01	2.0474775312097762E+01	7.1125902373066454E+00
H	1.2553190284361021E+01	1.9869949548614763E+01	8.7462825542835194E+00
H	1.4468941431703655E+01	1.8574271139194227E+01	6.7186274436093560E+00
H	1.4792357607461506E+01	1.8902259151377287E+01	8.4297049963999235E+00
O	5.5710411162637072E+00	1.7512681704042290E+01	8.5695329093961163E+00
O	7.0552045105675107E+00	1.7058766129165786E+01	6.2266682704083056E+00
C	7.3527517258753692E+00	1.8190993700210690E+01	7.0969952932574412E+00
C	5.6528866267427427E+00	1.6588509930157223E+01	6.3352304429918638E+00
C	5.3346763727500388E+00	1.6350669779692083E+01	7.7612398584435347E+00
C	7.0210585563211847E+00	1.7804647856535645E+01	8.5546208358037390E+00
H	4.2295114353038663E+00	1.6147863693725871E+01	7.9635551309772943E+00
H	5.8744552821376583E+00	1.5462415163903728E+01	8.0928978289332907E+00
H	5.6220063136766267E+00	1.5658133716239764E+01	8.4291089008601757E+00
H	4.9759346854007704E+00	1.7405747044134106E+01	5.8972730373322699E+00
H	7.1983264759666881E+00	1.8567324817843836E+01	9.2997836868052293E+00
H	7.5916970711693184E+00	1.6869270739993453E+01	8.6744473093573813E+00
H	6.7371336760608784E+00	1.9039964045196815E+01	6.7684782729852468E+00
H	8.4035382673699637E+00	1.8418405494412589E+01	6.9330213272612173E+00
O	2.0689515079301451E+01	1.2842790521295347E+01	1.3509277789127106E+01
O	1.9723930056620951E+01	1.3601788535517823E+01	1.1020820886498758E+01
C	2.0823477935262904E+01	1.2606212175713573E+01	1.1181880148669400E+01
C	1.9596276083106286E+01	1.4577824607924128E+01	1.2091302025669869E+01
C	1.9558540062342789E+01	1.3795086681609710E+01	1.3424208378372187E+01
C	2.0589968614494634E+01	1.1901741733071006E+01	1.2501161232734740E+01
H	1.9606150849244887E+01	1.4470810418183085E+01	1.4286366579640596E+01
H	1.8613909165231291E+01	1.3207788653299041E+01	1.3668222291560099E+01
H	1.8704411985640512E+01	1.5108970624441531E+01	1.1900698202437781E+01
H	2.0337938790454032E+01	1.5368599515313562E+01	1.2028019651720838E+01
H	2.1405611003884776E+01	1.1188999016636830E+01	1.2679096585398542E+01
H	1.9663583000269316E+01	1.1355706658309245E+01	1.2552731943245899E+01
H	2.1744571364046383E+01	1.3158509491742818E+01	1.1339196890637355E+01
H	2.0829389681038926E+01	1.2001494118123317E+01	1.0286626762187129E+01
O	8.6300187433837952E+00	1.5609160672435841E+01	1.7316339522493429E+01
O	7.1887997265727162E+00	1.5304385123253835E+01	1.9828512375575954E+01
C	7.3705857148667437E+00	1.4191432436682284E+01	1.8859244972338978E+01
C	7.5301736328257203E+00	1.6612853570444020E+01	1.9284302894589668E+01
C	8.7614266043278146E+00	1.6564370643124217E+01	1.8384539541090565E+01
C	8.5927728167820163E+00	1.4339299064441610E+01	1.7986397263136059E+01
H	8.8987782732596106E+00	1.7549715385859663E+01	1.7892230216730695E+01
H	9.6355848766736667E+00	1.6236894678058974E+01	1.8959183233141541E+01
H	7.6538156769162926E+00	1.7229536775987732E+01	2.0176931532954885E+01
H	6.6571152252661747E+00	1.7069266722367537E+01	1.8740750630349243E+01
H	8.5226532117027762E+00	1.3659518036258392E+01	1.7166614021246421E+01
H	9.6030813058645936E+00	1.4167776268258880E+01	1.8553519770595678E+01
H	6.5073942021450639E+00	1.4146615869528954E+01	1.8184840307543897E+01
H	7.4051112741955505E+00	1.3237858287799304E+01	1.9415251617591849E+01
O	1.0702033037051580E+01	5.1307311451717430E+00	1.6291331214964167E+01
O	8.7310620239847410E+00	6.7144156800652315E+00	1.7767433745774831E+01
C	8.6818993575520196E+00	5.2644927834472188E+00	1.7736044641278969E+01
C	9.4595457589248984E+00	7.1664030678010260E+00	1.6557828006065296E+01
C	1.0878150704103295E+01	6.5446857027876204E+00	1.6526636911991289E+01
C	1.0062834845137685E+01	4.6567414171728396E+00	1.7515208334404818E+01
H	1.1413864792970271E+01	6.8120555560733189E+00	1.5624993888432710E+01
H	1.1357196965861931E+01	6.8354154252905701E+00	1.7479120271772565E+01
H	9.5177746518611528E+00	8.2584480757085217E+00	1.6741106287052361E+01
H	8.9637396384991490E+00	6.7996815645002053E+00	1.5679125247608928E+01
H	1.0026070629682774E+01	3.5598499204117262E+00	1.7363737789179314E+01

H	1.0652000756095141E+01	4.7984393818070297E+00	1.8439182893183208E+01
H	8.0320377046251874E+00	4.9755281447639268E+00	1.6889114533645415E+01
H	8.1819781399484697E+00	4.9386159651207349E+00	1.8645182342068733E+01
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4.4142697006390808E-04 -1.4961936709119895E-05 3.1212512910617661E-04
-4.1850084718643242E-04 1.6518650590327666E-04 1.3541990510828412E-04
-1.1768713177980929E-03 -4.2422068379688581E-04 2.0824072036585112E-04
-5.2556371052553917E-04 -1.1275697024887494E-03 8.1854539250827247E-04
1.1748418031397078E-03 -2.7539710517086451E-04 -1.2646931160110740E-04
6.0324508345062930E-04 7.3332907433726617E-04 4.8281519206881820E-04
-1.3825424155022200E-04 -1.4124962628779431E-04 -2.4671193578874032E-04
2.5063826741181803E-04 -3.0154147949635799E-04 -1.3787506695656939E-04
-4.6095314209084718E-04 3.2342637605690554E-04 -3.0017140006818426E-05
1.8973995862919875E-04 1.5208495639189179E-04 1.1693985428335704E-04
-9.0530048210208343E-05 -2.2644427792907108E-04 -2.5379341024451169E-04
-1.2343207533134322E-05 1.4125140284566514E-04 -2.7129688590747398E-04
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-4.3570293732888557E-04 -1.0588519373305224E-03 3.4921586058945397E-04
3.8098218399831553E-04 7.1353970202895460E-05 -1.0571408448559450E-03
-2.0616948341775480E-04 3.1408387550955558E-04 2.5466895063466473E-04
8.9196014195739247E-05 9.1509145424867148E-04 1.2257065240374617E-03
8.4679017179782004E-05 -9.7301018669609081E-06 -3.7910722485171548E-04
3.3218875205901199E-04 -2.8907137732672641E-04 -1.2990122682957796E-04
-3.7906633542773057E-04 5.0398997926394495E-05 -7.7165942688558196E-04
-1.2373668718371271E-04 -2.5924024593001555E-04 -3.8876889243393505E-05
-4.6007959236939563E-05 1.6960156513620649E-04 -1.9461402929304636E-04
4.6950308390214640E-05 -2.0543433467037504E-04 -4.7207776257856496E-04
-1.0226228882602616E-04 -5.7540775384741852E-04 -3.0420873594920168E-04
2.7311143547614011E-05 1.1181760622160563E-04 6.1156380538601303E-05
1.6882083719751224E-04 -1.1086101390037877E-04 -1.4373765922187886E-04
-2.4347918742680815E-04 2.9933178193549689E-04 3.8118990618017857E-04
-2.851011529314304E-04 -6.1403044507627109E-04 4.8379890306853501E-04
1.4584383026296051E-04 6.8587257858268873E-04 2.3312075180531664E-04
9.3360240097179145E-05 -4.1412234649356990E-04 5.3864602039311509E-04
-2.5605194520214775E-05 2.0837933157931201E-04 7.8193619681600165E-04
&END VELOCITY
&KIND C
BASIS_SET DZVP-MOLOPT-SR-GTH
POTENTIAL GTH-PBE-q4
&POTENTIAL
2 2
0.3384712400000000E+00 2 -0.8803673979999999E+01 0.1339210850000000E+01
2
0.3025757500000000E+00 1 0.9622486650000001E+01
0.2915069400000000E+00 0
&END POTENTIAL
&END KIND
&KIND O
BASIS_SET DZVP-MOLOPT-SR-GTH
POTENTIAL GTH-PBE-q6
&POTENTIAL
2 4
0.2445543000000000E+00 2 -0.1666721480000000E+02 0.2487311320000000E+01
2
0.2209592000000000E+00 1 0.1833745811000000E+02
0.2113324700000000E+00 0
&END POTENTIAL
&END KIND
&KIND H
BASIS_SET DZVP-MOLOPT-SR-GTH
POTENTIAL GTH-PBE-q1
&POTENTIAL
1
0.2000000000000000E+00 2 -0.4178900440000000E+01 0.7244633100000000E+00
0
&END POTENTIAL
&END KIND
&KIND Rh
BASIS_SET DZVP-MOLOPT-SR-GTH
POTENTIAL GTH-PBE-q17
&POTENTIAL
3 6 8
0.4200000000000000E+00 2 0.2620679340000000E+02 -0.4937383350000000E+01
3
0.3454462200000000E+00 2 -0.4524823200000000E+00 0.3892804380000000E+01
-0.5025588850000000E+01
0.3783801400000000E+00 2 -0.9411124199999999E+00 -0.5699310000000000E-02
0.6743510000000000E-02

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0.433747250000000E+00 2 0.157423622000000E+01 -0.301217170000000E+01
0.341548166000000E+01
&END POTENTIAL
&END KIND
&KIND B
BASIS_SET DZVP-MOLOPT-SR-GTH
POTENTIAL GTH-PBE-q3
&POTENTIAL

2 1
0.418991450000000E+00 2 -0.585946171000000E+01 0.903756430000001E+00
2
0.371320460000000E+00 1 0.629728018000000E+01
0.364563080000000E+00 0
&END POTENTIAL
&END KIND
&TOPOLOGY
NUMBER_OF_ATOMS 773
MULTIPLE_UNIT_CELL 1 1 1
&END TOPOLOGY
&END SUBSYS
&END FORCE_EVAL

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Simulation S3

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&GLOBAL
PRINT_LEVEL MEDIUM
PROJECT_NAME MD
RUN_TYPE MD
&END GLOBAL
&MOTION
&MD
ENSEMBLE NVT
STEPS 20750
TIMESTEP 9.999999999999978E-01
STEP_START_VAL 5000
TIME_START_VAL 4.9999999999995689E+03
ECONS_START_VAL -3.3822048546363776E+03
TEMPERATURE 3.000000000000000E+02
&THERMOSTAT
TYPE NOSE
REGION GLOBAL
&NOSE
LENGTH 4
YOSHIDA 3
MTS 2
&COORD
-1.1835258888451117E-01 5.2719086090882419E+00 2.1946574346032071E+00
7.4540454851586366E+00
&END COORD
&VELOCITY
-9.3447278993970193E-08 -9.1648307781750363E-06 -1.3892360895187544E-05
2.1249831312603600E-05
&END VELOCITY
&MASS
3.6826194659470329E+09 1.6237299232570694E+06 1.6237299232570694E+06
1.6237299232570694E+06
&END MASS
&FORCE
-4.3489553692858236E-12 -5.6529506901932782E-10 -5.0110601530846617E-10 -
3.9210244725891461E-10
&END FORCE
&END NOSE
&CSVR
TIMECON 9.999999999999986E+01
&END CSVR
&END THERMOSTAT
&AVERAGES T
&RESTART_AVERAGES
ITIMES_START 1
AVECPU 1.4770361784357650E+02
AVEHUGONIOT 0.000000000000000E+00
AVETEMP_BARO 0.000000000000000E+00
AVEPOT -3.3830779397144302E+03
AVEKIN 1.0362883327953922E+00

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AVETEMP      2.8793365207549323E+02
AVEKIN_QM    0.0000000000000000E+00
AVETEMP_QM   0.0000000000000000E+00
AVEVOL       5.4800532563775429E+04
AVECELL_A    3.7983495271001452E+01
AVECELL_B    3.7983495271001452E+01
AVECELL_C    3.7983495271001452E+01
AVEALPHA     9.0000000000000000E+01
AVEBETA      9.0000000000000000E+01
AVEGAMMA     9.0000000000000000E+01
AVE_ECONS    5.0757463617513414E+00
AVE_PRESS    0.0000000000000000E+00
AVE_PXX      0.0000000000000000E+00
&END RESTART_AVERAGES
&END AVERAGES
&END MD
&PRINT
&TRAJECTORY SILENT
  ADD_LAST NUMERIC
  LOG_PRINT_KEY T
  FORMAT DCD_ALIGNED_CELL
  &EACH
    MD 1
  &END EACH
&END TRAJECTORY
&VELOCITIES OFF
  ADD_LAST NUMERIC
  LOG_PRINT_KEY T
  FORMAT XMOL
  &EACH
    MD 1
  &END EACH
&END VELOCITIES
&RESTART SILENT
  ADD_LAST NUMERIC
  LOG_PRINT_KEY T
  BACKUP_COPIES 0
  &EACH
    MD 10
  &END EACH
&END RESTART
&END PRINT
&END MOTION
&FORCE_EVAL
METHOD QS
&DFT
  BASIS_SET_FILE_NAME insert basis set path here
  POTENTIAL_FILE_NAME insert basis set path here
  MULTIPLICITY 1
  CHARGE 0
&SCF
  MAX_SCF 60
  EPS_SCF 9.999999999999995E-07
  SCF_GUESS ATOMIC
  &OT T
    MINIMIZER DIIS
    PRECONDITIONER FULL_SINGLE_INVERSE
  &END OT
  &OUTER_SCF T
    EPS_SCF 9.999999999999995E-07
    MAX_SCF 5
  &END OUTER_SCF
  &PRINT
    &RESTART SILENT
      ADD_LAST NUMERIC
      COMMON_ITERATION_LEVELS 1
      FILENAME =./WFn_restart.wfn
      LOG_PRINT_KEY T
    &EACH
      QS_SCF 0
    &END EACH
  &END RESTART
&END PRINT
&END SCF

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&QS
  EPS_DEFAULT      9.999999999999998E-13
&END QS
&MGRID
  NGRIDS  5
  CUTOFF   3.000000000000000E+02
  REL_CUTOFF 5.000000000000000E+01
&END MGRID
&XC
  DENSITY_CUTOFF  1.000000000000000E-10
  GRADIENT_CUTOFF 1.000000000000000E-10
  TAU_CUTOFF      1.000000000000000E-10
  &XC_FUNCTIONAL  NO_SHORTCUT
  &PBE T
  &END PBE
  &END XC_FUNCTIONAL
  &VDW_POTENTIAL
  POTENTIAL_TYPE PAIR_POTENTIAL
  &PAIR_POTENTIAL
  TYPE DFTD3(BJ)
  PARAMETER_FILE_NAME dftd3.dat
  REFERENCE_FUNCTIONAL PBE
  &END PAIR_POTENTIAL
  &END VDW_POTENTIAL
&END XC
&POISSON
&END POISSON
&LOCALIZE T
&END LOCALIZE
&END DFT
&SUBSYS
&CELL
  A  2.0100000000000001E+01  0.000000000000000E+00  0.000000000000000E+00
  B  0.000000000000000E+00  2.0100000000000001E+01  0.000000000000000E+00
  C  0.000000000000000E+00  0.000000000000000E+00  2.0100000000000001E+01
  PERIODIC XYZ
  MULTIPLE_UNIT_CELL 1 1 1
&END CELL
&COORD
Rh  9.6875292299262057E+00  1.1382353828217857E+01  1.0807645997671756E+01
C   8.0413407318752270E+00  1.3072059089492026E+01  1.0742148243697809E+01
C   1.0152238058732566E+01  1.3897393155771336E+01  1.1697426986704549E+01
C   1.3016932114900410E+01  1.3534198704840048E+01  1.1688347794371104E+01
C   6.7519834093509177E+00  1.2305173713662521E+01  1.0583280596579513E+01
C   5.9325093776819440E+00  1.2063446785269361E+01  1.1762909097165503E+01
C   8.8465075973189702E+00  1.3109966486964108E+01  1.1869660180306596E+01
C   8.6774263302004595E+00  1.3789414524522876E+01  9.5110136202216076E+00
C   5.2629675636974884E+00  1.0886065475089042E+01  2.807529323835389E+00
C   1.5145604028662598E+01  1.3211888634599269E+01  1.0599850564533984E+01
C   9.8346357578429267E+00  1.5368428078124625E+01  1.1294186400405980E+01
C   1.0023848045969817E+01  1.3047291585808216E+01  9.3987387457328371E+00
C   4.7634157706093072E+00  1.1305481196479336E+01  1.1634505372989869E+01
C   1.0845506240516173E+01  1.3171446343814591E+01  1.0568513703376640E+01
C   1.3061998784411148E+01  1.2696167686498940E+01  9.4366477583259893E+00
C   6.3650646063458423E+00  1.1760056180136372E+01  9.3384845700594159E+00
C   9.0163323703293639E+00  1.5320682940458646E+01  9.9752983034018285E+00
C   4.4525973769161196E+00  1.0616891904524508E+01  1.0456206098300946E+01
C   1.2354087434478974E+01  1.3097395679038607E+01  1.0566093021917220E+01
C   1.4435912011561363E+01  1.2665867637119026E+01  9.4648571280431604E+00
C   1.4370126202952537E+01  1.3631077964860584E+01  1.1724244188858435E+01
C   1.2473694856002149E+01  1.3871740653178382E+01  1.2585645928431575E+01
H   1.6232817544267316E+01  1.3240971356089402E+01  1.0570551442754677E+01
H   1.2572321378402856E+01  1.2465693434872048E+01  8.4974550771868795E+00
H   1.4967194432291084E+01  1.2372676050330757E+01  8.5266854404497501E+00
H   1.4723729777505703E+01  1.3972275009763651E+01  1.2710252715803831E+01
H   6.1264713115339910E+00  1.2428096897494834E+01  1.2741496823140348E+01
H   4.9653604998495586E+00  1.0423362529062577E+01  8.3246542936376979E+00
H   4.2008844487173240E+00  1.1184429952691392E+01  1.2557998282850718E+01
H   6.8407617261769431E+00  1.2051045029671000E+01  8.3860195866202751E+00
H   3.7103897352030217E+00  9.8868849218456134E+00  1.0393052061677832E+01
H   1.0819697832713118E+01  1.3867575162831951E+01  1.2494954546659732E+01
H   8.0961480151057259E+00  1.3689399198776831E+01  8.6083859260772542E+00
H   9.3422904224195840E+00  1.5793179859805083E+01  1.2189855165923897E+01
H   1.0829687780323715E+01  1.5804900144223220E+01  1.1103135038547377E+01

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H	9.6766116988410680E+00	1.5824745994306181E+01	9.2443613289183286E+00
H	8.1395639134226201E+00	1.5987376816290032E+01	1.0055789515981770E+01
H	1.0285567613714052E+01	1.2536202900492373E+01	8.4077039985949504E+00
H	8.4409945376313296E+00	1.2825643061911492E+01	1.2805230727313699E+01
C	1.0587753631100085E+01	1.0051229718156744E+01	9.4374682836700732E+00
C	1.1906974357485334E+01	9.5673835267028924E+00	9.4383239964294141E+00
C	9.8272697347367401E+00	9.7681272592366479E+00	8.3017036375256001E+00
C	1.2539204433457018E+01	9.0414717639721456E+00	8.2957538192580209E+00
H	1.2485198859928664E+01	9.6694590984931263E+00	1.0368196999748100E+01
C	1.0395665166744049E+01	9.2391295088990351E+00	7.0765603113349052E+00
H	8.7320665296953219E+00	1.0029193982214670E+01	8.1961163123530945E+00
C	1.1757699832309134E+01	8.9177854832153791E+00	7.1446946390908161E+00
H	1.3521653890696664E+01	8.6396602341736664E+00	8.3369287707519444E+00
H	9.7249072592013555E+00	8.9640677278952055E+00	6.2437645137789044E+00
H	1.2312671727471855E+01	8.4881857929554005E+00	6.2848674435492118E+00
C	9.5178968958342054E+00	9.3062413048520121E+00	1.1618066541888986E+01
C	8.6345180464317401E+00	1.0088205823300319E+01	1.2378097278763251E+01
H	9.0361649905425754E+00	8.7634898620910509E+00	1.0807192852424649E+01
H	7.6253996477458550E+00	1.0279082438018500E+01	1.2001594335176646E+01
C	8.9748489411947343E+00	1.0472109089069091E+01	1.3737956856743601E+01
O	8.1851436012269456E+00	1.1204552689486672E+01	1.4405377229818278E+01
C	1.0267573830509374E+01	9.9247825169520976E+00	1.4334676164957518E+01
H	1.0708605239104314E+01	1.0756635127385957E+01	1.4945189282912748E+01
C	1.0669506536778112E+01	8.5900233759111675E+00	1.2368895915865261E+01
C	1.1346620688475394E+01	9.5252247681619302E+00	1.3326173234301276E+01
H	1.0018749507844973E+01	9.0805206022799183E+00	1.4967104819461056E+01
H	1.1667895517960154E+01	1.0486774042049836E+01	1.2856644884127515E+01
H	1.2236217749597898E+01	9.1241262594595476E+00	1.3848661231388828E+01
H	1.0243161393347194E+01	7.7247630736246906E+00	1.2809343839254591E+01
H	1.1406392847961978E+01	8.2131374603819474E+00	1.1615473373403230E+01
H	1.9075483641773676E+01	7.5153758090887353E+00	1.3552886667824760E+01
O	9.6526070427420372E+00	1.4049155585543682E+01	1.6247565105051539E+01
H	9.8027437176391796E+00	1.3237298450613293E+01	1.6741332037243929E+01
H	8.6915941673026023E+00	1.4005268990805106E+01	1.6059288125946075E+01
O	1.9631837657987717E+01	7.6918791016701604E+00	1.4297001920217475E+01
H	1.9513816177026342E+01	8.6300989861763622E+00	1.4527390328261871E+01
O	6.1279817166139310E+00	1.0597064963682712E+01	1.9786735422542780E+01
B	5.6386399271949790E+00	1.0074899922929308E+01	1.6567612825302124E+01
O	2.9388382880043151E+00	9.2865893260688956E+00	1.4915138066770576E+01
O	5.5746775356511353E+00	1.0146229649194241E+01	1.5172483500209417E+01
H	5.3053304392697420E+00	1.0854093509637988E+01	2.0183230997471853E+01
H	6.3868305968184247E+00	9.7635068303327817E+00	2.0280462526464820E+01
O	2.3704008423118097E+00	6.6964446573572491E+00	1.3886966021570775E+01
O	6.6787456722781400E+00	1.0566345772542258E+01	1.7258964388244557E+01
O	4.5354827568305627E+00	9.4052535867456761E+00	1.7177469368630430E+01
H	1.4423772674655186E+00	6.8124221776090632E+00	1.4134584205525590E+01
H	6.4191385213839549E+00	1.0661740290668096E+01	1.8309707514447449E+01
H	3.8730711357719438E+00	9.2689146995397955E+00	1.6412435987325058E+01
H	2.6965158450210254E+00	6.2324179166453986E+00	1.4714608284931941E+01
H	2.7379556251235768E+00	8.5544396735935742E+00	1.4301594809926968E+01
H	6.3866189596456424E+00	1.0571845469671864E+01	1.4811374828374023E+01
C	3.8704487166069712E+00	9.4304661504762546E+00	1.4611973559225770E+01
H	6.8601805912845597E+00	6.2401250071358643E+00	1.6593254803700077E+01
H	6.6682854961601059E+00	7.8864402302958592E+00	1.4016224568400688E+01
H	7.3896664136338330E+00	8.3061319501223032E+00	1.5555326003979937E+01
O	1.7302788947881783E+01	9.2903444145055669E+00	4.3775531950618500E+00
O	1.7634956653833683E+01	6.7257688417119024E+00	5.6465932202067677E+00
C	1.6897554101790067E+01	7.8102139586510493E+00	6.2604479702063074E+00
C	1.8648989600833328E+01	7.2385219657402482E+00	4.7384297538328104E+00
C	1.8179836453814374E+01	8.3471923279783127E+00	3.8133719962054342E+00
C	1.6307788625877009E+01	8.8368588630583513E+00	5.3197290179147272E+00
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H	1.7699875936559366E+01	8.0124403510287312E+00	2.8974867665571722E+00
H	1.9002522034336366E+01	6.4438759473435043E+00	4.1040258176976465E+00
H	1.9490826716004751E+01	7.7166509638711247E+00	5.3120754759933462E+00
H	1.6067881672220906E+01	9.8295637791548689E+00	5.8243872309697187E+00
H	1.5430727959082221E+01	8.4860537107468001E+00	4.8050070486742609E+00
H	1.7586776626693055E+01	8.1183691767671338E+00	7.0612140206684053E+00
H	1.6169269900592319E+01	7.2781057811494980E+00	6.8743606270754913E+00
O	3.3888756574246020E+00	2.0983384895691739E+01	1.9572843216985291E+01
O	3.9416411437577414E+00	1.8742482689348904E+01	1.7938524780976728E+01
C	2.6483984863288219E+00	1.9361605590228358E+01	1.7999031067165696E+01
C	4.5626615007039941E+00	1.8927842715127866E+01	1.9197115153910151E+01
C	4.6721117325578243E+00	2.0409573824604337E+01	1.9575578759163744E+01

C	2.7665457096087014E+00	2.0815566836428133E+01	1.8319370502583375E+01
H	4.9871645375195914E+00	2.0433971573913578E+01	2.0607249947789249E+01
H	5.4139700476361154E+00	2.0947883779798644E+01	1.8905178877460983E+01
H	5.5870634417337994E+00	1.8427861321931886E+01	1.9194529530308639E+01
H	3.9265725999203576E+00	1.8438510942600949E+01	1.9957463827676598E+01
H	1.7653462219509313E+00	2.1282013203411562E+01	1.8422106201869731E+01
H	3.2208260550480223E+00	2.1370833114856378E+01	1.7503666412031329E+01
H	2.0387421495284981E+00	1.8879023113012586E+01	1.8792549230132067E+01
H	2.0961352671617393E+00	1.9118889732422080E+01	1.7090065345772206E+01
O	4.5436416293303186E+00	2.0173548479546433E+01	8.3816905716427925E+00
O	5.4380592470361755E+00	2.2934092129074468E+01	8.7595122646859025E+00
C	4.9731485448691570E+00	2.2068906248978646E+01	9.8898010781131322E+00
C	4.9262047595894298E+00	2.2414792332617900E+01	7.4492458340629106E+00
C	5.1939832462170763E+00	2.0902958922145370E+01	7.3449849246076759E+00
C	5.1783311537958054E+00	2.0626317946214865E+01	9.5824022444076409E+00
H	4.7268248088896163E+00	2.0466097280240060E+01	6.4294882643017806E+00
H	6.2713071944563890E+00	2.0689031971401132E+01	7.3582186347940812E+00
H	5.3786957569052456E+00	2.3070378355166582E+01	6.6850211592080386E+00
H	3.8397340103143343E+00	2.2541087905397944E+01	7.3160554465900391E+00
H	4.9473854205480317E+00	1.9899602395068417E+01	1.0415347851820151E+01
H	6.2919708710254998E+00	2.0507902251235997E+01	9.4718404799678364E+00
H	3.8943006847337265E+00	2.2414810462587553E+01	1.0142491082210325E+01
H	5.5427028038383455E+00	2.2250365896843412E+01	1.0776176582448738E+01
O	1.1844611906552252E+01	1.7673087334191585E+01	8.5356781244557745E+00
O	1.4398010224408571E+01	1.8289836804204047E+01	9.5337567766576647E+00
C	1.3615208975832982E+01	1.9300697873404257E+01	8.8839449077631532E+00
C	1.4097576019334189E+01	1.6938402929813115E+01	9.1100151384111943E+00
C	1.2588265303812035E+01	1.6666218948827552E+01	9.1785436827887992E+00
C	1.2117332742273177E+01	1.8991037691261234E+01	9.0909609853349949E+00
H	1.2406719646556708E+01	1.5732912456396283E+01	8.6294429308345766E+00
H	1.2242958311291639E+01	1.6470592049938720E+01	1.0172757757372862E+01
H	1.4723222314350119E+01	1.6236913868398595E+01	9.6843709070484536E+00
H	1.4486549124167270E+01	1.6789126627814930E+01	8.1130732219108062E+00
H	1.1405721983861772E+01	1.9654050058209815E+01	8.6420509073675795E+00
H	1.1989528020895346E+01	1.9013733696933869E+01	1.0192985448399247E+01
H	1.3790263470988837E+01	1.9296141611832379E+01	7.8316850352978795E+00
H	1.3980254857937942E+01	2.0260581293728933E+01	9.2960919080883766E+00
O	2.4777375660606880E+00	1.7871583656873160E+01	5.3372421718524050E+00
O	3.9514070892503561E+00	1.9201340124726553E+01	3.2823384106390403E+00
C	2.7806684616995869E+00	1.9800122278287354E+01	3.8053831383656944E+00
C	3.8058580088787259E+00	1.7760294065219664E+01	3.2260137398685460E+00
C	3.5904990472948755E+00	1.7261089467963398E+01	4.6829608718330675E+00
C	2.4713965308424983E+00	1.9264858915877472E+01	5.2323928374805799E+00
H	3.3723489130535800E+00	1.6154371283260183E+01	4.7890766406786742E+00
H	4.5028819625687584E+00	1.7472912288643546E+01	5.2418812135598998E+00
H	4.7113488071740059E+00	1.7348730192832701E+01	2.7354957965808437E+00
H	2.9709224762582265E+00	1.7547601182905996E+01	2.5932859428981847E+00
H	1.4944909795258763E+00	1.9650840405026418E+01	5.5574490961515659E+00
H	3.2012255798615832E+00	1.9628915208424608E+01	5.9167484037287812E+00
H	1.8924135357378715E+00	1.9580190987890770E+01	3.2121798114144307E+00
H	3.0220735060746602E+00	2.0840816285383170E+01	3.8463187053428536E+00
O	1.6048907844046582E+01	2.0761999247955418E+00	2.0240191900039246E+01
O	1.3691060733543829E+01	1.7873633921726642E+00	1.8885434198685331E+01
C	1.3691341538640382E+01	1.7391869011436476E+00	2.0319280242685625E+01
C	1.4924026449173958E+01	1.4397395832241358E+00	1.8318121466452922E+01
C	1.5914478912573642E+01	2.3664387054729406E+00	1.8833948696208559E+01
C	1.4817903572712439E+01	2.6528060381388143E+00	2.0835635119257791E+01
H	1.6893133858240539E+01	2.2926384692880686E+00	1.8392991574118756E+01
H	1.5629734341390304E+01	3.4163262898861690E+00	1.8721222064265447E+01
H	1.4767566537471733E+01	1.4979779251385663E+00	1.7187316112372752E+01
H	1.5282628502876614E+01	3.9370203584323210E-01	1.8565371124185273E+01
H	1.4895601108215114E+01	2.5325356222370039E+00	1.1922884667303389E+01
H	1.4683158447597943E+01	3.7084763951631756E+00	2.0569585931393700E+01
H	1.3861068625664766E+01	6.8902338767395699E-01	2.0578554570030906E+01
H	1.2639103948003969E+01	1.9846794382860136E+00	2.0646333396990290E+01
O	1.4965645595517609E+01	2.7645750247208363E+00	2.165625853879085E+00
O	1.5323696817444100E+01	5.5814901615143082E+00	8.5440033405684357E+00
C	1.3959732285096925E+01	4.9565874383609918E+00	8.5576202536816215E+00
C	1.6297028701071717E+01	4.6074755101267186E+00	8.2626244143748568E+00
C	1.6304095563386522E+01	3.2824745661593093E+00	9.1285463911292943E+00
C	1.3928718713798238E+01	3.7380784800348477E+00	9.5704999345266302E+00
H	1.6927227192131760E+01	2.5554668718568676E+00	8.6160607743987434E+00
H	1.6583040743334873E+01	3.5106509913374819E+00	1.0112559409529696E+01
H	1.7145630853355037E+01	5.2204470555023059E+00	8.3939877248422867E+00

H 1.6202649270166280E+01 4.3057999625826167E+00 7.2434963458242256E+00
H 1.2977393229551080E+01 3.1737797039411491E+00 9.5662440575987979E+00
H 1.4073953532553709E+01 4.1064337068585521E+00 1.0605457595776809E+01
H 1.3718436950016065E+01 4.5921521899932971E+00 7.5563406525897250E+00
H 1.3331981955435314E+01 5.6966193161011951E+00 8.9661488818391319E+00
O 3.7425962149355412E+00 1.7314442259374331E+01 1.0875273886404720E+01
O 3.8256565970883409E+00 1.6003328509953473E+01 8.3012163549298617E+00
C 2.7535311954160298E+00 1.6968667198245111E+01 8.655216472723160E+00
C 5.0133276533611921E+00 1.6314938477608880E+01 9.1273454540108432E+00
C 4.6256847147004416E+00 1.6289776071538384E+01 1.0559215171630415E+01
C 2.5504405658674183E+00 1.7141952180843848E+01 1.0166903939748437E+01
H 4.2339705117840207E+00 1.5236943232623307E+01 1.0803307475835760E+01
H 5.4867495743092380E+00 1.6492311869174610E+01 1.1270535270158380E+01
H 5.4781306143588049E+00 1.7292851864497905E+01 8.7621444004857434E+00
H 5.7292421174688721E+00 1.5504433252587308E+01 8.8155290085798672E+00
H 1.9250006600452021E+00 1.6429152918266883E+01 1.0661353397961737E+01
H 1.9803364270002928E+00 1.8112397837831796E+01 1.0260443101708466E+01
H 1.8401504616023561E+00 1.6564709475805717E+01 8.2144786980351441E+00
H 3.0079608194048766E+00 1.7960737314709561E+01 8.3410132463720501E+00
O 4.3346700942285077E+00 7.5727760669112172E+00 9.2577797982395360E+00
O 6.4037444971638608E+00 6.7128772971902615E+00 1.1000863848559991E+01
C 5.1786869422667010E+00 7.2147902588861497E+00 1.1524123538253692E+01
C 6.7504814195014289E+00 7.4298997125560042E+00 9.7444109944419175E+00
C 5.6408530610340559E+00 7.2272063866115177E+00 8.7406895792999162E+00
C 4.0847788783306600E+00 6.8974412931931246E+00 1.0547866334529392E+01
H 5.8239715263571812E+00 7.8326095014077124E+00 7.8065029000412478E+00
H 5.7392493872486332E+00 6.1817194021602120E+00 8.4489026045518294E+00
H 7.5802926104334460E+00 6.9068139097785064E+00 9.3298042541297868E+00
H 6.9749195405126558E+00 8.5153962288025351E+00 9.9806926093402488E+00
H 3.0724573215157198E+00 7.1614852621722722E+00 1.0834452636008843E+01
H 4.1668537350354162E+00 5.7632763989125877E+00 1.0401052729482785E+01
H 5.3025045061559180E+00 8.2398391464371681E+00 1.1832716608657773E+01
H 5.1431581311534984E+00 6.7309093279841683E+00 1.2491900634635074E+01
O 1.2159940138172534E+01 1.0397407618308439E+01 1.9727991330818035E+01
O 1.1064841224549090E+01 1.2375952275305766E+01 1.7872867724867834E+01
C 1.1022563853552807E+01 1.0886098471192822E+01 1.7602213205685459E+01
C 1.2164017981962289E+01 1.2739850284537404E+01 1.8791640326519801E+01
C 1.2197204256988803E+01 1.1807070856412473E+01 2.0069281606965312E+01
C 1.1109756649824481E+01 1.0089850217608822E+01 1.8873963574349549E+01
H 1.3113139022065353E+01 1.1936683053089945E+01 2.0638396369582953E+01
H 1.1470632005170946E+01 1.2013366045255971E+01 2.0822478900457131E+01
H 1.1904059896840971E+01 1.3827394275366409E+01 1.8899137910065985E+01
H 1.3096383174911344E+01 1.2599950086803368E+01 1.8310314012680152E+01
H 1.1355514062543779E+01 9.0349250859137822E+00 1.8641944255536067E+01
H 1.0153416113830087E+01 1.0193556394208755E+01 1.9430330346397824E+01
H 1.1839267185519645E+01 1.0628660738593567E+01 1.6870811880838612E+01
H 1.0041645547042819E+01 1.0664997728717561E+01 1.7191550642466183E+01
O 1.9086015964603451E+01 1.3979708349774778E+01 1.4474217012728456E+01
O 1.8580440142069051E+01 1.1203157910090503E+01 1.4089704502849406E+01
C 1.7518798427698748E+01 1.2133698659513364E+01 1.4199247071719418E+01
C 1.9817588362560037E+01 1.1628288040290792E+01 1.4679767484039411E+01
C 2.0186946949412054E+01 1.3036679711412201E+01 1.4262195759267819E+01
C 1.7907680455116605E+01 1.3523683462185327E+01 1.3794683169749264E+01
H 2.0968196081306566E+01 1.3488499736181932E+01 1.4811993708381808E+01
H 2.0480629879257741E+01 1.2979090078433750E+01 1.3198844169540317E+01
H 2.0576034553856509E+01 1.0923348929544714E+01 1.4368503240233977E+01
H 1.9830927707776599E+01 1.1679914873768389E+01 1.5775376049776215E+01
H 1.7115860986399461E+01 1.4281753713591515E+01 1.3906937583689576E+01
H 1.8085020276572898E+01 1.3470528153785612E+01 1.2721454780740547E+01
H 1.7051436918265342E+01 1.2098373200937992E+01 1.5195849478254800E+01
H 1.6794660483436317E+01 1.1665092110832655E+01 1.3482215052473432E+01
O 2.6616766824799765E+00 1.3347275732937097E+01 5.5668879763551207E+00
O 5.0019288387120060E+00 1.2219060280615073E+01 4.6238854062978190E+00
C 5.0536350109244585E+00 1.3061543063955003E+01 5.7956146454035053E+00
C 4.1522534766927084E+00 1.2783257331550839E+01 3.6813304415360704E+00
C 2.6895438861925354E+00 1.2939507556719235E+01 4.1764236178534402E+00
C 3.6849727863890669E+00 1.2940224199691363E+01 6.4882835159846648E+00
H 2.1245669051409104E+00 1.3795931480011850E+01 3.7052143920482270E+00
H 2.0955854071205957E+00 1.1988206599254761E+01 3.9216221023469169E+00
H 4.1797279544400521E+00 1.2124016841081266E+01 2.7771157181363435E+00
H 4.5891907087027910E+00 1.3848685609827955E+01 3.4467444285116327E+00
H 3.6215821135034494E+00 1.3688562112374099E+01 7.2963112586204577E+00
H 3.4502603618270773E+00 1.1893148198598606E+01 6.7885398044169856E+00
H 5.2471660569084300E+00 1.4150907891639555E+01 5.5953731432474916E+00

H	5.8956769964744220E+00	1.2739493086966087E+01	6.4543440556796838E+00
O	1.8257335490917491E+01	1.6089469845598721E+01	1.2051253173999955E+01
O	1.9056916920680770E+01	1.5510886000575352E+01	9.3462181461223235E+00
C	1.7668284737576172E+01	1.5808444796804071E+01	9.7343789209906078E+00
C	1.9770051701398877E+01	1.4869600182443870E+01	1.0411684667875848E+01
C	1.9632508189797065E+01	1.5695333966325826E+01	1.1761733053384564E+01
C	1.7677034056826553E+01	1.6728784775410521E+01	1.0910994367674764E+01
H	1.9903011923323302E+01	1.5169450195788677E+01	1.2695949816859054E+01
H	2.0327949730470024E+01	1.6556088185889784E+01	1.1651432712981009E+01
H	2.0794614616620702E+01	1.4717230038560274E+01	1.0114379150611093E+01
H	1.9428294563948945E+01	1.3844911232692603E+01	1.0533430613494568E+01
H	1.6687534728438493E+01	1.6973876101566130E+01	1.1170124227859262E+01
H	1.8261978033274737E+01	1.7637653460808249E+01	1.0698429034750601E+01
H	1.7090066293237626E+01	1.4944476996086282E+01	1.0010943322501840E+01
H	1.7205466861299850E+01	1.6342924656233045E+01	8.8978366634881212E+00
O	3.8837066243801739E+00	1.4809234208548176E+01	1.6642912507928891E+01
O	6.6214592834780694E+00	1.4772794105195249E+01	1.5687824108114475E+01
C	6.0166529317065720E+00	1.6057709391739607E+01	1.6116413128902199E+01
C	5.5548890324404052E+00	1.3976246338848714E+01	1.5068618501835431E+01
C	4.4247435846888941E+00	1.3653041048659286E+01	1.6045049953570281E+01
C	4.9637345801005841E+00	1.5710310550936514E+01	1.7138722624226173E+01
H	3.5386509831835653E+00	1.3016977106178631E+01	1.5669744030328497E+01
H	4.9240394710985242E+00	1.3049994702253956E+01	1.6849316799252708E+01
H	6.0234835171372225E+00	1.3069496051660112E+01	1.4677699050860650E+01
H	5.2050624225121291E+00	1.4513349569599900E+01	1.4176958229700473E+01
H	4.5384923580232703E+00	1.6670043114348431E+01	1.7368068936031754E+01
H	5.5172930969258491E+00	1.5179156389361449E+01	1.7919216157950522E+01
H	5.6167720718355696E+00	1.6661372843127047E+01	1.5281672492316146E+01
H	6.8081837980514424E+00	1.6760719736156489E+01	1.6479258964382520E+01
O	1.0727884379558532E+01	4.7987180172905894E+00	9.3014063393503346E+00
O	8.6179242690340558E+00	5.0641484946633204E+00	7.3839209872918623E+00
C	8.6789465470786773E+00	3.9547575097214369E+00	8.2471071307691339E+00
C	9.8772787093205299E+00	5.7171558365939825E+00	7.2377237744491874E+00
C	1.0500474908708833E+01	5.9893273463055854E+00	8.5597473635907413E+00
C	9.4456532732818186E+00	4.2832414902054632E+00	9.5490160374880979E+00
H	1.1417550358583686E+01	6.6121845066299834E+00	8.4052306720182184E+00
H	9.7942432033827238E+00	6.6821849608671409E+00	9.1141825807869186E+00
H	9.6047487436634587E+00	6.6960444189656192E+00	6.7798091389906618E+00
H	1.0556912172053597E+01	5.1203849569943847E+00	6.6329477622840276E+00
H	9.5550318485665180E+00	3.3359587825772676E+00	1.0045445326917216E+01
H	8.8699153103868280E+00	4.9180002943126651E+00	1.0236428368940160E+01
H	9.1983436179991145E+00	3.0794100679332943E+00	7.7868429441575824E+00
H	7.6294312507727016E+00	3.7835210614333246E+00	8.4590089898001484E+00
O	3.3840995395490512E+00	1.0626709586824875E+01	2.1121993713205708E+01
O	8.7794570137017247E-01	1.0109887804442092E+01	2.0209863705412360E+01
C	1.1489590127564584E+00	1.1364587912501680E+01	2.0799394304223469E+01
C	1.6599813722490280E+00	9.0674277235163014E+00	2.0766996962086232E+01
C	3.1494412521232787E+00	9.3254687033838639E+00	2.0577260360628230E+01
C	2.5472298307455490E+00	1.1676328415349651E+01	2.0556589465087612E+01
H	3.7470519853132522E+00	8.7176053521816623E+00	2.1240897610503332E+01
H	3.4140356708704198E+00	9.2988141811258753E+00	1.9452935131019238E+01
H	1.3048498645009317E+00	8.0753415864411338E+00	2.0383166397666056E+01
H	1.443596226071727E+00	9.0620019917843155E+00	2.1825423016845043E+01
H	2.9562870110914283E+00	1.2591806778552524E+01	2.0950370719605708E+01
H	2.7699097300382212E+00	1.1661830320381055E+01	1.9511212277056561E+01
H	8.3726041081805003E-01	1.1415571295553706E+01	2.1856925036766434E+01
H	5.3959837337539307E-01	1.2123857476985819E+01	2.0300407127031072E+01
O	9.6246499449790495E+00	1.9527814491534105E+01	3.7465183176895511E+00
O	7.9368694050280428E+00	1.9163354376352988E+01	1.3926846015094538E+00
C	7.4117603574093023E+00	1.9260641895360607E+01	2.6956366901851108E+00
C	9.2889468196560916E+00	1.8516608665510983E+01	1.4351659005807047E+00
C	1.0201998610095483E+01	1.9296643086431718E+01	2.4104820682468144E+00
C	8.3071319120630811E+00	2.0207783621485728E+01	3.5311195423178376E+00
H	1.1132722602911883E+01	1.8716080252839006E+01	2.5484313460025874E+00
H	1.0365405495729538E+01	2.0216662385120301E+01	1.8373631095346983E+00
H	9.6773735860496135E+00	1.8740451446219392E+01	4.6217628946691414E-01
H	9.2129492290211701E+00	1.7423810395676615E+01	1.5599250220389067E+00
H	7.8634312537515845E+00	2.0495740050740981E+01	4.4514329512414674E+00
H	8.5227488216084630E+00	2.1118301281093700E+01	2.9545995463352601E+00
H	7.2282148189606552E+00	1.8304035778604582E+01	3.2472103401613008E+00
H	6.4577674407147097E+00	1.9757383690959109E+01	2.5665222667185899E+00
O	1.4334614992717766E+01	1.8755585593886035E+01	5.2921872036483393E+00
O	1.5982184596385446E+01	1.8189548900654454E+01	3.0043076612058166E+00
C	1.6471312136720314E+01	1.8136318591633486E+01	4.3565799082842229E+00

C	1.4814071346712584E+01	1.9100558990724554E+01	2.9298984153947272E+00
C	1.3802371076190255E+01	1.8640879490961865E+01	3.9770584333259662E+00
C	1.5413105813910292E+01	1.7799327900122567E+01	5.4341680150903695E+00
H	1.2989560704284560E+01	1.9366777219239456E+01	3.9218414697895634E+00
H	1.3463325795362564E+01	1.7621483416693199E+01	3.8584239057446958E+00
H	1.4350528929773223E+01	1.9013213054731178E+01	1.9881579392048740E+00
H	1.5182349335393688E+01	2.0077874808048101E+01	3.2582546611198837E+00
H	1.5866049065061173E+01	1.7861925569397869E+01	6.4043910817824425E+00
H	1.4927418963615915E+01	1.6772156041053094E+01	5.4714639607904738E+00
H	1.6887855326546411E+01	1.9144849014607466E+01	4.6222927520775805E+00
H	1.7230129601425656E+01	1.7271932880375157E+01	4.3403669033704446E+00
O	1.1017368872076560E+01	2.4098020176036221E+00	1.5496005278458149E+01
O	1.1014775854315534E+01	1.5747357081329234E+00	1.2594392525043833E+01
C	1.2123579244390449E+01	2.3797464435419378E+00	1.3220156431859833E+01
C	9.8322960995704971E+00	1.8573651662931212E+00	1.3354302464536756E+01
C	9.9489237997843318E+00	1.6062429375684684E+00	1.4889893611055339E+01
C	1.2189227319245971E+01	2.2965195821352520E+00	1.4721162511504922E+01
H	9.0596906753906765E+00	2.0104878667442354E+00	1.5361294901543088E+01
H	1.0078589492989172E+01	5.5681575402843175E-01	1.5015546873545960E+01
H	8.9879223522553353E+00	1.3177141239340249E+00	1.2960044230294576E+01
H	9.6327799901206745E+00	2.9268491651081621E+00	1.3173566218929937E+01
H	1.2934139498959794E+01	3.0860548315713858E+00	1.4966331648748927E+01
H	1.2773777755258054E+01	1.3982673885545585E+00	1.4970602667724270E+01
H	1.1935156215391585E+01	3.4127176690073222E+00	1.2908848387906778E+01
H	1.3036476427856480E+01	1.9804826400143862E+00	1.2733467431622648E+01
O	6.9062731745252819E+00	2.0782898052679972E+01	1.2770422977844685E+01
O	6.669690339536124E+00	1.8800734089919100E+01	1.4850712288265120E+01
C	6.4131470226176752E+00	2.0223535073407806E+01	1.5034108613569570E+01
C	7.5320446086028525E+00	1.8630503696315348E+01	1.3756115695513738E+01
C	7.1951872548285998E+00	1.9412733177593005E+01	1.2498159529935579E+01
C	5.8730167987923441E+00	2.0815475209958077E+01	1.3758080032135936E+01
H	8.0806229783828680E+00	1.9221878169071907E+01	1.1848989723769000E+01
H	6.2593617144622531E+00	1.9059309722746704E+01	1.1929546118841921E+01
H	7.5822088187692840E+00	1.7472534667288862E+01	1.3579454173364221E+01
H	8.5709027917163141E+00	1.8887959383593522E+01	1.3971968856364583E+01
H	5.5783872012870885E+00	2.1884666594551113E+01	1.3902253659544433E+01
H	4.9782473226975847E+00	2.0253655017237108E+01	1.3353663866021369E+01
H	7.3721030637877902E+00	2.0583236361942028E+01	1.5330996631379504E+01
H	5.6850834202367020E+00	2.0358575454203919E+01	1.5884011228957144E+01
O	1.1629165202201520E+01	2.2257953125004196E+01	6.7038511352618118E+00
O	1.3114667733242714E+01	2.1687956176471538E+01	4.1931225656660214E+00
C	1.3762283492639440E+01	2.2152404469558057E+01	5.3916343149276598E+00
C	1.1752360632946694E+01	2.2139018159507536E+01	4.2145941441182782E+00
C	1.0972518719224214E+01	2.1769397997448880E+01	5.4888887307510954E+00
C	1.2982896960343632E+01	2.1781790984139295E+01	6.6431096298205565E+00
H	9.9238028188746572E+00	2.2078567915975132E+01	5.5286398376717161E+00
H	1.0837856863462576E+01	2.0662769893508845E+01	5.5712257061756034E+00
H	1.1233791581932621E+01	2.1747542587248468E+01	3.4003323336564852E+00
H	1.1696234972647051E+01	2.3197874564586261E+01	4.1473148162779472E+00
H	1.3627006644898122E+01	2.2158874312875028E+01	7.4580903887426899E+00
H	1.2915794982015433E+01	2.0731852845157565E+01	6.7437666439247224E+00
H	1.3846905790629785E+01	2.3248759947138005E+01	5.4074443320070049E+00
H	1.4673279062267177E+01	2.1568818610341225E+01	5.4565478426639347E+00
O	2.1656353190585769E+01	1.0740753048040473E+01	8.3576932812766174E+00
O	1.8866678434406747E+01	1.0868645183911260E+01	9.3604108750047335E+00
C	1.9721851564613612E+01	9.7167133394028298E+00	9.5742922144457996E+00
C	1.9232278165108227E+01	1.1463074964945447E+01	8.1295296627206266E+00
C	2.0722173784738747E+01	1.1840415613313805E+01	8.1753053194808381E+00
C	2.1206505160392357E+01	9.9935931988433051E+00	9.5440252187806625E+00
H	2.0967602085902634E+01	1.2278022230221284E+01	7.1981963632365433E+00
H	2.0946457160266728E+01	1.2438154430047895E+01	9.0167743036690844E+00
H	1.8737421483434481E+01	1.2444159373283304E+01	8.0486122395871593E+00
H	1.8817146007811228E+01	1.0903433724762271E+01	7.2800079237346109E+00
H	2.1766914510151320E+01	9.0896580186397564E+00	9.5521002993498971E+00
H	2.1445186397766246E+01	1.0619697929275381E+01	1.0421906489931985E+01
H	1.9506442130022947E+01	8.8888973796551962E+00	8.8757460974616702E+00
H	1.9498623211760396E+01	9.3056369948921738E+00	1.0600906443586075E+01
O	1.5377361397755386E+01	1.1964864656104526E+01	2.1036650498562945E+01
O	1.6823508413133123E+01	9.6220904009818362E+00	2.1376969046792439E+01
C	1.6825938842738655E+01	1.0185598384683761E+01	2.0032716191369321E+01
C	1.5495343435151483E+01	9.7626164697505793E+00	2.1920192532354655E+01
C	1.5375648871339603E+01	1.1260727844514584E+01	2.2311129930192049E+01
C	1.6595803355118459E+01	1.1653426801383054E+01	2.0238365363369724E+01
H	1.4407974445381692E+01	1.1497098190393139E+01	2.2790215292862406E+01

H	1.6189086590683161E+01	1.1582977916281150E+01	2.3017659064480771E+01
H	1.5385252960601354E+01	9.0316264555363652E+00	2.2704230746064873E+01
H	1.4686889922243209E+01	9.4828472243627910E+00	2.1221393017294819E+01
H	1.6441815125411523E+01	1.2172043157163289E+01	1.9305467300299252E+01
H	1.7470286619012487E+01	1.2121683461616678E+01	2.0775360158445075E+01
H	1.6080599117956993E+01	9.6528967129424093E+00	1.9324678155289163E+01
H	1.7886128319792878E+01	9.9706738351585074E+00	1.9661072221640026E+01
O	1.6828251991077895E+01	2.3746888359257823E+00	1.3190547408391495E+01
O	1.6328849877354244E+01	-3.5982247056815170E-01	1.3848915866627459E+01
C	1.5844018703671935E+01	2.3676662818791547E-01	1.2633822724133122E+01
C	1.6380842680731305E+01	6.6460461273322280E-01	1.4817503180774477E+01
C	1.7307264616338422E+01	1.8848474195571243E+00	1.4449111746320151E+01
C	1.6695271565454544E+01	1.3809260060360762E+00	1.2127032807742898E+01
H	1.7117506769709877E+01	2.7388096993907616E+00	1.5176677795215152E+01
H	1.8363098128952924E+01	1.5907218638645597E+00	1.4383418756494386E+01
H	1.6710428658692244E+01	2.7462905972150348E-01	1.5783729007501623E+01
H	1.5378946535352516E+01	1.0916403655716636E+00	1.4920644520189475E+01
H	1.6135113192461013E+01	1.9263661552721447E+00	1.1314475354773476E+01
H	1.7649690075415226E+01	1.1044964867205553E+00	1.1634814666283297E+01
H	1.4879118192220748E+01	6.8923910986265213E-01	1.2953684777404449E+01
H	1.5676089587943885E+01	-5.4250307089203598E-01	1.1901051922095972E+01
O	1.3468746362205483E+01	5.6059242109431757E+00	1.6241740455921764E+01
O	1.3216591360124717E+01	7.2847916164690112E+00	1.8538745604584179E+01
C	1.3981161248848531E+01	7.6393732444950500E+00	1.7422020950559475E+01
C	1.3269194318422917E+01	5.8580090696591887E+00	1.8646703716063211E+01
C	1.2740998267707360E+01	5.1846041869104722E+00	1.7363199331031591E+01
C	1.3438728416099046E+01	7.0205133300703659E+00	1.6094990993605386E+01
H	1.2829740649977419E+01	4.1082956748053343E+00	1.7489237295599189E+01
H	1.1573849449067559E+01	5.4603528599541118E+00	1.7240415024158466E+01
H	1.2636259060222580E+01	5.6419314939102119E+00	1.9479610198865181E+01
H	1.4263956086824358E+01	5.5355349332195720E+00	1.8886652208754537E+01
H	1.4100246563914082E+01	7.2511441755038382E+00	1.5227913033365017E+01
H	1.2429309907528490E+01	7.3771089070627385E+00	1.5838307660293339E+01
H	1.5056142922866538E+01	7.4050254304491733E+00	1.7575980365015738E+01
H	1.3941102114194784E+01	8.7215378751507391E+00	1.7348027322828546E+01
O	1.4925424878268695E+01	1.2459078476150411E+01	6.4462337893535242E+00
O	1.3037811021419673E+01	1.2470077964822396E+01	4.3019219840989793E+00
C	1.3831692608847453E+01	1.3665967810812001E+01	4.5214066034772973E+00
C	1.2802609479638116E+01	1.1869595616417332E+01	5.5791650404232769E+00
C	1.4075742433879238E+01	1.1375577699230332E+01	6.1897574173340635E+00
C	1.5114057050946748E+01	1.3373434920861691E+01	5.3000150630923448E+00
H	1.3838756074761644E+01	1.0852309599645235E+01	7.1525683382089209E+00
H	1.4550163773231120E+01	1.0678140361771918E+01	5.4602705953256416E+00
H	1.2198264480140438E+01	1.0954859854489845E+01	5.4308139857433266E+00
H	1.2366840022977049E+01	1.2617142085782991E+01	6.2297629606803619E+00
H	1.5642932041046169E+01	1.4249341744853185E+01	5.7214661949085031E+00
H	1.5838189309346673E+01	1.2810133417662765E+01	4.6497137354160829E+00
H	1.3182993567804617E+01	1.4422284536713267E+01	4.9564514882174491E+00
H	1.4002148931020329E+01	1.4122458261215042E+01	3.5013260097129546E+00
O	3.1557740754657676E-01	4.1687680592129359E+00	1.3561422515931444E+01
O	2.3167360214136421E+00	2.6725611232327799E+00	1.2058259844528969E+01
C	2.4314311492140628E+00	2.8727640425304055E+00	1.3458901319809717E+01
C	1.5432299997667560E+00	3.8070483216252060E+00	1.1515920023568615E+01
C	2.1787771019629470E-01	4.0182897386119727E+00	1.2156622319807457E+01
C	1.127685698333663E+00	3.0864120748303105E+00	1.4138999354150897E+01
H	-1.6545302131528886E-01	4.9788213638606118E+00	1.1732467283897579E+01
H	-5.6884345135638359E-01	3.2463873265522771E+00	1.1936254824537084E+01
H	1.4036564790628596E+00	3.5404159055335302E+00	1.0488339120450469E+01
H	2.1484295367562245E+00	4.7043851549114493E+00	1.1642644067207570E+01
H	1.2121785744498133E+00	3.2908534889397791E+00	1.5201418152662356E+01
H	6.7550845732258002E-01	2.0891570490784916E+00	1.4043295301507985E+01
H	3.0089579264360955E+00	3.8217880720700621E+00	1.3604997759724489E+01
H	2.9804371514334749E+00	1.9756791228873130E+00	1.3773921223588220E+01
O	1.4401604747864508E-01	1.8911728653218411E+01	8.7216201677529579E+00
O	-1.6648662199600703E+00	2.1231468199357799E+01	9.1613911939250201E+00
C	-3.3853799010920255E-01	2.1153742940322314E+01	7.108857393922481E+00
C	-2.0873611041695157E+00	1.9930258509451978E+01	9.0360246930618331E+00
C	-1.1238086991224718E+00	1.9042765753947332E+01	8.2257473266992314E+00
C	7.0057352017762664E-01	2.0309552509339401E+01	8.8632566127264365E+00
H	-1.593129228356586E+00	1.8064199447206594E+01	8.2214739632507605E+00
H	-1.1365897371674449E+00	1.9473719384360606E+01	7.2490495111528856E+00
H	-3.0076725485690354E+00	1.9951101536517733E+01	8.4294555793219086E+00
H	-2.3515884704742396E+00	1.9555197908428454E+01	1.0023665442515286E+01
H	1.6885997797859191E+00	2.0204811512601005E+01	9.3304810103768752E+00

H	8.5521295365945083E-01	2.0706730224908380E+01	7.8351241102510345E+00
H	-3.7252103694441263E-01	2.0724066276202358E+01	1.0724017431378456E+01
H	-4.2718100873863414E-02	2.2212363145470572E+01	9.7969114445279466E+00
O	7.8469147261989249E+00	2.1481331307301804E+01	1.8227022300456923E+01
O	1.0354533946706903E+01	2.1378619451080073E+01	1.9671165311659355E+01
C	9.4661558217699451E+00	2.2553249298888101E+01	1.9735381747009590E+01
C	1.0203765586514079E+01	2.0797735718227006E+01	1.8422779371087415E+01
C	8.7597532800896367E+00	2.0371991179773637E+01	1.8037832814981982E+01
C	8.0360895416950324E+00	2.2085668658499323E+01	1.9532129869433636E+01
H	8.8007067259660321E+00	2.0007050435546041E+01	1.6984441735246406E+01
H	8.3980179928808614E+00	1.9495843946298343E+01	1.8613241713715318E+01
H	1.0900830882258250E+01	1.9935644199523789E+01	1.8366338939884610E+01
H	1.0495340006736747E+01	2.1564727935774286E+01	1.7621017138319214E+01
H	7.3479321810159961E+00	2.2931202113846556E+01	1.9636190832719638E+01
H	7.7771538317480156E+00	2.1261859020429025E+01	2.0239983026260365E+01
H	9.8559387513660841E+00	2.3358646395570663E+01	1.9074932165791104E+01
H	9.5278204946222207E+00	2.2931582733453784E+01	2.0786386073631260E+01
O	8.7098265354132689E+00	5.8219602722514301E+00	1.9825201426732232E+01
O	7.3652311616343935E+00	8.1716251936738118E+00	2.0624120113605411E+01
C	8.8208610226740234E+00	8.1194055690175659E+00	2.0534811552613046E+01
C	6.7412213927846549E+00	6.8506058298053185E+00	2.0900414824919356E+01
C	7.2394338261576801E+00	5.8685024875719769E+00	1.9877648585256114E+01
C	9.2335547130683739E+00	7.1148634954034078E+00	1.9483017169508056E+01
H	6.9245918523803578E+00	4.7903770773603194E+00	1.9896923871741688E+01
H	6.7828541816572319E+00	6.2159279632891113E+00	1.8921624999857976E+01
H	5.6692412082066248E+00	6.8502336192266702E+00	2.0871918674954465E+01
H	7.1120998387259728E+00	6.5289708673894653E+00	2.1923195072689790E+01
H	1.0341882700247989E+01	7.0229488152577195E+00	1.9490773682867598E+01
H	8.9114438414554247E+00	7.3812984780586195E+00	1.8489331946013682E+01
H	9.1920432958708922E+00	7.8905009581252719E+00	2.1546905471608401E+01
H	9.1686790435565371E+00	9.1765312693483772E+00	2.0376270551137353E+01
O	1.4730056699182116E+01	1.6053525987013753E+01	1.8035979439929680E+01
O	1.4145785108003745E+01	1.7597844023093884E+01	2.0477237793116718E+01
C	1.4200627891818609E+01	1.8208682540646180E+01	1.9119829095343981E+01
C	1.5041435805439376E+01	1.6415245395878046E+01	2.0479638075148340E+01
C	1.4576784944325508E+01	1.5396810117134395E+01	1.9403989748921163E+01
C	1.3906026162842560E+01	1.7204717677611075E+01	1.7989315410805709E+01
H	1.5318252510871874E+01	1.4599935963317629E+01	1.9419861003983758E+01
H	1.3576079248983353E+01	1.4915000608700590E+01	1.9490980122626162E+01
H	1.4931282058819146E+01	1.6057006571012348E+01	2.1493004922375739E+01
H	1.6076989482915749E+01	1.6661531412652320E+01	2.0231296906331057E+01
H	1.4138914116247264E+01	1.7789392335087260E+01	1.7048276786644170E+01
H	1.2858107987357988E+01	1.6818876225645290E+01	1.8016620541242563E+01
H	1.5283465508060111E+01	1.8525081414919335E+01	1.8977979539667814E+01
H	1.3581745332161370E+01	1.9076483464218658E+01	1.9240221078905936E+01
O	-5.0785723228355262E-01	1.5963456177101767E+01	1.8559658572047361E+01
O	5.6926348097031781E-01	1.3454409931414068E+01	1.8599098058788254E+01
C	-8.5809690435573765E-01	1.3635602529748279E+01	1.8682038572809383E+01
C	1.3313505699829771E+00	1.4509986357835075E+01	1.9075234639681508E+01
C	9.1522798181467502E-01	1.5832308586285423E+01	1.8382554340677057E+01
C	-1.1820038715003300E+00	1.4885219954991731E+01	1.7894413237341723E+01
H	1.4307176065417728E+00	1.6681421973422374E+01	1.8902681601126918E+01
H	1.1561884278478238E+00	1.5782924397464090E+01	1.7296859842185768E+01
H	2.3111936626070007E+00	1.4129276791720224E+01	1.8817562341438830E+01
H	1.2861111792023285E+00	1.4549240285831690E+01	2.0175575244156587E+01
H	-2.2729860593306599E+00	1.5100740631621782E+01	1.7869699452876901E+01
H	-8.6411999769834713E-01	1.4810627073226589E+01	1.6874672574553401E+01
H	-1.2846103207730721E+00	1.3764827254563462E+01	1.9691966220892425E+01
H	-1.3205753234307414E+00	1.2739997619223640E+01	1.8290775853108581E+01
O	6.4253156053818135E+00	4.2590861815443288E+00	4.3797039510647204E+00
O	7.8016893453737319E+00	2.8924332680649685E+00	2.2194461055998680E+00
C	8.4837692831859108E+00	3.8631660770696978E+00	3.0484210454366147E+00
C	6.4010926233829935E+00	3.2437153879615783E+00	2.1017568731905625E+00
C	5.7953822674751265E+00	3.3024514643211380E+00	3.4889078624810259E+00
C	7.8268062417875104E+00	3.9852792111539554E+00	4.4642334589561559E+00
H	4.7391649980270811E+00	3.6371442856812890E+00	3.2689508413321651E+00
H	5.7115814079419103E+00	2.2088814977080791E+00	3.9481731995029548E+00
H	6.0300563778803529E+00	2.5288507532992823E+00	1.3201319130617386E+00
H	6.3176011016619196E+00	4.2641732936797414E+00	1.6440960305732149E+00
H	8.2656342288339957E+00	4.8353770992180118E+00	5.0581418457063716E+00
H	8.0407057727035465E+00	3.0441836975729584E+00	5.0187286512389830E+00
H	8.5946095131937792E+00	4.8246541259654938E+00	2.5714886420775125E+00
H	9.5200279693380629E+00	3.5429862214070793E+00	3.0553677762349878E+00
O	-2.5469729793683404E-01	4.5707193720196866E+00	8.5433355460325409E+00

O	1.8229084183195470E+00	5.6022069347824672E+00	6.9735293953177306E+00
C	1.6374960104080247E+00	4.1677746630944155E+00	7.1129895591719796E+00
C	1.3914408950812938E+00	6.3528986587928049E+00	8.0787798711834160E+00
C	2.4454309064577209E-02	5.9715411928737483E+00	8.5113514946774753E+00
C	1.4958426098705802E-01	3.8297283170649208E+00	7.3420036717088264E+00
H	-6.3618116618903084E-02	6.2576647020793654E+00	9.5689109254074687E+00
H	-7.3114926845909090E-01	6.5185217185364923E+00	7.8920478264102227E+00
H	1.2836222550314940E+00	7.3052107486828470E+00	7.5950558003421715E+00
H	2.1305075469055237E+00	6.2242022381790774E+00	8.8862782409927501E+00
H	-1.3205603305454633E-01	2.7972289668005224E+00	7.5709163777152346E+00
H	-4.4306777106551964E-01	4.1473018337738630E+00	6.4504226757011498E+00
H	2.2686280610014444E+00	3.7233874132778353E+00	7.9436850104306949E+00
H	1.9999874810169860E+00	3.7138269720437291E+00	6.1695747611839495E+00
O	-2.9984132519457409E+00	1.4282982040767702E+00	2.9921284479472789E+00
O	-1.1535516253593807E+00	1.8987391377098111E+00	5.1027382666968446E+00
C	-1.1440826264343205E+00	6.1486555686446509E-01	4.3909089461448625E+00
C	-2.5413253374384190E+00	2.2859486376213032E+00	5.2364345454244390E+00
C	-2.9899924287156909E+00	2.6164350541249655E+00	3.8109617973014247E+00
C	-1.7194841374820196E+00	7.5185751125138012E-01	2.9980548940162604E+00
H	-4.0719404692691450E+00	2.9910605394699461E+00	3.8348059189192027E+00
H	-2.2576928178657192E+00	3.2892991323537433E+00	3.746669535843679E+00
H	-2.7578964853172909E+00	3.1557506845034560E+00	5.8344866559918955E+00
H	-3.1601800371932924E+00	1.4694922094096206E+00	5.6401144586779308E+00
H	-1.9670056400327542E+00	-2.4396282115848680E-01	2.5710126690879025E+00
H	-1.0414000141700130E+00	1.2650200200624457E+00	2.2471994777718542E+00
H	-1.7966519861231516E+00	-1.5211019418871234E-02	5.0535621626857230E+00
H	-1.3213396956320722E-01	1.6797738822325467E-01	4.3986125523886681E+00
O	1.3870147723717972E+01	7.8042705007275943E+00	3.3497807459624345E+00
O	1.1548082153333400E+01	6.3635826880528308E+00	2.7860593818374211E+00
C	1.2805051618162249E+01	5.7040834057662115E+00	2.7971043223922285E+00
C	1.1689806718138550E+01	7.7467858819538629E+00	2.3279328133328736E+00
C	1.2573699054162825E+01	8.3686969693307685E+00	3.3273224418280796E+00
C	1.3841208304233545E+01	6.3753639199306296E+00	3.6358530222116046E+00
H	1.2808777923005033E+01	9.3891453048795128E+00	3.0405532542536338E+00
H	1.2058624466893953E+01	8.2392815547794527E+00	4.2899793561010222E+00
H	1.0728039275955412E+01	8.2864547606227266E+00	2.1974139883648296E+00
H	1.2123461478921602E+01	7.7079772400162803E+00	1.2853180775302380E+00
H	1.4857307216213927E+01	5.9750049628549888E+00	3.4892977068058353E+00
H	1.3678984849294928E+01	6.2364213301707681E+00	4.7335494904668121E+00
H	1.3040694613267817E+01	5.6819245473872657E+00	1.7315360673574212E+00
H	1.2565005797305940E+01	4.7106070354748972E+00	3.1267215122361653E+00
O	2.9823512072997058E+00	5.6376975787561001E+00	1.6614604238458824E+01
O	4.6391626285543799E+00	4.4406931900407240E+00	1.8688549102619564E+01
C	4.2017458879083422E+00	5.8632897951121272E+00	1.8851880748103355E+01
C	4.4936707003140466E+00	3.7959824713740935E+00	1.7409693958712126E+01
C	3.1631844479098667E+00	4.1592983608702427E+00	1.6757536089826008E+01
C	2.9811832176407056E+00	6.2069451066087344E+00	1.7971073307107343E+01
H	3.1106234002683588E+00	3.7708781424354583E+00	1.5736037926500796E+01
H	2.3369136179741470E+00	3.8211252178471971E+00	1.7410186105254230E+01
H	4.5427741194454647E+00	2.6543125328027690E+00	1.7519708723924797E+01
H	5.2261009993516723E+00	4.1474847495206655E+00	1.6657513813984593E+01
H	3.0417319112072718E+00	7.2589479430475405E+00	1.7767379265946758E+01
H	2.0864797758543636E+00	5.9487225557789163E+00	1.8543387372219765E+01
H	5.0554982464754659E+00	6.5837856728494906E+00	1.8630968881422550E+01
H	3.9364829768198923E+00	5.9471002079768658E+00	1.9918733223970118E+01
O	8.7724384717662236E+00	1.4058666425924685E+01	2.1006043473914730E+01
O	6.7026402166183914E+00	1.5832590349709850E+01	2.0152753729819892E+01
C	6.4437682698529812E+00	1.4821613582359401E+01	2.1040620882092508E+01
C	7.5963299840446634E+00	1.5233959185356037E+01	1.9103715344247625E+01
C	8.9022502734608420E+00	1.4959275320544771E+01	1.9749208706869897E+01
C	7.7269128990144056E+00	1.4506521171212528E+01	2.1867672612874554E+01
H	9.6230353525369754E+00	1.4369142609696924E+01	1.9086654853607239E+01
H	9.3711201096598984E+00	1.5880052455405636E+01	2.0111765953727254E+01
H	7.7261575473912734E+00	1.5878641798862985E+01	1.8225458740034405E+01
H	7.0973059870136472E+00	1.4352651859452829E+01	1.8659746208685640E+01
H	7.3621875896610964E+00	1.3708478974710689E+01	2.2491062068035038E+01
H	8.0901693228277747E+00	1.5349521300625078E+01	2.2460659713565725E+01
H	6.1169963612039844E+00	1.3926895465268521E+01	2.0496249148039059E+01
H	5.6207429823267931E+00	1.5117599324933336E+01	2.1659924131884303E+01
O	1.6918252510785326E+01	6.5376715701715629E+00	1.7943660625232546E+01
O	1.9603658245134469E+01	6.1896075436365665E+00	1.8917068754602589E+01
C	1.8562717896523427E+01	6.7172450113164874E+00	1.9769150610002942E+01
C	1.9352582983895761E+01	6.4300169805123764E+00	1.7549889574612745E+01
C	1.7950008451513000E+01	5.9294540189547433E+00	1.7200037684011171E+01

C	1.7135926410360447E+01	6.2821207846332934E+00	1.9287750183410118E+01
H	1.7758306266965086E+01	6.1220760055713015E+00	1.6188579844532264E+01
H	1.7837015554644772E+01	4.8315551109212667E+00	1.7380373841573512E+01
H	2.0162840534860262E+01	5.9052522216762275E+00	1.7005950612193345E+01
H	1.9481637816924295E+01	7.4892208094874402E+00	1.7262547882783643E+01
H	1.6461906674869070E+01	6.8919845377151931E+00	1.9906592564395019E+01
H	1.6839075135964936E+01	5.1641776512651987E+00	1.9514502805980555E+01
H	1.8658772186125805E+01	7.8038323966509786E+00	1.9894784907060817E+01
H	1.8760950783564397E+01	6.2131763250153149E+00	2.0720921861501498E+01
O	1.1927646603332674E+01	1.6884833608777619E+01	1.2533086006139335E+01
O	1.3272820070266260E+01	1.8282321962517578E+01	1.4713959989832139E+01
C	1.3977380882615373E+01	1.7310004912121290E+01	1.3894167675607488E+01
C	1.1900911529133616E+01	1.7958420781489789E+01	1.4701194885421781E+01
C	1.1269942041362548E+01	1.7845367000325005E+01	1.3324489665546489E+01
C	1.3348830166305122E+01	1.7203166490075443E+01	1.2505591516599031E+01
H	1.0216606673820269E+01	1.7427808663673769E+01	1.3470273085363520E+01
H	1.1281603891847688E+01	1.8790108819251138E+01	1.2785324417222933E+01
H	1.1455021386004045E+01	1.8870164939987774E+01	1.5207827967670816E+01
H	1.1695641955368492E+01	1.7020621706939220E+01	1.5244403852419007E+01
H	1.3872657876077417E+01	1.6446006922527129E+01	1.1906123213924472E+01
H	1.3557167645407379E+01	1.8182069957267746E+01	1.2023327111119114E+01
H	1.3883904045397173E+01	1.6294881138837905E+01	1.4402344010533451E+01
H	1.5032893014187477E+01	1.7650764048676816E+01	1.3867499457919665E+01
O	3.4989152226898250E+00	7.6810444633704584E+00	3.5067444654134383E+00
O	5.0662961466856640E+00	8.3454912986832444E+00	5.9236259370383673E+00
C	5.6099285717980694E+00	7.4148789569596651E+00	4.8731726846593784E+00
C	3.7000536728714186E+00	8.0164748315834835E+00	5.9814058228660425E+00
C	2.9498276953127212E+00	8.4238554542409290E+00	4.6320480010902010E+00
C	5.0735526904309243E+00	7.8293027179210153E+00	3.5923618174800347E+00
H	1.8733326862247370E+00	8.2237825921419958E+00	4.6037480004817199E+00
H	2.9755999560806750E+00	9.5288332360742860E+00	4.4847222131807341E+00
H	3.2378613466359085E+00	8.4852580580860248E+00	6.8527640664053466E+00
H	3.5193707370368266E+00	6.8660164350635684E+00	5.9487996300895363E+00
H	5.5851819089755095E+00	7.3312240632472641E+00	2.7973355290123889E+00
H	5.2321238123350424E+00	8.8946797201215446E+00	3.7141683819571338E+00
H	5.2949388521077108E+00	6.4150970326002605E+00	5.2017805949179285E+00
H	6.7101569269583825E+00	7.4368921681958859E+00	4.9011402465746698E+00
O	1.8109119720765161E+01	1.5143032464483491E+01	2.3657083788351962E+01
O	2.0840095760332748E+01	1.5723476992065295E+01	2.3878350625161698E+01
C	2.0029114678662058E+01	1.5731852993670547E+01	2.5060703618249942E+01
C	2.0135341934654164E+01	1.5971470675396857E+01	2.2647313189486137E+01
C	1.8912402328749376E+01	1.4998832245189989E+01	2.2488561939282960E+01
C	1.8838970521877229E+01	1.4770228749715285E+01	2.4811069341250548E+01
H	1.8159868001319108E+01	1.5303286846205056E+01	2.1698319889617867E+01
H	1.9138507408503326E+01	1.3933663602279468E+01	2.2314260020485129E+01
H	2.0810839086943952E+01	1.5779871496489919E+01	2.1881784346557723E+01
H	1.9782280465900225E+01	1.6988652063571848E+01	2.2696987273819786E+01
H	1.8107899704294855E+01	1.4711416525873096E+01	2.5596391055708807E+01
H	1.9256861205037435E+01	1.3773871196841011E+01	2.4738853520107305E+01
H	1.9681131379382570E+01	1.6727747076423871E+01	2.5160417135775681E+01
H	2.0706002960830471E+01	1.5424725167896717E+01	2.5917736487020171E+01
O	9.6838497918298572E-01	1.8975441605562747E+01	1.2360197097411922E+01
O	1.0511845729745224E+00	1.8343483896406156E+01	1.5139763949618903E+01
C	2.1408548995100429E+00	1.8127400339274953E+01	1.4293991400822467E+01
C	-2.1318180722878813E-01	1.8400960506383797E+01	1.4329502270655730E+01
C	-1.4490776107661987E-01	1.9360824291725436E+01	1.3164719678871052E+01
C	2.1147888642641357E+00	1.9085376882372412E+01	1.3143690609888674E+01
H	-9.9111766010547664E-01	1.9029417845971935E+01	1.2465466440310756E+01
H	-1.0310492977082036E-01	2.0455336834461246E+01	1.3329058360453869E+01
H	-9.0371534879309690E-01	1.8739414261489379E+01	1.5099573252287072E+01
H	-3.2563997015413776E-01	1.7358617664589922E+01	1.4042577839748914E+01
H	3.0108383900011124E+00	1.8911412870296225E+01	1.2494732697962762E+01
H	2.1331037500644565E+00	2.0185257480119269E+01	1.3444197380930044E+01
H	2.0034486918308643E+00	1.7111506561945639E+01	1.3853273249241619E+01
H	3.0393278070098755E+00	1.8131171148716415E+01	1.4933094690848087E+01
O	-5.4929710726786496E-01	-5.3986280396483488E-01	1.9775046190004790E+01
O	-1.727282322492393E+00	2.9105835258776697E-01	1.7305365593955433E+01
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H	-2.7301196012623317E+00	-6.2192205790637445E-01	1.9850328211210904E+01
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-3.9568847006989713E-07 -1.0858382925148504E-04 1.3168106326114497E-04

```

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2
0.302575750000000E+00 1 0.9622486650000001E+01
0.291506940000000E+00 0
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&END KIND
&KIND O
  BASIS_SET DZVP-MOLOPT-SR-GTH
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  &POTENTIAL
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2
0.220955920000000E+00 1 0.183374581100000E+02
0.211332470000000E+00 0
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&END KIND
&KIND H
  BASIS_SET DZVP-MOLOPT-SR-GTH
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  &POTENTIAL
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&END KIND
&KIND Rh
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-0.502558885000000E+01

```

```

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&END KIND
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POTENTIAL GTH-PBE-q3
&POTENTIAL

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&END KIND
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MULTIPLE_UNIT_CELL 1 1 1
&END TOPOLOGY
&END SUBSYS
&END FORCE_EVAL

```

To carry out WTMetaD simulations, take the appropriate restart file generated by CP2K (usually named MD-1.restart for the current file and MD-XXXX.restart for the earlier XXXX-th step) and insert the “&FREE ENERGY” section after “&END MD” line and “&COLVAR” section at the very end after “&END TOPOLOGY”. These sections for **M1**, **M2** and **M3** are given below.

Simulation M1

```

&FREE_ENERGY
&METADYN
NT_HILLS 100
MIN_DISP -1.0000000000000001E-01
WW 1.0000000000000000E-02
DO_HILLS T
WELL_TEMPERED T
DELTA_T 7.500000000000000E+02
&METAVAR
SCALE 1.0000000000000001E-01
COLVAR 1
&END METAVAR
&PRINT
&COLVAR SILENT
COMMON_ITERATION_LEVELS 3
&EACH
MD 1
&END EACH
&END COLVAR
&END PRINT
&END METADYN
&END FREE_ENERGY

&COLVAR
&COORDINATION
ATOMS_FROM 56
ATOMS_TO 69
R0 7.099999999999999E+00
&END COORDINATION
&END COLVAR

```

Simulation M2

```

&FREE_ENERGY
&METADYN
NT_HILLS 100
MIN_DISP -1.0000000000000001E-01
WW 1.0000000000000000E-02
DO_HILLS T
WELL_TEMPERED T
DELTA_T 7.500000000000000E+02

```

```

&METAVAR
  SCALE 1.0000000000000001E-01
  COLVAR 1
&END METAVAR
&PRINT
  &COLVAR SILENT
  COMMON_ITERATION_LEVELS 3
  &EACH
    MD 1
  &END EACH
&END COLVAR
&END PRINT
&END METADYN
&END FREE_ENERGY

```

```

&COLVAR
  &COORDINATION
  ATOMS_FROM 56
  ATOMS_TO 75
  R0 7.0999999999999996E+00
&END COORDINATION
&END COLVAR

```

Simulation M3

```

&FREE_ENERGY
  &METADYN
  NT_HILLS 100
  MIN_DISP -1.0000000000000001E-01
  WW 1.0000000000000000E-02
  DO_HILLS T
  WELL_TEMPERED T
  DELTA_T 7.500000000000000E+02
  &METAVAR
  SCALE 1.0000000000000001E-01
  COLVAR 1
&END METAVAR
  &METAVAR
  SCALE 1.0000000000000001E-01
  COLVAR 2
&END METAVAR
  &PRINT
  &COLVAR SILENT
  COMMON_ITERATION_LEVELS 3
  &EACH
    MD 1
  &END EACH
&END COLVAR
  &HILLS SILENT
  COMMON_ITERATION_LEVELS 3
  &EACH
    MD 1
  &END EACH
&END HILLS
&END PRINT
&END METADYN
&END FREE_ENERGY

```

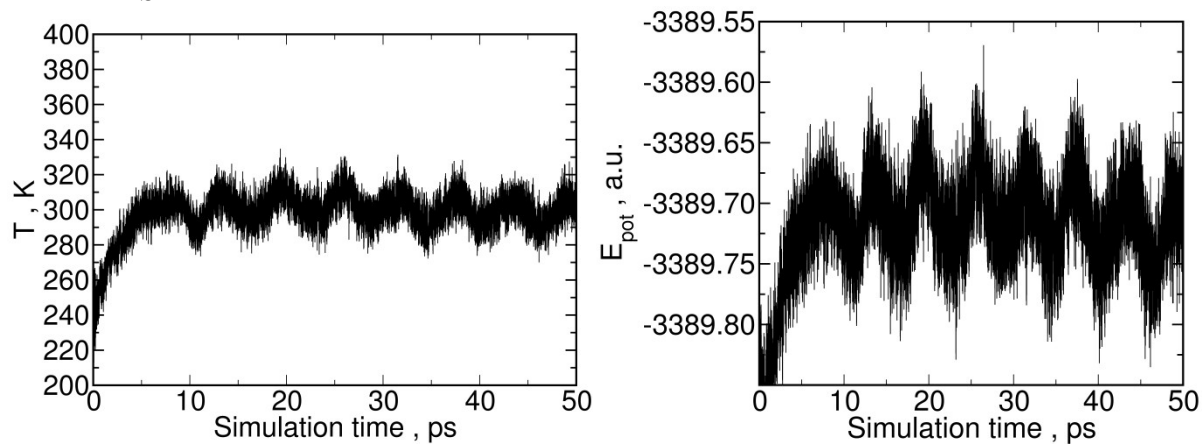
```

&COLVAR
  &COORDINATION
  ATOMS_FROM 56
  ATOMS_TO 73
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&END COORDINATION
&END COLVAR
  &COLVAR
  &COORDINATION
  ATOMS_FROM 56
  ATOMS_TO 67
  R0 8.1600000000000001E+00
&END COORDINATION
&END COLVAR

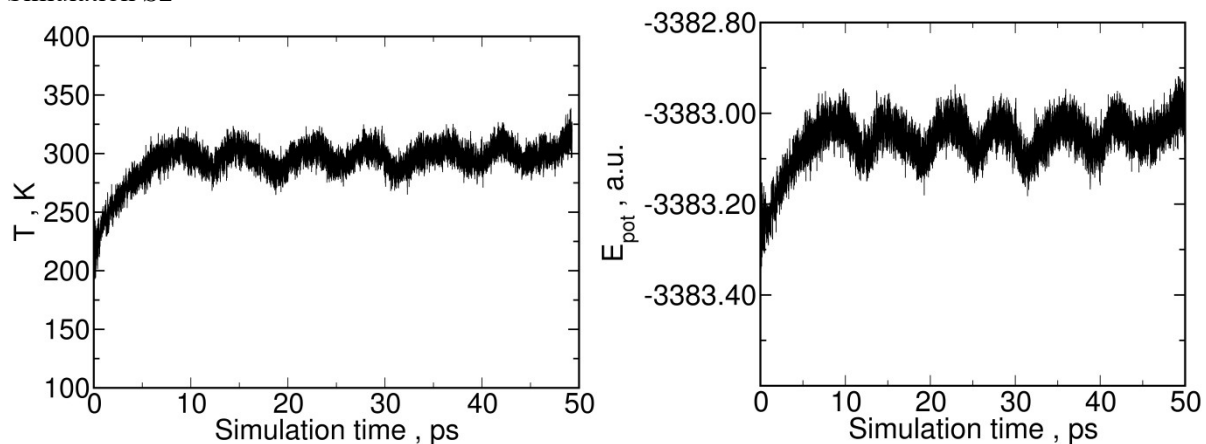
```

3. Temperature and potential energy plots over the BOMD trajectories

Simulation S1



Simulation S2



Simulation S3

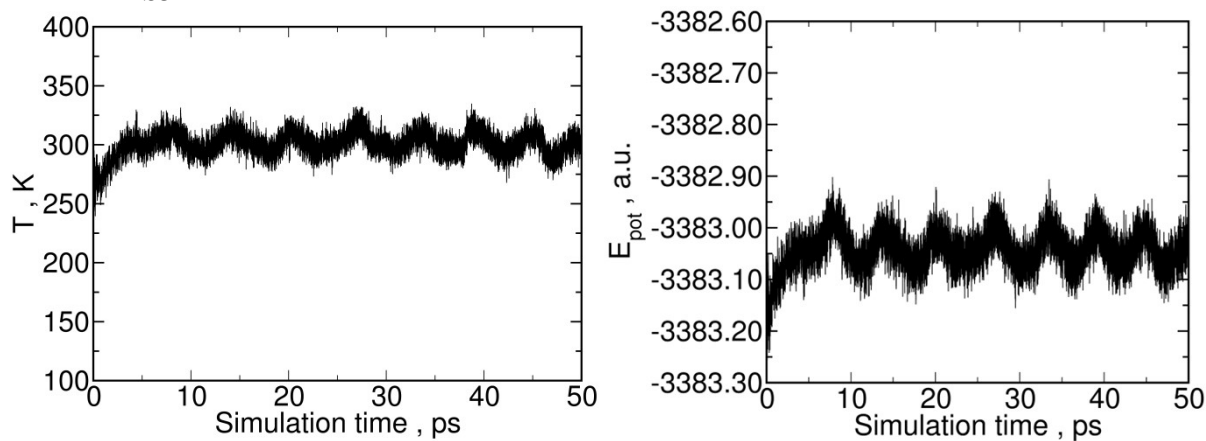


Figure S1. Plots of temperature (left) and potential energy (right) over BOMD simulations S1-3.

4. Single-CV well-tempered metadynamics results

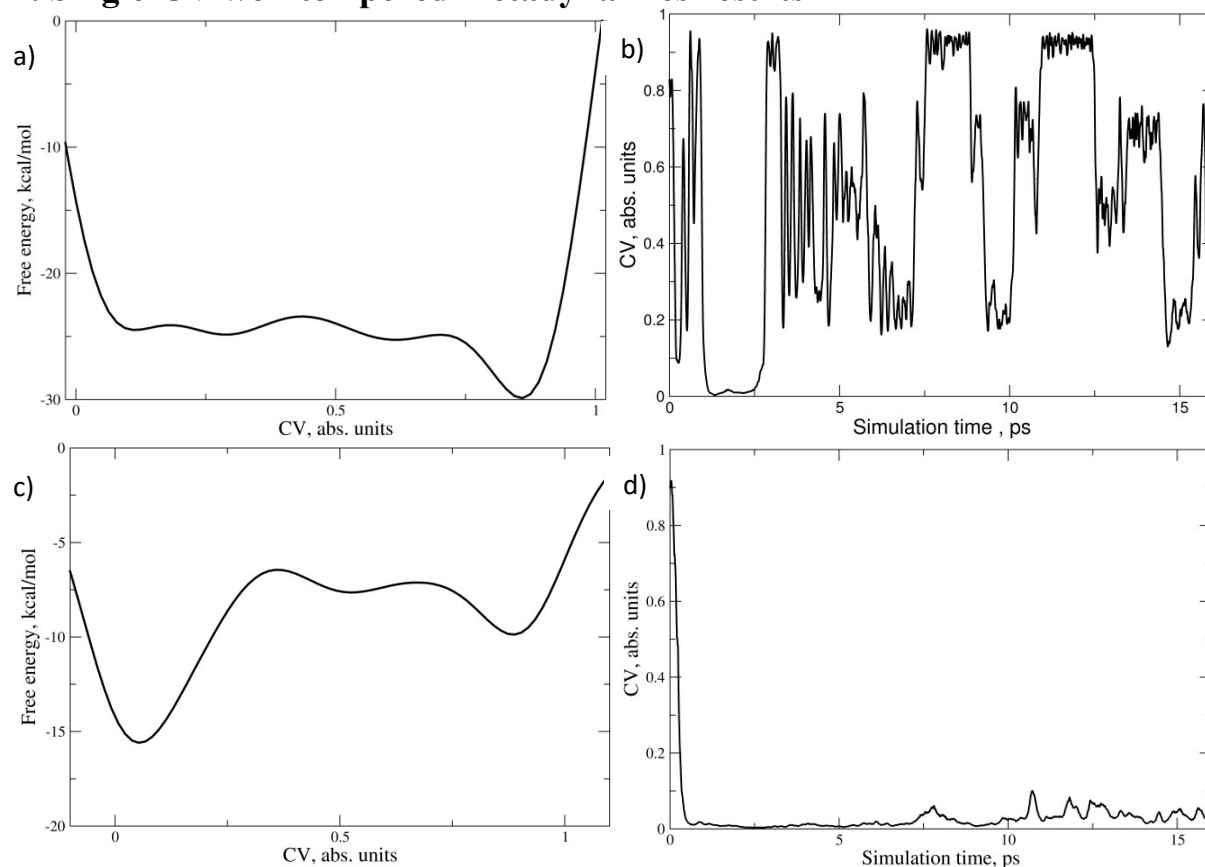
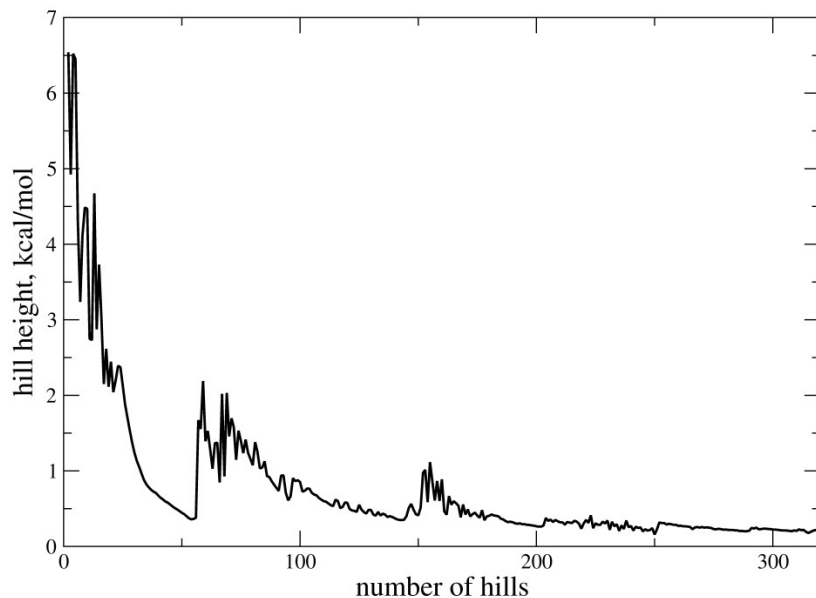


Figure S2. WTMetaD simulations **M1** (a: Free energy/CV (FES) plot; b: CV/time plot) and **M2** (c: Free energy/CV (FES) plot; d: CV/time plot).

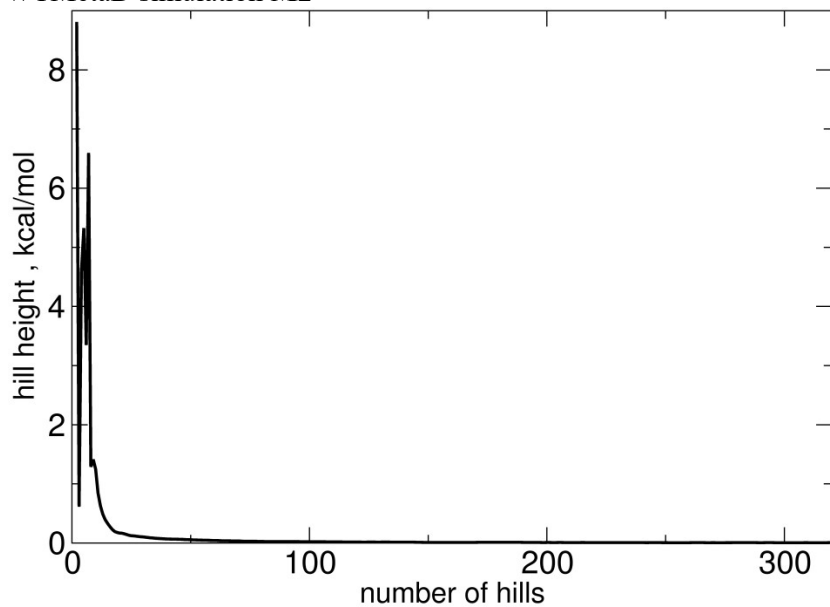
5. Well-tempered metadynamics – convergence assessment

a) Hills magnitude and convergence. The hill magnitude in kcal mol⁻¹ is plotted against the hill number. At deposition rate of 100 steps, for 16 ps or 32000 steps, hills with variable height were deposited 320 times. At the end of the simulation, the hill height is very close to 0, indicating convergence of the value of the total energy deposited and the barrier height.

WTMetaD simulation **M1**



WTMetaD simulation **M2**



WTMetaD simulation **M3**

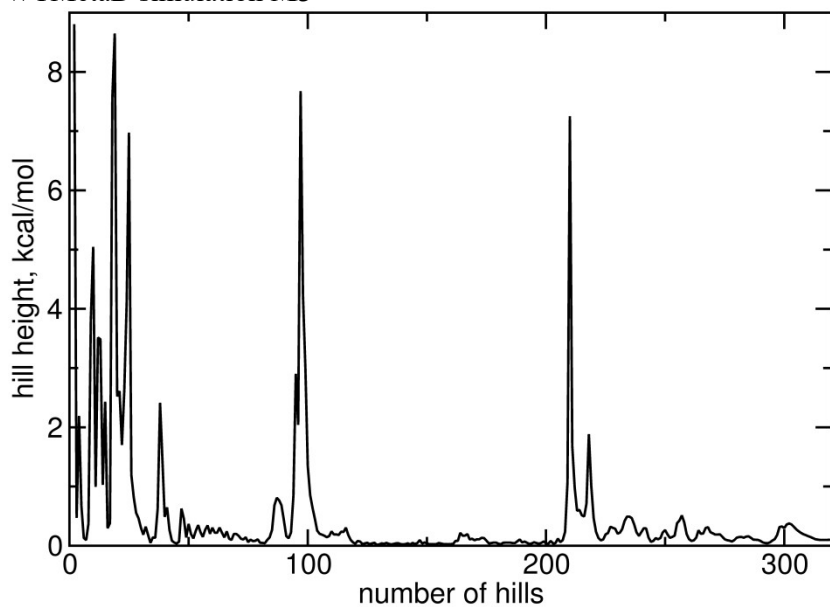
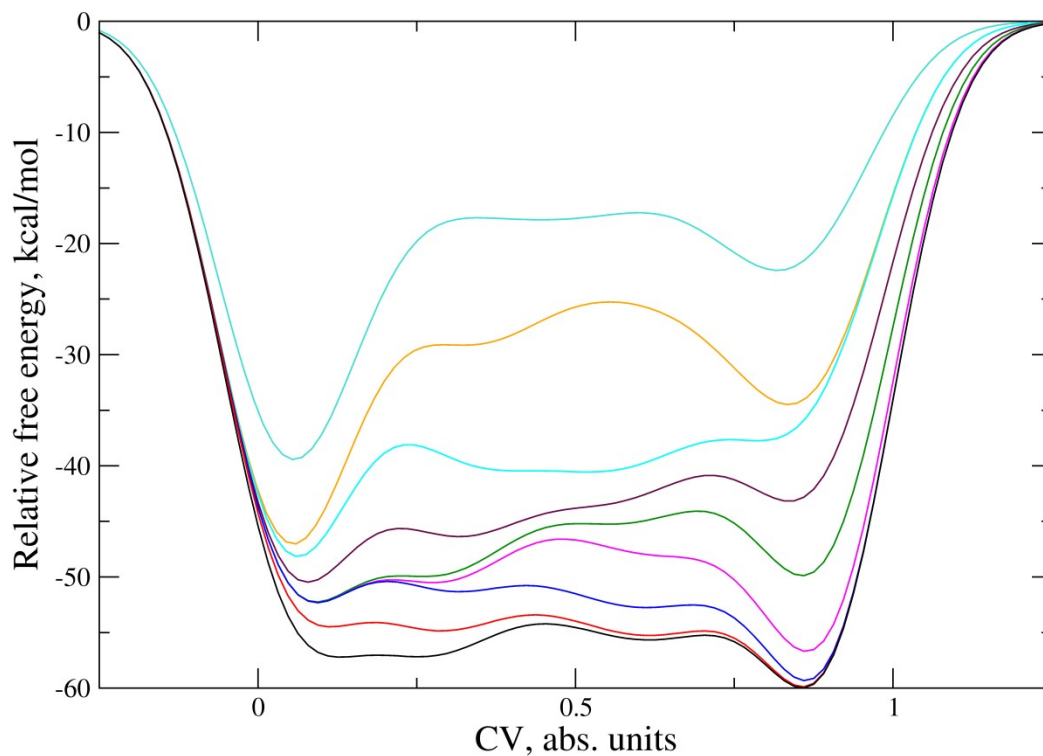


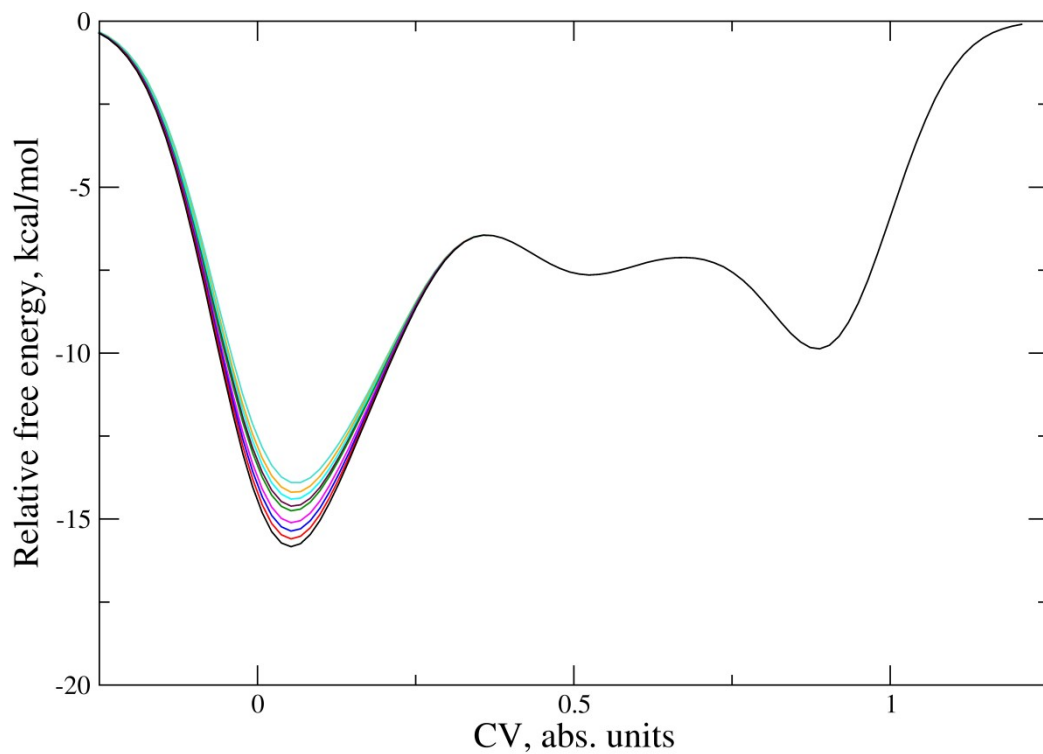
Figure S3. Magnitude of the deposited hills during WTMetaD simulations **M1-3**.

b) FES plots at selected timepoints. The FES was generated from the respective restart files starting at 2 ps to 18 ps spaced by 2 ps. These plots track the evolution of the FES with time. In the case of H₂O-containing systems (**M1**, **M3**) due to the high mobility of H₂O and the very flat nature of the FES exhibiting a multitude of shallow minima, the dissociated states diverge quite significantly from one another. The H-bonded state, being more geometrically well-defined and constrained generally assumes the final curve shape at earlier time point.

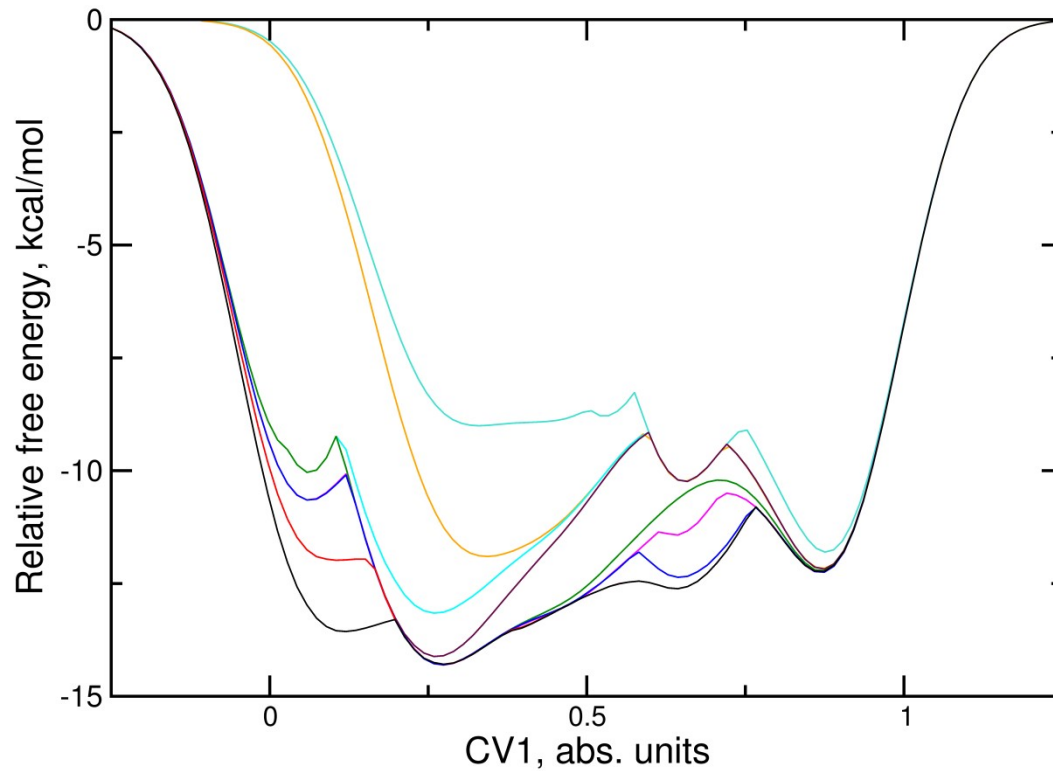
WTMetaD simulation **M1**



WTMetaD simulation **M2**



WTMetaD simulation **M3**: CV1



WTMetaD simulation **M3**: CV2

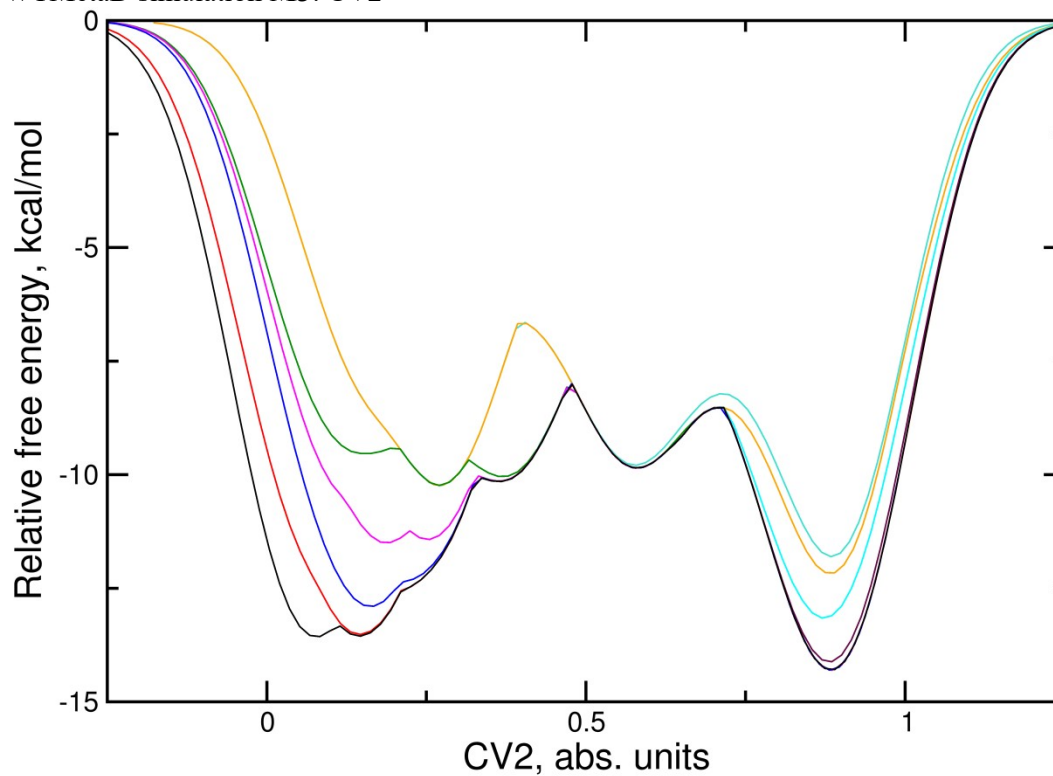


Figure S4. Evolution of FES from 2 ps (turquoise) to 18ps (black) at timepoints taken 2 ps apart during WTMetaD simulations **M1-3**.

6. Static DFT methods

All computations were executed on Gaussian 09 (revision A.02)¹² using default PBE0,⁴ M06L,¹³ M06,¹⁴ and ω B97xD¹⁵ functionals and IEFPCM¹⁶ and SMD¹⁷ implicit solvation methods. DGDZVP basis set¹⁸ was used as implemented in Gaussian09. Def2-TZVP basis set¹⁹ was used as downloaded from Basis Set Exchange (<https://www.basissetexchange.org>). All structures were optimized at IEFPCM(1,4-dioxane, 303.15K)/PBE0/DGDZVP with cutoff values for Maximum Force = 0.001500, RMS Force = 0.001000, Maximum Displacement = 0.006000, RMS Displacement = 0.004000 for all Rh-containing species and cutoff values for Maximum Force = 0.000150, RMS Force = 0.000100, Maximum Displacement = 0.00600, RMS Displacement = 0.00400 for the others. In all cases, the predicted change in energy at the last optimization step was $< 1 \times 10^{-6}$. All stationary points were confirmed to reside in their respective PES minima by having only positive vibrational frequencies after frequency calculation at the optimization level of theory. Thereafter, single-point calculations at SMD/M06L/def2-TZVP, SMD/M06/def2-TZVP, and IEFPCM/ ω B97xD/def2-TZVP (solvent = 1,4-dioxane) were performed.

7. H-bond energies by static DFT calculations (extended results)

The initial H-bonded structures were derived from step 20 000 of simulations **S1** and **S2**, respectively, after solvent particles and distal water molecules were stripped and then subjected to structure optimization, frequency calculation, and higher level of theory single point calculations as described in section 6 above. The results show that O_k in both **4a** and **4b** forms H-bonds in the optimized structures with the H-bond acceptors positioning themselves opposite the bulky chiral diene ligand (Figure S5). In **4a**, the 3 H₂O molecules form an H-bonded cluster. The one that is closest to the carbonyl O atom serves as a lynchpin by participating in 3 H-bonds, once as acceptor and twice as donor (the structural optimization of internally H-bonded (H₂O)₃ cluster without the ketone failed). The calculated DFT reaction energies and enthalpies (ΔE , ΔH ; Table S1) were both negative but adding the entropy term ($-T\Delta S$) to ΔH caused the resultant Gibbs free energy (ΔG) to become positive due to ΔH having smaller values. Thus, static DFT calculations on model systems in implicit solvation do not attain even qualitative agreement with the free energy calculated by the more sophisticated BOMD + WTMetaD simulations in full explicit solvent. Whereas the former predict both **4a** and **4b** to be unstable relative to **4** + 3H₂O and **4** + H₃BO₃, respectively, the latter showed that the H-bonded state in the first case is more but in the second case less stable than the non-H-bonded state. DFT calculations also showed that H-bonding of uncomplexed 2-cyclohexenone with H₃BO₃ and 3H₂O (reactions 5 and 6) proceeded with about the same free energy as the complex (reactions 2 and 1). There was no improvement in reaction ΔG (Table S1) after correction of the electronic energy at SMD/M06 or M06L/def2-TZVP

and IEFPCM// ω B97xD/def2-TZVP levels of theory even with these dispersion-corrected modern DFT functionals and a triple- ζ basis set specifically developed for calculating reaction energies.

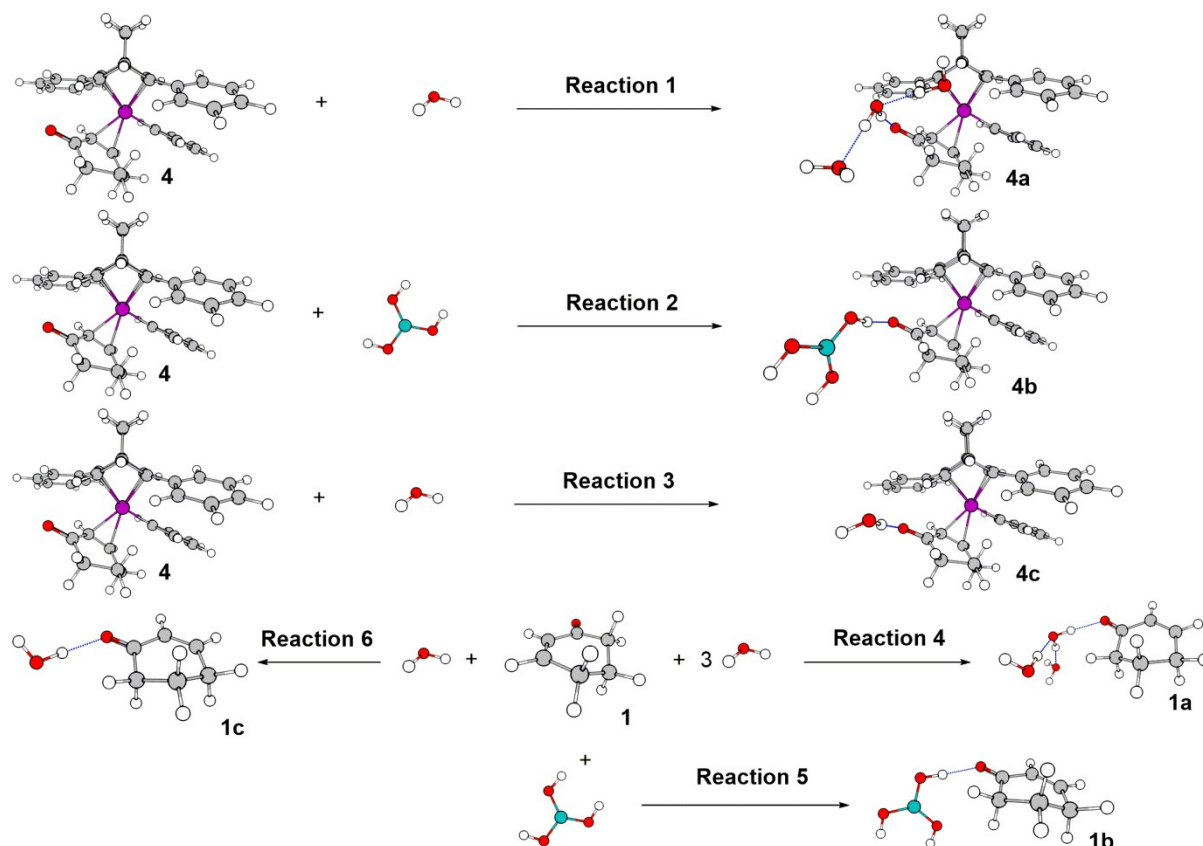


Figure S5. Model reaction equations 1-6 for evaluation of H-bonding energies (Table S1).

	Reaction energy, kcal mol ⁻¹					
	ΔE^1	ΔH^1	ΔG^1	$\Delta G_{\text{corr}}(1)^2$	$\Delta G_{\text{corr}}(2)^3$	$\Delta G_{\text{corr}}(3)^4$
Reaction 1	-23.0	-18.0	8.2	10.4	11.0	8.1
Reaction 2	-7.3	-6.1	2.3	2.3	2.7	1.4
Reaction 3	-6.8	-5.2	1.8	2.0	2.2	1.5
Reaction 4	-21.0	-15.9	8.1	11.0	11.4	9.1
Reaction 5	-6.6	-5.2	4.0	3.7	4.1	3.2
Reaction 6	-6.4	-4.8	2.8	3.1	3.3	2.6

¹at IEFPCM(1,4-dioxane, 303.15K)/PBE0/DGDZVP level of theory

²at SMD(1,4-dioxane)/M06L/def2-TZVP//IEFPCM(1,4-dioxane, 303.15K)/PBE0/DGDZVP level of theory

³at SMD(1,4-dioxane)/M06/def2-TZVP//IEFPCM(1,4-dioxane, 303.15K)/PBE0/DGDZVP level of theory

⁴at IEFPCM(1,4-dioxane)/ ω B97xD/def2-TZVP//IEFPCM(1,4-dioxane, 303.15K)/PBE0/DGDZVP level of theory

Table S1. Reaction energies for equations 1 - 6 (Figure S5) at different level of theory.

8. Cartesian coordinates, first 3 frequencies, electronic energies, enthalpies and Gibbs free energies for all DFT structures

Complex 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	45	0	-0.166185	-0.324353	-0.061371
2	6	0	-1.813642	1.263833	-0.322855
3	6	0	-0.012791	2.313211	0.929366
4	6	0	2.876011	1.428011	1.590555
5	6	0	-3.160894	0.721249	-0.589750
6	6	0	-4.175010	0.788906	0.376239
7	6	0	-1.246781	1.439337	0.925873
8	6	0	-1.011364	1.970497	-1.408210
9	6	0	-4.721235	-0.400191	-2.081100
10	6	0	5.166844	1.627061	0.851072
11	6	0	-0.362314	3.692260	0.314237
12	6	0	0.382774	1.394598	-1.266745
13	6	0	-5.440533	0.269995	0.118265
14	6	0	0.960661	1.610306	-0.010390
15	6	0	3.353758	1.809343	-0.735952
16	6	0	-3.456594	0.119659	-1.823061
17	6	0	-0.976979	3.485164	-1.081916
18	6	0	-5.720886	-0.325369	-1.111004
19	6	0	2.408183	1.608724	0.279607
20	6	0	4.716931	1.817574	-0.454434
21	6	0	4.238114	1.431762	1.873753
22	1	0	2.167936	1.258496	2.397494
23	1	0	6.231090	1.633291	1.071074
24	1	0	3.020335	1.965240	-1.757588
25	1	0	5.430603	1.975230	-1.258848
26	1	0	4.576462	1.279760	2.895505
27	1	0	-3.972124	1.250119	1.337654
28	1	0	-4.926190	-0.868757	-3.040203
29	1	0	-6.211648	0.333098	0.881442
30	1	0	-2.681202	0.033302	-2.580017
31	1	0	-6.709898	-0.728639	-1.311573
32	1	0	0.393573	2.429300	1.934538
33	1	0	-1.419491	1.796412	-2.404192
34	1	0	-1.061104	4.205649	0.982216
35	1	0	0.545496	4.302274	0.264558
36	1	0	-0.390522	3.994967	-1.852980
37	1	0	-1.994891	3.884926	-1.132854
38	1	0	0.968175	1.138202	-2.144803
39	1	0	-1.749028	1.163108	1.848257
40	6	0	1.288429	-1.371925	-1.098718
41	6	0	2.633694	-1.493701	-0.724361
42	6	0	0.927503	-1.888470	-2.356504
43	6	0	3.576299	-2.093930	-1.564791

44	1	0	2.969873	-1.112652	0.238021
45	6	0	1.864659	-2.481713	-3.204765
46	1	0	-0.108928	-1.831057	-2.689612
47	6	0	3.199594	-2.588726	-2.811908
48	1	0	4.612240	-2.168838	-1.239376
49	1	0	1.548763	-2.865192	-4.173300
50	1	0	3.932339	-3.053820	-3.466987
51	6	0	-0.428724	-2.522912	0.564149
52	6	0	-1.449985	-1.735206	1.087536
53	1	0	-0.609838	-3.042900	-0.373879
54	1	0	-2.400976	-1.635254	0.567352
55	6	0	-1.470716	-1.369629	2.518458
56	8	0	-2.427218	-0.779115	3.016742
57	6	0	-0.320181	-1.837390	3.385335
58	1	0	-0.157040	-1.090569	4.167903
59	6	0	0.656953	-3.083428	1.439691
60	6	0	0.955213	-2.173870	2.622267
61	1	0	-0.694209	-2.736670	3.895898
62	1	0	1.415517	-1.251030	2.247546
63	1	0	1.679922	-2.645540	3.294969
64	1	0	0.311454	-4.064855	1.800954
65	1	0	1.557439	-3.268978	0.848948

```

-----
                1                2                3
                A                A                A
Frequencies --  24.7900          38.5193          39.9303
SCF Done:  E(RPBE1PBE) = -5999.08904453  A.U. after  1 cycles
                Conv g =   0.6309D-08          -V/T =  2.0047
Zero-point correction=                0.545455 (Hartree/Particle)
Thermal correction to Energy=                0.575734
Thermal correction to Enthalpy=                0.576694
Thermal correction to Gibbs Free Energy=                0.483204
Sum of electronic and zero-point Energies=                -5998.543590
Sum of electronic and thermal Energies=                -5998.513311
Sum of electronic and thermal Enthalpies=                -5998.512351
Sum of electronic and thermal Free Energies=                -5998.605840
SCF Done:  E(RM06L) = -1424.26367204  A.U. after  24 cycles
                Conv g =   0.6660D-08          -V/T =  2.0564
SCF Done:  E(RM06) = -1423.36288747  A.U. after  23 cycles
                Conv g =   0.4920D-08          -V/T =  2.0572
SCF Done:  E(RwB97XD) = -1423.95354902  A.U. after  25 cycles
                Conv g =   0.6705D-08          -V/T =  2.0572

```

H₂O

```

-----
Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type      X           Y           Z
-----
   1         8         0      0.000000   0.000000   0.117139
   2         1         0      0.000000   0.767242  -0.468555
   3         1         0      0.000000  -0.767242  -0.468555

```

```

-----
                1                2                3
                A1                A1                B2
Frequencies -- 1686.5450          3820.9379          3953.8733
SCF Done: E(RPBE1PBE) = -76.3516415090  A.U. after 1 cycles
                Conv = 0.2157D-09          -V/T = 2.0095

Zero-point correction= 0.021555 (Hartree/Particle)
Thermal correction to Energy= 0.024437
Thermal correction to Enthalpy= 0.025397
Thermal correction to Gibbs Free Energy= 0.003544
Sum of electronic and zero-point Energies= -76.330087
Sum of electronic and thermal Energies= -76.327204
Sum of electronic and thermal Enthalpies= -76.326244
Sum of electronic and thermal Free Energies= -76.348098
SCF Done: E(RM06L) = -76.4474389288  A.U. after 9 cycles
                Conv = 0.6223D-09          -V/T = 2.0033
SCF Done: E(RM06) = -76.4263679514  A.U. after 8 cycles
                Conv = 0.5488D-08          -V/T = 2.0033
SCF Done: E(RwB97XD) = -76.4409290788  A.U. after 9 cycles
                Conv = 0.5875D-08          -V/T = 2.0040

```

Complex 4a

```

-----
Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type     X           Y           Z
-----
  1       45       0       -0.154337  -0.667559  -0.317542
  2        6       0        1.303911  -1.343317   1.323110
  3        6       0        0.142970   0.616829   2.185284
  4        6       0       -2.272464   2.240004   1.232181
  5        6       0        2.435690  -2.156227   0.833189
  6        6       0        3.735722  -1.631582   0.784736
  7        6       0        1.255471   0.038293   1.342542
  8        6       0        0.170271  -1.951806   2.138533
  9        6       0        3.295978  -4.239950  -0.081028
 10       6       0       -4.679201   2.448845   1.372641
 11       6       0        0.272582   0.076342   3.632037
 12       6       0       -1.080902  -1.355946   1.522893
 13       6       0        4.796701  -2.396872   0.309434
 14       6       0       -1.133284   0.041395   1.584621
 15       6       0       -3.623353   0.305765   1.727499
 16       6       0        2.235560  -3.474784   0.395357
 17       6       0        0.303180  -1.462868   3.603069
 18       6       0        4.583275  -3.704559  -0.125056
 19       6       0       -2.355692   0.864404   1.506052
 20       6       0       -4.772443   1.087854   1.661438
 21       6       0       -3.423924   3.019191   1.159787
 22       1       0       -1.305577   2.711203   1.068123
 23       1       0       -5.576247   3.060543   1.320081
 24       1       0       -3.714038  -0.751649   1.957373
 25       1       0       -5.743638   0.632343   1.837060

```

26	1	0	-3.337762	4.079890	0.937610
27	1	0	3.917662	-0.615462	1.120754
28	1	0	3.116314	-5.256149	-0.422487
29	1	0	1.235308	-3.900394	0.403107
30	1	0	5.412723	-4.301737	-0.494418
31	1	0	0.165171	1.706314	2.158275
32	1	0	1.187991	0.481822	4.074532
33	1	0	-0.567231	0.447157	4.228771
34	1	0	-0.519451	-1.887548	4.187518
35	1	0	1.234903	-1.851783	4.026829
36	1	0	-1.961019	-1.970107	1.357991
37	1	0	2.058509	0.666038	0.970292
38	6	0	-1.917797	-1.214366	-1.265100
39	6	0	-3.033764	-0.388942	-1.459501
40	6	0	-2.055671	-2.567147	-1.625744
41	6	0	-4.231629	-0.887117	-1.981108
42	1	0	-2.983325	0.666816	-1.200209
43	6	0	-3.251331	-3.073991	-2.138994
44	1	0	-1.213343	-3.248967	-1.507208
45	6	0	-4.350391	-2.233301	-2.321006
46	1	0	-5.076459	-0.214253	-2.116249
47	1	0	-3.321476	-4.127996	-2.401945
48	1	0	-5.282124	-2.622001	-2.725056
49	6	0	0.254503	-0.437440	-2.562112
50	6	0	1.415817	-0.211373	-1.823505
51	1	0	0.096622	-1.432317	-2.972709
52	1	0	2.138614	-1.006702	-1.651702
53	6	0	1.906133	1.154421	-1.599182
54	8	0	2.997646	1.356573	-1.050421
55	6	0	1.101409	2.311783	-2.144220
56	1	0	1.190022	3.152622	-1.450522
57	6	0	-0.469672	0.689452	-3.243989
58	6	0	-0.352380	1.988624	-2.462585
59	1	0	-0.915628	1.890719	-1.527266
60	1	0	-0.801118	2.815880	-3.022914
61	1	0	-0.021367	0.808599	-4.243090
62	1	0	-1.516812	0.420119	-3.401469
63	8	0	3.893428	5.916096	-1.448873
64	8	0	0.709936	3.985087	1.365009
65	8	0	3.260655	3.791666	0.329974
66	1	0	3.343305	6.705995	-1.355111
67	1	0	4.806270	6.226393	-1.372971
68	1	0	0.792493	4.424802	2.221092
69	1	0	1.631990	3.927242	1.015738
70	1	0	3.477507	4.522669	-0.282814
71	1	0	3.282898	2.972867	-0.211344
72	1	0	5.795649	-1.969638	0.281434
73	1	0	1.630003	2.613012	-3.060618
74	1	0	0.162869	-3.041261	2.089800

	1	2	3
	A	A	A
Frequencies --	13.3824	24.7685	27.5052
SCF Done: E(RPBE1PBE) =	-6228.18062251	A.U. after	1 cycles

```

          Conv g =    0.8343D-08          -V/T = 2.0049
Zero-point correction=                0.619860 (Hartree/Particle)
Thermal correction to Energy=          0.659959
Thermal correction to Enthalpy=        0.660919
Thermal correction to Gibbs Free Energy= 0.543497
Sum of electronic and zero-point Energies= -6227.560763
Sum of electronic and thermal Energies= -6227.520664
Sum of electronic and thermal Enthalpies= -6227.519704
Sum of electronic and thermal Free Energies= -6227.637126
SCF Done: E(RM06L) = -1653.63908696      A.U. after 24 cycles
          Conv g =    0.3245D-08          -V/T = 2.0487
SCF Done: E(RM06) = -1652.67418380      A.U. after 23 cycles
          Conv g =    0.3114D-08          -V/T = 2.0494
SCF Done: E(RwB97XD) = -1653.31308111   A.U. after 26 cycles
          Conv g =    0.4209D-08          -V/T = 2.0495

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H₃BO₃

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-----
Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type      X           Y           Z
-----
      1         5         0      -0.008359   -0.029776    0.001869
      2         8         0       0.053191    1.349415   -0.000142
      3         8         0       1.075091   -0.873030   -0.000227
      4         1         0       1.923128   -0.415363   -0.001265
      5         8         0      -1.240364   -0.625256   -0.000355
      6         1         0       0.948673    1.707519   -0.001184
      7         1         0      -1.933360    0.047689   -0.001103
-----
                    1           2           3
                    A           A           A
Frequencies --   304.6954          445.1695          468.0771
SCF Done: E(RPBE1PBE) = -252.246651981   A.U. after 1 cycles
          Conv g =    0.4784D-09          -V/T = 2.0107
Zero-point correction=                0.048892 (Hartree/Particle)
Thermal correction to Energy=          0.053513
Thermal correction to Enthalpy=        0.054473
Thermal correction to Gibbs Free Energy= 0.021814
Sum of electronic and zero-point Energies= -252.197760
Sum of electronic and thermal Energies= -252.193139
Sum of electronic and thermal Enthalpies= -252.192179
Sum of electronic and thermal Free Energies= -252.224838
SCF Done: E(RM06L) = -252.559817676      A.U. after 11 cycles
          Conv g =    0.4020D-08          -V/T = 2.0037
SCF Done: E(RM06) = -252.488796521      A.U. after 10 cycles
          Conv g =    0.6535D-08          -V/T = 2.0039
SCF Done: E(RwB97XD) = -252.525558279   A.U. after 11 cycles
          Conv g =    0.8625D-08          -V/T = 2.0042

```

Complex 4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	45	0	0.553326	0.454419	-0.338916
2	6	0	-0.460796	1.807275	1.220754
3	6	0	0.221135	-0.213890	2.390320
4	6	0	1.993190	-2.613985	1.584846
5	6	0	-1.376433	2.819611	0.657082
6	6	0	-2.764158	2.719056	0.830323
7	6	0	-0.790464	0.498417	1.520928
8	6	0	0.887665	2.195432	1.813422
9	6	0	-1.729519	4.862702	-0.614247
10	6	0	4.250537	-3.468603	1.676949
11	6	0	0.421895	0.590561	3.700117
12	6	0	1.845737	1.162068	1.256837
13	6	0	-3.620340	3.673496	0.288795
14	6	0	1.521041	-0.155377	1.597125
15	6	0	3.848490	-1.086034	1.689817
16	6	0	-0.873677	3.909569	-0.071087
17	6	0	0.805480	2.040443	3.352984
18	6	0	-3.108337	4.749613	-0.434869
19	6	0	2.463329	-1.291717	1.616451
20	6	0	4.732028	-2.160993	1.719363
21	6	0	2.874722	-3.690055	1.609265
22	1	0	0.925561	-2.805935	1.519522
23	1	0	4.940188	-4.308199	1.700125
24	1	0	4.240570	-0.074354	1.729502
25	1	0	5.801430	-1.975891	1.777106
26	1	0	2.486822	-4.704839	1.574521
27	1	0	-3.177872	1.887575	1.392179
28	1	0	-1.319899	5.694097	-1.182090
29	1	0	-4.692699	3.575520	0.434872
30	1	0	0.196739	4.000985	-0.237755
31	1	0	-3.778054	5.494596	-0.856181
32	1	0	-0.087588	-1.236588	2.607850
33	1	0	1.184038	3.208264	1.539240
34	1	0	-0.506920	0.553659	4.277680
35	1	0	1.196979	0.104909	4.301800
36	1	0	1.776033	2.308086	3.782734
37	1	0	0.071063	2.751612	3.744524
38	1	0	2.835317	1.452797	0.917540
39	1	0	-1.779564	0.085017	1.349747
40	6	0	2.272734	0.292295	-1.483676
41	6	0	3.089560	-0.841402	-1.586542
42	6	0	2.728724	1.468220	-2.106506
43	6	0	4.307653	-0.804572	-2.272411
44	1	0	2.785234	-1.778633	-1.124703
45	6	0	3.948295	1.514783	-2.784496
46	1	0	2.121576	2.372812	-2.067511
47	6	0	4.747029	0.373625	-2.872595
48	1	0	4.915489	-1.705507	-2.331659
49	1	0	4.271426	2.444100	-3.250000
50	1	0	5.694547	0.402854	-3.405137
51	6	0	-0.139436	-0.081820	-2.459271

52	6	0	-1.222287	0.285964	-1.661105
53	1	0	0.301052	0.675982	-3.102359
54	1	0	-1.603474	1.305589	-1.665083
55	6	0	-2.140448	-0.729889	-1.131305
56	8	0	-3.172803	-0.400281	-0.535183
57	6	0	-1.853524	-2.185361	-1.418139
58	6	0	0.085564	-1.511312	-2.864277
59	6	0	-0.411233	-2.485326	-1.806728
60	1	0	-2.186095	-2.779001	-0.561282
61	1	0	-2.529593	-2.447088	-2.244760
62	1	0	0.232761	-2.401814	-0.922988
63	1	0	-0.331246	-3.516421	-2.167367
64	1	0	-0.458143	-1.672270	-3.808387
65	1	0	1.143757	-1.674754	-3.083612
66	8	0	-4.844505	-2.134794	0.794950
67	1	0	-4.282631	-1.553524	0.233644
68	5	0	-5.720729	-2.873727	0.069665
69	8	0	-5.700949	-2.796424	-1.314469
70	8	0	-6.587924	-3.680346	0.780446
71	1	0	-6.379556	-3.329914	-1.744167
72	1	0	-7.178747	-4.195936	0.220647

```

-----
                1                2                3
                A                A                A
Frequencies --   8.6743           12.9896           16.9124
SCF Done: E(RPBE1PBE) = -6251.34729757   A.U. after   1 cycles
              Convg =   0.6925D-08           -V/T =   2.0050
Zero-point correction=                   0.595241 (Hartree/Particle)
Thermal correction to Energy=             0.632155
Thermal correction to Enthalpy=           0.633115
Thermal correction to Gibbs Free Energy=   0.520334
Sum of electronic and zero-point Energies= -6250.752057
Sum of electronic and thermal Energies=    -6250.715142
Sum of electronic and thermal Enthalpies=  -6250.714182
Sum of electronic and thermal Free Energies= -6250.826964
SCF Done: E(RM06L) = -1676.83519069   A.U. after   23 cycles
              Convg =   0.6000D-08           -V/T =   2.0481
SCF Done: E(RM06) = -1675.86266866   A.U. after   23 cycles
              Convg =   0.4264D-08           -V/T =   2.0488
SCF Done: E(RwB97XD) = -1676.49216314   A.U. after   22 cycles
              Convg =   0.8290D-08           -V/T =   2.0489

```

Complex 4c

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-----
Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type     X           Y           Z
-----
   1         45         0       0.055412   -0.345457   -0.261131
   2         6          0       1.676996   -0.298415   1.368188
   3         6          0       0.044339   1.403520   1.964035
   4         6          0      -2.755948   2.102014   0.863545
   5         6          0       2.979770   -0.859928   0.957845

```

6	6	0	4.091714	-0.031965	0.746502
7	6	0	1.256851	1.001863	1.155523
8	6	0	0.765628	-1.028781	2.346661
9	6	0	4.357026	-2.778170	0.373810
10	6	0	-5.116536	1.710897	1.195209
11	6	0	0.340990	1.186543	3.470064
12	6	0	-0.612229	-0.905354	1.728039
13	6	0	5.314736	-0.567839	0.354103
14	6	0	-1.039059	0.414847	1.550502
15	6	0	-3.499100	0.048890	1.873523
16	6	0	3.134817	-2.242250	0.767852
17	6	0	0.791234	-0.267793	3.696398
18	6	0	5.454462	-1.942468	0.166491
19	6	0	-2.442634	0.852670	1.421726
20	6	0	-4.820245	0.472036	1.761506
21	6	0	-4.076223	2.524784	0.746059
22	1	0	-1.960553	2.745737	0.497159
23	1	0	-6.148042	2.041670	1.107853
24	1	0	-3.286901	-0.916526	2.322979
25	1	0	-5.621538	-0.168784	2.119984
26	1	0	-4.293622	3.492805	0.302089
27	1	0	3.999472	1.039840	0.890933
28	1	0	4.452567	-3.850672	0.225339
29	1	0	6.163604	0.092354	0.197190
30	1	0	2.284828	-2.905590	0.906391
31	1	0	6.410661	-2.359605	-0.137954
32	1	0	-0.240422	2.437672	1.770180
33	1	0	1.053403	-2.071712	2.481440
34	1	0	1.116927	1.894329	3.777558
35	1	0	-0.558750	1.421117	4.048038
36	1	0	0.130047	-0.783213	4.400313
37	1	0	1.803153	-0.311813	4.111854
38	1	0	-1.296634	-1.748346	1.730480
39	1	0	1.858214	1.741576	0.636551
40	6	0	-1.508519	-1.510143	-0.965580
41	6	0	-2.812992	-1.067950	-1.222519
42	6	0	-1.269901	-2.892633	-1.067963
43	6	0	-3.834563	-1.961606	-1.559515
44	1	0	-3.054408	-0.008417	-1.159051
45	6	0	-2.286918	-3.791312	-1.395457
46	1	0	-0.268259	-3.285343	-0.891938
47	6	0	-3.579735	-3.328787	-1.645569
48	1	0	-4.835831	-1.580896	-1.752199
49	1	0	-2.066080	-4.855162	-1.460459
50	1	0	-4.373873	-4.023994	-1.906848
51	6	0	0.302488	-0.421256	-2.539001
52	6	0	1.421519	0.155515	-1.938217
53	1	0	0.343048	-1.479766	-2.783700
54	1	0	2.302870	-0.438315	-1.703180
55	6	0	1.628870	1.609001	-1.979683
56	8	0	2.679271	2.113993	-1.564646
57	6	0	0.574356	2.470659	-2.635778
58	6	0	-0.680533	0.407145	-3.317672
59	6	0	-0.796343	1.816969	-2.759020

60	1	0	0.537004	3.431163	-2.113045
61	1	0	0.973300	2.688062	-3.637598
62	1	0	-1.269263	1.764000	-1.770840
63	1	0	-1.444059	2.430301	-3.394541
64	1	0	-0.323777	0.444494	-4.358933
65	1	0	-1.654013	-0.089000	-3.340175
66	8	0	2.652962	4.864744	-0.899724
67	1	0	3.365469	5.317005	-1.368977
68	1	0	2.724145	3.926463	-1.170657

```

-----
              1                      2                      3
              A                      A                      A
Frequencies -- 7.9724                23.2423                27.8674
SCF Done: E(RPBE1PBE) = -6075.45158816  A.U. after 1 cycles
              Conv = 0.3870D-08          -V/T = 2.0048
Zero-point correction= 0.569702 (Hartree/Particle)
Thermal correction to Energy= 0.603641
Thermal correction to Enthalpy= 0.604601
Thermal correction to Gibbs Free Energy= 0.500599
Sum of electronic and zero-point Energies= -6074.881886
Sum of electronic and thermal Energies= -6074.847947
Sum of electronic and thermal Enthalpies= -6074.846987
Sum of electronic and thermal Free Energies= -6074.950990
SCF Done: E(RM06L) = -1500.72179662  A.U. after 23 cycles
              Conv = 0.5650D-08          -V/T = 2.0536
SCF Done: E(RM06) = -1499.79952977  A.U. after 23 cycles
              Conv = 0.4846D-08          -V/T = 2.0543
SCF Done: E(RwB97XD) = -1500.40592805  A.U. after 25 cycles
              Conv = 0.8948D-08          -V/T = 2.0544

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2-cyclohexenone (1)

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Center   Atomic   Atomic   Coordinates (Angstroms)
Number   Number   Type     X           Y           Z
-----
  1         6         0     -0.962786   1.316500   0.026452
  2         1         0     -1.472304   2.279416   0.022905
  3         6         0         0.378388   1.285575  -0.058478
  4         1         0         0.965700   2.195826  -0.153244
  5         6         0         1.134987   0.021818   0.015786
  6         8         0         2.356376   0.001849  -0.074855
  7         6         0     -1.810895   0.087597   0.133428
  8         1         0     -2.735892   0.230605  -0.435904
  9         1         0     -2.124409  -0.027400   1.181831
 10        6         0         0.327111  -1.233624   0.267527
 11        1         0         0.254269  -1.345523   1.358615
 12        1         0         0.896279  -2.090369  -0.102278
 13        6         0     -1.068843  -1.157153  -0.341705
 14        1         0     -1.639526  -2.058480  -0.096772
 15        1         0     -0.982898  -1.123150  -1.434372
-----
              1                      2                      3

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Frequencies --      A              A              A
              103.2147          246.0748          307.9643
SCF Done: E(RPBE1PBE) = -308.332694733 A.U. after 1 cycles
              Conv = 0.2930D-08          -V/T = 2.0137
Zero-point correction=          0.128507 (Hartree/Particle)
Thermal correction to Energy=          0.134787
Thermal correction to Enthalpy=          0.135747
Thermal correction to Gibbs Free Energy=          0.097953
Sum of electronic and zero-point Energies=          -308.204188
Sum of electronic and thermal Energies=          -308.197907
Sum of electronic and thermal Enthalpies=          -308.196947
Sum of electronic and thermal Free Energies=          -308.234742
SCF Done: E(RM06L) = -308.743983765 A.U. after 13 cycles
              Conv = 0.4379D-08          -V/T = 2.0045
SCF Done: E(RM06) = -308.568231805 A.U. after 12 cycles
              Conv = 0.8364D-08          -V/T = 2.0052
SCF Done: E(RwB97XD) = -308.684808704 A.U. after 13 cycles
              Conv = 0.3554D-08          -V/T = 2.0052

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2-cyclohexenone×3*H₂O (1a)*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.305622	-0.728823	0.144604
2	6	0	2.250795	-1.358471	-0.403830
3	1	0	4.273541	-1.228644	0.150722
4	1	0	2.344046	-2.341261	-0.858903
5	6	0	0.902757	-0.775551	-0.369246
6	8	0	-0.050363	-1.376384	-0.868667
7	6	0	0.739283	0.538845	0.352809
8	1	0	-0.136067	1.066867	-0.035180
9	6	0	3.223922	0.630800	0.762851
10	6	0	1.997389	1.398300	0.283280
11	1	0	2.159042	1.713669	-0.754249
12	1	0	1.859557	2.309584	0.872527
13	1	0	3.201645	0.510187	1.856563
14	1	0	4.143510	1.185948	0.547606
15	8	0	-4.218079	-1.063731	1.343715
16	8	0	-2.240919	2.380578	-0.505555
17	8	0	-2.686465	-0.305620	-0.923380
18	1	0	-4.415011	-0.240585	1.812410
19	1	0	-5.078984	-1.437960	1.110887
20	1	0	-2.397850	2.830879	-1.345181
21	1	0	-2.444277	1.431933	-0.682913
22	1	0	-3.174148	-0.663569	-0.154756
23	1	0	-1.804771	-0.732254	-0.911346
24	1	0	0.517762	0.285870	1.400099

	1	2	3
	A	A	A
Frequencies --	13.0532	19.9319	33.9712

SCF Done: E(RPBE1PBE) = -537.421086880 A.U. after 1 cycles
 Conv g = 0.3867D-08 -V/T = 2.0120
 Zero-point correction= 0.202848 (Hartree/Particle)
 Thermal correction to Energy= 0.219107
 Thermal correction to Enthalpy= 0.220067
 Thermal correction to Gibbs Free Energy= 0.154915
 Sum of electronic and zero-point Energies= -537.218238
 Sum of electronic and thermal Energies= -537.201980
 Sum of electronic and thermal Enthalpies= -537.201020
 Sum of electronic and thermal Free Energies= -537.266172
 SCF Done: E(RM06L) = -538.115064052 A.U. after 13 cycles
 Conv g = 0.9610D-08 -V/T = 2.0041
 SCF Done: E(RM06) = -537.875549386 A.U. after 12 cycles
 Conv g = 0.9336D-08 -V/T = 2.0045
 SCF Done: E(RwB97XD) = -538.039399066 A.U. after 13 cycles
 Conv g = 0.5740D-08 -V/T = 2.0048

2-cyclohexenone×*H₃BO₃* (1b)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.350365	0.422215	0.547377
2	6	0	-2.315377	1.262439	0.366757
3	1	0	-4.274523	0.808085	0.975792
4	1	0	-2.382686	2.317656	0.618268
5	6	0	-1.016020	0.785752	-0.121811
6	8	0	-0.070573	1.565025	-0.251215
7	6	0	-0.877189	-0.691854	-0.391986
8	6	0	-3.301462	-1.032061	0.201492
9	6	0	-2.195859	-1.338350	-0.802478
10	1	0	-0.095869	-0.839027	-1.142101
11	1	0	-0.500876	-1.137318	0.539372
12	1	0	-2.494366	-0.954456	-1.785052
13	1	0	-2.066626	-2.419507	-0.910742
14	1	0	-3.149688	-1.601651	1.130644
15	1	0	-4.276891	-1.349858	-0.182307
16	8	0	2.515206	0.713476	-0.843818
17	1	0	1.603280	0.991085	-0.608658
18	5	0	3.069788	-0.097490	0.091162
19	8	0	2.317067	-0.496991	1.186499
20	8	0	4.375917	-0.489091	-0.124032
21	1	0	2.808661	-1.034517	1.818457
22	1	0	4.717346	-1.081234	0.554938

	1	2	3
	A	A	A
Frequencies --	23.6666	34.7631	39.8876

SCF Done: E(RPBE1PBE) = -560.589911517 A.U. after 1 cycles
 Conv g = 0.2429D-08 -V/T = 2.0123
 Zero-point correction= 0.178857 (Hartree/Particle)
 Thermal correction to Energy= 0.191486

Thermal correction to Enthalpy= 0.192446
 Thermal correction to Gibbs Free Energy= 0.136722
 Sum of electronic and zero-point Energies= -560.411055
 Sum of electronic and thermal Energies= -560.398425
 Sum of electronic and thermal Enthalpies= -560.397465
 Sum of electronic and thermal Free Energies= -560.453189
 SCF Done: E(RM06L) = -561.314823144 A.U. after 14 cycles
 Convrg = 0.5256D-08 -V/T = 2.0042
 SCF Done: E(RM06) = -561.067495414 A.U. after 13 cycles
 Convrg = 0.3315D-08 -V/T = 2.0046
 SCF Done: E(RwB97XD) = -561.222233795 A.U. after 13 cycles
 Convrg = 0.7359D-08 -V/T = 2.0048

2-cyclohexenone×*H₂O* (1c)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.161534	0.820197	-0.004833
2	6	0	-0.947979	1.397383	-0.069818
3	1	0	-3.048345	1.452268	-0.029303
4	1	0	-0.830051	2.473444	-0.167954
5	6	0	0.285383	0.607816	0.039362
6	8	0	1.389014	1.151228	-0.024764
7	6	0	0.133708	-0.872175	0.293293
8	6	0	-2.367816	-0.656714	0.109971
9	6	0	-1.136361	-1.438764	-0.332988
10	1	0	1.033913	-1.386014	-0.053728
11	1	0	0.100801	-0.994921	1.385324
12	1	0	-1.054296	-1.384007	-1.424889
13	1	0	-1.242180	-2.496938	-0.075786
14	1	0	-2.617156	-0.888200	1.156519
15	1	0	-3.247912	-0.949200	-0.472909
16	8	0	3.706729	-0.522201	0.022549
17	1	0	4.356968	-0.101163	-0.553979
18	1	0	2.949903	0.096059	0.044505

 1 2 3
 A A A
 Frequencies -- 34.0411 50.5148 89.7408
 SCF Done: E(RPBE1PBE) = -384.694483735 A.U. after 1 cycles
 Convrg = 0.3675D-08 -V/T = 2.0129
 Zero-point correction= 0.152834 (Hartree/Particle)
 Thermal correction to Energy= 0.162721
 Thermal correction to Enthalpy= 0.163681
 Thermal correction to Gibbs Free Energy= 0.116079
 Sum of electronic and zero-point Energies= -384.541650
 Sum of electronic and thermal Energies= -384.531763
 Sum of electronic and thermal Enthalpies= -384.530802
 Sum of electronic and thermal Free Energies= -384.578405
 SCF Done: E(RM06L) = -385.201053402 A.U. after 13 cycles
 Convrg = 0.8525D-08 -V/T = 2.0043

SCF Done: E(RM06) = -385.003880612 A.U. after 12 cycles
 Convg = 0.6218D-08 -V/T = 2.0048
 SCF Done: E(RwB97XD) = -1423.95354902 A.U. after 25 cycles
 Convg = 0.6705D-08 -V/T = 2.0572

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